

Table 1. Crystal data and structure refinement for (2d) $C_{20}H_{22}F_{12}P_2S_2$.

Identification code	$C_{20}H_{22}F_{12}P_2S_2$
Empirical formula	$C_{20}H_{22}F_{12}P_2S_2$
Formula weight	616.44
Temperature	223 K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pna2(1)
Unit cell dimensions	
	$a = 13.281(3)$ Å
	$b = 16.488(3)$ Å
	$c = 10.945(2)$ Å
Volume	2396.7(8) Å ³
Z	4
Density (calculated)	1.708 Mg/m ³
Absorption coefficient	0.458 mm ⁻¹
F(000)	1248
Crystal size	0.50 x 0.35 x 0.30 mm
$\bar{\alpha}$ range for data collection	2.23 to 34.56°
Limiting indices	$0 \leq h \leq 21, 0 \leq k \leq 14, -14 \leq l \leq 0$
Reflections collected	2279
Independent reflections	2279 [R(int) = 0.0000]
Absorption correction	Psi scans
Max. and min. transmission	1.0000 and 0.9673
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2279 / 1 / 325
Goodness-of-fit on F ²	1.069
Final R indices [I > 2 σ (I)]	R1 = 0.0471, wR2 = 0.1286
R indices (all data)	R1 = 0.0775, wR2 = 0.1439
Absolute structure parameter	0.10(16)
Largest diff. peak and hole	0.418 and -0.407 e.Å ⁻³

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for (2d) $\text{C}_{20}\text{H}_{22}\text{F}_{12}\text{P}_2\text{S}_2$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
P(1)	-1226(1)	-1466(2)	-2784(2)	44(1)
F(1)	-2006(5)	-2035(8)	-3182(10)	165(5)
F(2)	-1768(5)	-616(6)	-2258(8)	113(3)
F(3)	-1261(4)	-2052(6)	-1518(6)	117(4)
F(4)	-665(5)	-2322(5)	-3301(7)	107(3)
F(5)	-1181(3)	-896(5)	-4066(5)	77(2)
F(6)	-432(4)	-889(8)	-2404(7)	145(4)
P(2)	-721(1)	-3421(1)	2559(2)	32(1)
F(7)	-1169(3)	-3095(3)	1318(4)	46(1)
F(8)	-296(3)	-4327(4)	1843(5)	63(2)
F(9)	16(3)	-2692(4)	2228(5)	67(2)
F(10)	-282(3)	-3741(4)	3794(4)	53(2)
F(11)	-1473(3)	-4131(4)	2888(5)	61(2)
F(12)	-1159(3)	-2516(4)	3258(4)	51(2)
S(1)	1821(1)	887(1)	6423(2)	31(1)
S(2)	3227(1)	-471(1)	5569(2)	29(1)
C(1)	1586(4)	-223(5)	5613(7)	31(2)
C(2)	783(4)	-465(6)	5351(7)	44(2)
C(3)	633(4)	-1365(6)	4788(7)	47(2)
C(4)	1251(5)	-2019(6)	4454(8)	47(3)
C(5)	2067(4)	-1769(6)	4701(7)	41(2)
C(6)	2215(4)	-873(5)	5275(6)	29(2)
C(7)	2498(4)	400(5)	7534(6)	29(2)
C(8)	2402(5)	639(6)	8760(6)	35(2)
C(9)	2996(5)	316(6)	9567(7)	40(2)
C(10)	3654(5)	-225(6)	9166(7)	47(3)
C(11)	3751(4)	-485(6)	7940(7)	34(2)
C(12)	3156(4)	-150(5)	7137(6)	29(2)
C(13)	2610(4)	1540(5)	5463(6)	29(2)
C(14)	3151(4)	780(5)	4784(6)	30(2)
C(15)	4017(4)	1131(6)	4491(8)	46(2)
C(16)	4067(5)	1856(7)	3417(8)	53(2)
C(17)	3638(5)	2867(7)	3590(8)	53(3)
C(18)	3846(5)	3400(6)	4771(8)	41(2)
C(19)	3192(5)	3321(6)	5788(8)	46(2)
C(20)	3019(4)	2287(5)	6328(7)	34(2)

Table 3. Bond lengths [Å] and angles [°] for (2d) C₂₀H₂₂F₁₂P₂S₂.

P(1)-F(1)	1.464(8)
P(1)-F(6)	1.479(9)
P(1)-F(2)	1.678(8)
P(1)-F(3)	1.689(7)
P(1)-F(5)	1.690(6)
P(1)-F(4)	1.693(8)
P(2)-F(10)	1.564(5)
P(2)-F(7)	1.577(5)
P(2)-F(11)	1.581(5)
P(2)-F(9)	1.592(5)
P(2)-F(12)	1.775(6)
P(2)-F(8)	1.779(6)
S(1)-C(7)	1.712(7)
S(1)-C(13)	1.833(7)
S(1)-C(1)	2.056(8)
S(2)-C(6)	1.533(6)
S(2)-C(12)	1.798(7)
S(2)-C(14)	2.238(8)
C(1)-C(2)	1.175(8)
C(1)-C(6)	1.408(10)
C(2)-C(3)	1.619(13)
C(3)-C(4)	1.404(13)
C(4)-C(5)	1.191(9)
C(5)-C(6)	1.618(12)
C(7)-C(12)	1.333(10)
C(7)-C(8)	1.404(10)
C(8)-C(9)	1.299(10)
C(9)-C(10)	1.323(13)
C(10)-C(11)	1.415(12)
C(11)-C(12)	1.304(9)
C(13)-C(14)	1.624(10)
C(13)-C(20)	1.645(10)
C(14)-C(15)	1.326(8)
C(15)-C(16)	1.678(13)
C(16)-C(17)	1.772(16)
C(17)-C(18)	1.588(13)
C(18)-C(19)	1.418(11)
C(19)-C(20)	1.819(13)

Table 3. Bond lengths [Å] and angles [°] for (2d) C₂₀H₂₂F₁₂P₂S₂. (contd.)

F(1)-P(1)-F(6)	179.0(5)
F(1)-P(1)-F(2)	109.5(6)
F(6)-P(1)-F(2)	70.9(5)
F(1)-P(1)-F(3)	81.9(5)
F(6)-P(1)-F(3)	99.0(5)
F(2)-P(1)-F(3)	100.6(4)
F(1)-P(1)-F(5)	97.7(5)
F(6)-P(1)-F(5)	81.4(4)
F(2)-P(1)-F(5)	80.5(4)
F(3)-P(1)-F(5)	178.9(4)
F(1)-P(1)-F(4)	71.2(6)
F(6)-P(1)-F(4)	108.5(5)
F(2)-P(1)-F(4)	179.2(5)
F(3)-P(1)-F(4)	79.0(4)
F(5)-P(1)-F(4)	99.8(4)
F(10)-P(2)-F(7)	179.6(3)
F(10)-P(2)-F(11)	77.8(3)
F(7)-P(2)-F(11)	102.1(3)
F(10)-P(2)-F(9)	102.8(3)
F(7)-P(2)-F(9)	77.2(3)
F(11)-P(2)-F(9)	178.7(3)
F(10)-P(2)-F(12)	91.9(3)
F(7)-P(2)-F(12)	87.7(3)
F(11)-P(2)-F(12)	108.5(3)
F(9)-P(2)-F(12)	70.4(3)
F(10)-P(2)-F(8)	88.8(3)
F(7)-P(2)-F(8)	91.5(3)
F(11)-P(2)-F(8)	71.3(3)
F(9)-P(2)-F(8)	109.8(3)
F(12)-P(2)-F(8)	179.2(2)
C(7)-S(1)-C(13)	112.4(3)
C(7)-S(1)-C(1)	88.2(3)
C(13)-S(1)-C(1)	111.2(3)
C(6)-S(2)-C(12)	106.3(3)
C(6)-S(2)-C(14)	106.1(3)
C(12)-S(2)-C(14)	95.4(3)
C(2)-C(1)-C(6)	102.5(7)
C(2)-C(1)-S(1)	123.0(6)
C(6)-C(1)-S(1)	134.5(4)
C(1)-C(2)-C(3)	121.1(7)
C(4)-C(3)-C(2)	137.0(5)
C(5)-C(4)-C(3)	102.0(8)
C(4)-C(5)-C(6)	121.0(8)
C(1)-C(6)-S(2)	97.8(5)
C(1)-C(6)-C(5)	136.5(5)
S(2)-C(6)-C(5)	125.7(5)
C(12)-C(7)-C(8)	124.2(6)

Table 3. Bond lengths [Å] and angles [°] for (2d) C₂₀H₂₂F₁₂P₂S₂. (contd.)

C(12)-C(7)-S(1)	115.6(5)
C(8)-C(7)-S(1)	120.0(6)
C(9)-C(8)-C(7)	118.7(8)
C(8)-C(9)-C(10)	116.9(8)
C(9)-C(10)-C(11)	125.4(7)
C(12)-C(11)-C(10)	117.1(8)
C(11)-C(12)-C(7)	117.8(7)
C(11)-C(12)-S(2)	119.1(6)
C(7)-C(12)-S(2)	123.1(5)
C(14)-C(13)-C(20)	134.0(4)
C(14)-C(13)-S(1)	93.6(5)
C(20)-C(13)-S(1)	107.4(5)
C(15)-C(14)-C(13)	99.2(6)
C(15)-C(14)-S(2)	117.1(5)
C(13)-C(14)-S(2)	123.7(4)
C(14)-C(15)-C(16)	120.9(6)
C(15)-C(16)-C(17)	125.6(7)
C(18)-C(17)-C(16)	123.5(7)
C(19)-C(18)-C(17)	118.8(7)
C(18)-C(19)-C(20)	114.7(7)
C(13)-C(20)-C(19)	123.8(6)

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for (2d) $\text{C}_{20}\text{H}_{22}\text{F}_{12}\text{P}_2\text{S}_2$.
The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12})]$$

Atom	U11	U22	U33	U23	U13	U12
P(1)	18(1)	80(2)	33(1)	5(1)	5(1)	4(1)
F(1)	58(4)	301(13)	135(8)	-3(9)	-10(5)	-99(6)
F(2)	76(4)	163(8)	101(6)	23(6)	56(4)	60(5)
F(3)	49(3)	235(10)	66(4)	59(6)	31(3)	43(5)
F(4)	79(4)	151(7)	90(5)	43(5)	47(4)	63(5)
F(5)	29(2)	160(7)	43(3)	34(4)	6(2)	24(3)
F(6)	34(2)	329(13)	71(5)	-6(7)	-5(3)	-49(5)
P(2)	12(1)	57(2)	27(1)	2(1)	2(1)	1(1)
F(7)	21(1)	86(4)	31(2)	5(3)	-6(2)	7(2)
F(8)	29(2)	107(5)	52(3)	-12(3)	-4(2)	26(3)
F(9)	18(2)	130(5)	52(3)	4(3)	8(2)	-22(3)
F(10)	19(2)	106(5)	35(2)	11(3)	-8(2)	3(2)
F(11)	17(2)	112(5)	54(3)	18(3)	-2(2)	-22(2)
F(12)	26(2)	88(5)	37(2)	-11(3)	2(2)	12(2)
S(1)	10(1)	54(2)	28(1)	-4(1)	1(1)	3(1)
S(2)	10(1)	48(1)	27(1)	-1(1)	2(1)	3(1)
C(1)	16(2)	47(5)	30(3)	-2(4)	-1(2)	0(3)
C(2)	11(2)	90(7)	33(4)	-3(4)	0(2)	0(3)
C(3)	14(2)	93(7)	34(4)	-7(5)	3(2)	-21(3)
C(4)	21(3)	78(8)	43(4)	-27(5)	2(3)	-11(4)
C(5)	17(2)	69(7)	37(4)	-5(5)	2(2)	-3(4)
C(6)	11(2)	51(6)	25(3)	-6(4)	3(2)	-3(3)
C(7)	17(2)	41(5)	31(3)	0(4)	-3(2)	0(3)
C(8)	21(2)	57(6)	27(3)	5(4)	4(2)	-6(3)
C(9)	32(3)	70(7)	20(3)	11(4)	-3(3)	-13(4)
C(10)	27(3)	81(8)	31(4)	15(5)	-15(3)	-14(4)
C(11)	16(2)	47(6)	38(4)	12(4)	-3(2)	2(3)
C(12)	14(2)	52(6)	22(3)	2(4)	1(2)	-3(3)
C(13)	12(2)	48(5)	28(3)	0(4)	-2(2)	5(3)
C(14)	11(2)	55(6)	25(3)	3(4)	0(2)	-3(3)
C(15)	9(2)	80(7)	51(5)	-9(5)	5(3)	-3(3)
C(16)	29(3)	86(7)	44(4)	5(6)	10(3)	-16(4)
C(17)	28(3)	87(9)	43(5)	22(5)	3(3)	-21(4)
C(18)	17(2)	54(6)	54(5)	12(5)	3(3)	-4(3)
C(19)	20(2)	62(7)	55(5)	3(5)	5(3)	-3(4)
C(20)	13(2)	57(6)	31(3)	-2(4)	0(2)	-2(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (2d) $\text{C}_{20}\text{H}_{22}\text{F}_{12}\text{P}_2\text{S}_2$.

Atom	x	y	z	U(eq)
H(2A)	224	-134	5467	53
H(3A)	-44	-1479	4649	56
H(4A)	1070	-2519	4126	57
H(5A)	2628	-2094	4561	49
H(8A)	1923	1022	8989	42
H(9A)	2960	457	10388	48
H(10A)	4088	-453	9737	56
H(11A)	4218	-878	7716	40
H(13A)	2159	1785	4859	35
H(14A)	2790	719	4008	37
H(15A)	4474	703	4239	56
H(15B)	4292	1361	5235	56
H(16A)	3711	1639	2715	64
H(16B)	4769	1895	3179	64
H(17A)	3906	3169	2903	63
H(17B)	2913	2852	3484	63
H(18A)	4523	3279	5049	50
H(18B)	3840	3965	4524	50
H(19A)	2539	3541	5569	55
H(19B)	3455	3646	6455	55
H(20A)	3664	2114	6651	41
H(20B)	2563	2318	7019	41

Table 1. Crystal data and structure refinement for $C_{29}H_{24}F_{12}S_4Sb_2$:

Identification code	$C_{29}H_{24}F_{12}S_4Sb_2$
Empirical formula	$C_{29}H_{24}F_{12}S_4Sb_2$
Formula weight	972.22
Temperature	298 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/n
Unit cell dimensions	
	$a = 14.672(3)$ Å $\alpha = 90^\circ$
	$b = 13.741(3)$ Å $\beta = 108.06(3)^\circ$
	$c = 17.658(4)$ Å $\gamma = 90^\circ$
Volume,	$3384.5(12)$ Å ³
Z	4
Density (calculated)	1.908 Mg/m ³
Absorption coefficient	1.931 mm ⁻¹
F(000)	1888
Crystal size	0.50 x 0.45 x 0.20 mm
$\bar{\alpha}$ range for data collection	2.08 to 27.42°
Limiting indices	$0 \leq h \leq 15, 0 \leq k \leq 17, -22 \leq l \leq 21$
Reflections collected	4831
Independent reflections	4535 ($R_{int} = 0.0378$)
Absorption correction	Psi scans
Max. and min. transmission	1.0000 and 0.6232
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4535 / 0 / 424
Goodness-of-fit on F^2	1.039
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0479, wR2 = 0.1234$
R indices (all data)	$R1 = 0.0805, wR2 = 0.1377$
Largest diff. peak and hole	1.103 and -0.864 e.Å ⁻³

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $\text{C}_{29}\text{H}_{24}\text{F}_{12}\text{S}_4\text{Sb}_2$.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	$U(\text{eq})$
Sb(1)	2384(1)	4049(1)	2202(1)	62(1)
F(11)	2489(8)	3979(7)	3270(4)	160(4)
F(12)	3575(7)	3619(11)	2410(7)	220(6)
F(13)	2257(8)	4064(6)	1134(4)	150(4)
F(14)	1174(7)	4493(13)	1993(8)	240(7)
F(15)	2729(9)	5323(6)	2271(7)	196(5)
F(16)	1981(12)	2808(7)	2124(5)	227(7)
Sb(2)	6345(1)	3042(1)	1172(1)	62(1)
F(21)	7574(4)	2503(5)	1602(4)	98(2)
F(22)	6789(6)	3998(6)	650(6)	147(4)
F(23)	5130(4)	3606(4)	774(3)	77(2)
F(24)	5884(7)	2219(13)	1737(11)	349(13)
F(25)	6601(6)	3887(12)	2006(5)	247(8)
F(26)	6120(9)	2272(8)	345(7)	281(10)
S(1)	8378(1)	1879(1)	4488(1)	41(1)
S(2)	8743(2)	3847(2)	3571(1)	61(1)
S(3)	5402(1)	2641(2)	3711(1)	44(1)
S(4)	6002(2)	3392(2)	5583(1)	68(1)
C(1)	9197(5)	1896(6)	3921(4)	45(2)
C(2)	9672(6)	1040(7)	3893(5)	54(2)
C(3)	10295(6)	1011(8)	3457(6)	70(3)
C(4)	10439(7)	1828(9)	3051(6)	73(3)
C(5)	9965(7)	2670(8)	3091(5)	64(3)
C(6)	9330(6)	2726(6)	3528(5)	49(2)
C(7)	8715(6)	3856(6)	4564(5)	51(2)
C(8)	8847(6)	4731(6)	4980(6)	62(2)
C(9)	8816(7)	4761(9)	5752(7)	80(3)
C(10)	8662(7)	3938(9)	6133(6)	73(3)
C(11)	8546(6)	3058(7)	5739(5)	56(2)
C(12)	8550(5)	3038(6)	4960(5)	44(2)
C(13)	5821(5)	3819(6)	4006(5)	46(2)
C(14)	5923(7)	4435(7)	3405(6)	65(3)
C(15)	6319(8)	5336(8)	3599(8)	84(3)
C(16)	6588(8)	5636(7)	4362(9)	86(4)
C(17)	6469(7)	5074(8)	4963(7)	75(3)
C(18)	6085(6)	4121(6)	4797(5)	52(2)
C(19)	5021(7)	2655(7)	5145(6)	61(3)
C(20)	4498(9)	2285(7)	5615(7)	78(3)
C(21)	3708(10)	1734(9)	5317(10)	99(4)
C(22)	3365(8)	1520(8)	4515(10)	88(4)
C(23)	3869(7)	1855(7)	4007(7)	72(3)
C(24)	4692(6)	2387(6)	4339(6)	53(2)
C(25)	6445(5)	1844(6)	4174(5)	44(2)
C(26)	7189(5)	1943(5)	3727(4)	38(2)

C(27)	7068(6)	1061(6)	3176(5)	51(2)
C(28)	6178(7)	543(7)	3224(6)	71(3)
C(29)	6134(7)	785(6)	4051(6)	57(2)

Table 3. Bond lengths [Å] and angles [°] for C₂₉H₂₄F₁₂S₄Sb₂.

Sb(1)-F(12)	1.772(9)
Sb(1)-F(16)	1.796(8)
Sb(1)-F(14)	1.804(10)
Sb(1)-F(15)	1.816(9)
Sb(1)-F(13)	1.838(7)
Sb(1)-F(11)	1.846(7)
Sb(2)-F(26)	1.749(8)
Sb(2)-F(24)	1.775(8)
Sb(2)-F(25)	1.821(10)
Sb(2)-F(22)	1.835(7)
Sb(2)-F(23)	1.870(5)
Sb(2)-F(21)	1.878(6)
S(1)-C(12)	1.780(8)
S(1)-C(1)	1.786(8)
S(1)-C(26)	1.843(7)
S(2)-C(7)	1.766(8)
S(2)-C(6)	1.778(9)
S(3)-C(13)	1.751(8)
S(3)-C(24)	1.776(9)
S(3)-C(25)	1.853(8)
S(4)-C(19)	1.733(11)
S(4)-C(18)	1.746(9)
C(1)-C(2)	1.375(11)
C(1)-C(6)	1.381(11)
C(2)-C(3)	1.366(12)
C(3)-C(4)	1.384(14)
C(4)-C(5)	1.363(14)
C(5)-C(6)	1.383(11)
C(7)-C(12)	1.385(11)
C(7)-C(8)	1.391(12)
C(8)-C(9)	1.378(14)
C(9)-C(10)	1.370(15)
C(10)-C(11)	1.379(13)
C(11)-C(12)	1.378(11)
C(13)-C(18)	1.393(11)
C(13)-C(14)	1.401(12)
C(14)-C(15)	1.365(15)
C(15)-C(16)	1.346(16)
C(16)-C(17)	1.366(15)
C(17)-C(18)	1.420(13)
C(19)-C(20)	1.389(12)
C(19)-C(24)	1.404(13)
C(20)-C(21)	1.347(17)
C(21)-C(22)	1.380(17)
C(22)-C(23)	1.404(14)
C(23)-C(24)	1.378(12)
C(25)-C(29)	1.521(11)
C(25)-C(26)	1.538(10)

C(26)-C(27)	1.530(10)
C(27)-C(28)	1.513(12)
C(28)-C(29)	1.518(13)
F(12)-Sb(1)-F(16)	88.8(7)
F(12)-Sb(1)-F(14)	179.7(8)
F(16)-Sb(1)-F(14)	91.5(8)
F(12)-Sb(1)-F(15)	94.1(7)
F(16)-Sb(1)-F(15)	177.1(7)
F(14)-Sb(1)-F(15)	85.6(7)
F(12)-Sb(1)-F(13)	89.8(5)
F(16)-Sb(1)-F(13)	90.4(4)
F(14)-Sb(1)-F(13)	90.3(5)
F(15)-Sb(1)-F(13)	89.7(5)
F(12)-Sb(1)-F(11)	90.4(5)
F(16)-Sb(1)-F(11)	87.1(4)
F(14)-Sb(1)-F(11)	89.5(5)
F(15)-Sb(1)-F(11)	92.8(5)
F(13)-Sb(1)-F(11)	177.5(4)
F(26)-Sb(2)-F(24)	94.4(10)
F(26)-Sb(2)-F(25)	177.3(8)
F(24)-Sb(2)-F(25)	88.3(9)
F(26)-Sb(2)-F(22)	91.1(7)
F(24)-Sb(2)-F(22)	173.8(8)
F(25)-Sb(2)-F(22)	86.2(6)
F(26)-Sb(2)-F(23)	91.5(4)
F(24)-Sb(2)-F(23)	89.4(4)
F(25)-Sb(2)-F(23)	88.4(3)
F(22)-Sb(2)-F(23)	87.7(3)
F(26)-Sb(2)-F(21)	90.5(4)
F(24)-Sb(2)-F(21)	90.4(4)
F(25)-Sb(2)-F(21)	89.6(4)
F(22)-Sb(2)-F(21)	92.3(3)
F(23)-Sb(2)-F(21)	178.0(3)
C(12)-S(1)-C(1)	103.2(4)
C(12)-S(1)-C(26)	105.2(3)
C(1)-S(1)-C(26)	103.9(3)
C(7)-S(2)-C(6)	102.0(4)
C(13)-S(3)-C(24)	102.5(4)
C(13)-S(3)-C(25)	104.4(4)
C(24)-S(3)-C(25)	99.9(4)
C(19)-S(4)-C(18)	103.5(4)
C(2)-C(1)-C(6)	122.4(7)
C(2)-C(1)-S(1)	116.5(6)
C(6)-C(1)-S(1)	121.1(6)
C(3)-C(2)-C(1)	118.8(9)
C(2)-C(3)-C(4)	120.3(9)
C(5)-C(4)-C(3)	119.9(9)
C(4)-C(5)-C(6)	121.3(9)
C(1)-C(6)-C(5)	117.3(8)
C(1)-C(6)-S(2)	123.3(6)
C(5)-C(6)-S(2)	119.4(7)
C(12)-C(7)-C(8)	116.9(8)

C(12)-C(7)-S(2)	123.9(6)
C(8)-C(7)-S(2)	119.2(7)
C(9)-C(8)-C(7)	120.4(9)
C(10)-C(9)-C(8)	121.5(9)
C(9)-C(10)-C(11)	119.2(9)
C(12)-C(11)-C(10)	118.9(9)
C(11)-C(12)-C(7)	123.0(8)
C(11)-C(12)-S(1)	116.2(7)
C(7)-C(12)-S(1)	120.8(6)
C(18)-C(13)-C(14)	121.2(8)
C(18)-C(13)-S(3)	122.4(6)
C(14)-C(13)-S(3)	116.4(7)
C(15)-C(14)-C(13)	119.7(10)
C(16)-C(15)-C(14)	119.9(11)
C(15)-C(16)-C(17)	122.4(10)
C(16)-C(17)-C(18)	120.0(10)
C(13)-C(18)-C(17)	116.8(9)
C(13)-C(18)-S(4)	124.1(7)
C(17)-C(18)-S(4)	119.1(7)
C(20)-C(19)-C(24)	115.4(10)
C(20)-C(19)-S(4)	118.9(9)
C(24)-C(19)-S(4)	125.6(6)
C(21)-C(20)-C(19)	122.7(12)
C(20)-C(21)-C(22)	121.1(11)
C(21)-C(22)-C(23)	119.2(11)
C(24)-C(23)-C(22)	118.0(11)
C(23)-C(24)-C(19)	123.4(9)
C(23)-C(24)-S(3)	116.5(8)
C(19)-C(24)-S(3)	119.8(7)
C(29)-C(25)-C(26)	103.9(6)
C(29)-C(25)-S(3)	109.4(6)
C(26)-C(25)-S(3)	110.0(5)
C(27)-C(26)-C(25)	107.2(6)
C(27)-C(26)-S(1)	108.8(5)
C(25)-C(26)-S(1)	106.5(5)
C(28)-C(27)-C(26)	105.6(7)
C(27)-C(28)-C(29)	104.2(7)
C(28)-C(29)-C(25)	104.3(7)

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $\text{C}_{29}\text{H}_{24}\text{F}_{12}\text{S}_4\text{Sb}_2$.
The anisotropic displacement factor exponent takes the form:

$$-2\Pi^2 [(h^2 a^2 U_{11} + \dots + 2hka^* b^* U_{12})]$$

Atom	U11	U22	U33	U23	U13	U12
Sb(1)	66(1)	62(1)	61(1)	-12(1)	23(1)	-6(1)
F(11)	243(11)	166(8)	72(5)	-29(5)	50(6)	28(7)
F(12)	110(7)	325(16)	231(12)	65(12)	62(7)	97(9)
F(13)	258(11)	129(7)	78(5)	19(4)	74(6)	31(7)
F(14)	107(8)	381(19)	243(13)	67(13)	70(8)	70(10)
F(15)	88(14)	82(6)	198(11)	-18(6)	44(9)	-41(7)
F(16)	460(20)	109(7)	107(6)	-33(5)	74(9)	-140(10)
Sb(2)	48(1)	77(1)	52(1)	10(1)	3(1)	-8(1)
F(21)	65(4)	117(5)	103(5)	15(4)	12(3)	21(4)
F(22)	98(5)	111(6)	261(11)	68(6)	99(7)	19(5)
F(23)	50(3)	96(4)	71(3)	14(3)	0(3)	-9(3)
F(24)	90(6)	460(20)	450(20)	410(20)	20(9)	5(10)
F(25)	110(7)	500(20)	97(6)	-136(10)	-17(5)	100(10)
F(26)	252(13)	176(9)	265(13)	-177(10)	-140(10)	138(9)
S(1)	36(1)	42(1)	42(1)	3(1)	10(1)	2(1)
S(2)	64(2)	56(1)	65(1)	17(1)	23(1)	3(1)
S(3)	38(1)	46(1)	45(1)	-1(1)	10(1)	3(1)
S(4)	72(2)	84(2)	47(1)	-2(1)	16(1)	10(1)
C(1)	37(4)	57(5)	41(4)	-1(4)	11(4)	1(4)
C(2)	42(5)	58(6)	59(5)	-6(4)	13(4)	11(4)
C(3)	46(5)	85(8)	77(7)	-26(6)	17(5)	8(5)
C(4)	57(6)	101(9)	68(6)	-21(6)	32(5)	-6(6)
C(5)	60(6)	86(7)	51(5)	7(5)	25(5)	-5(5)
C(6)	44(5)	62(6)	39(4)	0(4)	7(4)	-4(4)
C(7)	42(5)	55(6)	51(5)	-5(4)	9(4)	3(4)
C(8)	47(5)	47(5)	89(7)	-9(5)	19(5)	2(4)
C(9)	48(6)	85(8)	97(9)	-45(7)	9(6)	-1(6)
C(10)	54(6)	99(9)	63(6)	-32(7)	15(5)	2(6)
C(11)	41(5)	81(7)	43(5)	-6(5)	10(4)	3(5)
C(12)	31(4)	52(5)	48(5)	-6(4)	10(3)	-1(4)
C(13)	39(4)	42(5)	54(5)	-2(4)	11(4)	6(4)
C(14)	64(6)	51(6)	80(7)	20(5)	24(5)	17(5)
C(15)	72(7)	61(8)	117(10)	28(7)	25(7)	9(6)
C(16)	65(7)	36(6)	148(12)	14(7)	20(8)	-1(5)
C(17)	56(6)	70(7)	87(7)	-25(6)	4(5)	10(5)
C(18)	38(5)	54(5)	62(6)	-1(4)	14(4)	13(4)
C(19)	68(6)	60(6)	73(7)	24(5)	50(5)	31(5)
C(20)	105(9)	56(6)	99(8)	19(6)	70(8)	27(6)
C(21)	109(11)	60(7)	164(14)	20(8)	95(11)	13(7)
C(22)	70(7)	55(7)	155(12)	6(8)	55(8)	-3(6)
C(23)	57(6)	54(6)	105(8)	6(6)	24(6)	-2(5)
C(24)	42(5)	46(5)	72(6)	12(4)	21(4)	6(4)
C(25)	40(4)	50(5)	41(4)	2(4)	13(3)	0(4)
C(26)	35(4)	42(4)	35(4)	6(3)	9(3)	6(4)
C(27)	57(5)	50(5)	46(5)	-5(4)	13(4)	9(4)

C(28)	59(6)	53(6)	98(8)	-18(5)	19(5)	-3(5)
C(29)	59(6)	45(5)	74(6)	8(4)	33(5)	0(4)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{C}_{29}\text{H}_{24}\text{F}_{12}\text{S}_4\text{Sb}_2$.

Atom	x	y	z	U(eq)
H(2)	9571	492	4165	65
H(3)	10624	439	3433	84
H(4)	10859	1803	2750	87
H(5)	10070	3218	2820	77
H(8)	8957	5300	4736	74
H(9)	8903	5353	6020	96
H(10)	8635	3972	6652	87
H(11)	8467	2488	5995	67
H(14)	5721	4232	2877	78
H(15)	6402	5742	3204	101
H(16)	6866	6248	4484	104
H(17)	6640	5316	5480	90
H(20)	4700	2424	6157	93
H(21)	3389	1494	5658	119
H(22)	2807	1157	4312	106
H(23)	3653	1722	3464	87
H(25)	6731	1993	4742	52
H(26)	7107	2554	3428	45
H(27B)	6989	1266	2634	62
H(27A)	7622	636	3351	62
H(28B)	6230	-154	3160	86
H(28A)	5611	779	2817	86
H(29B)	6566	372	4449	68
H(29A)	5489	704	4079	68

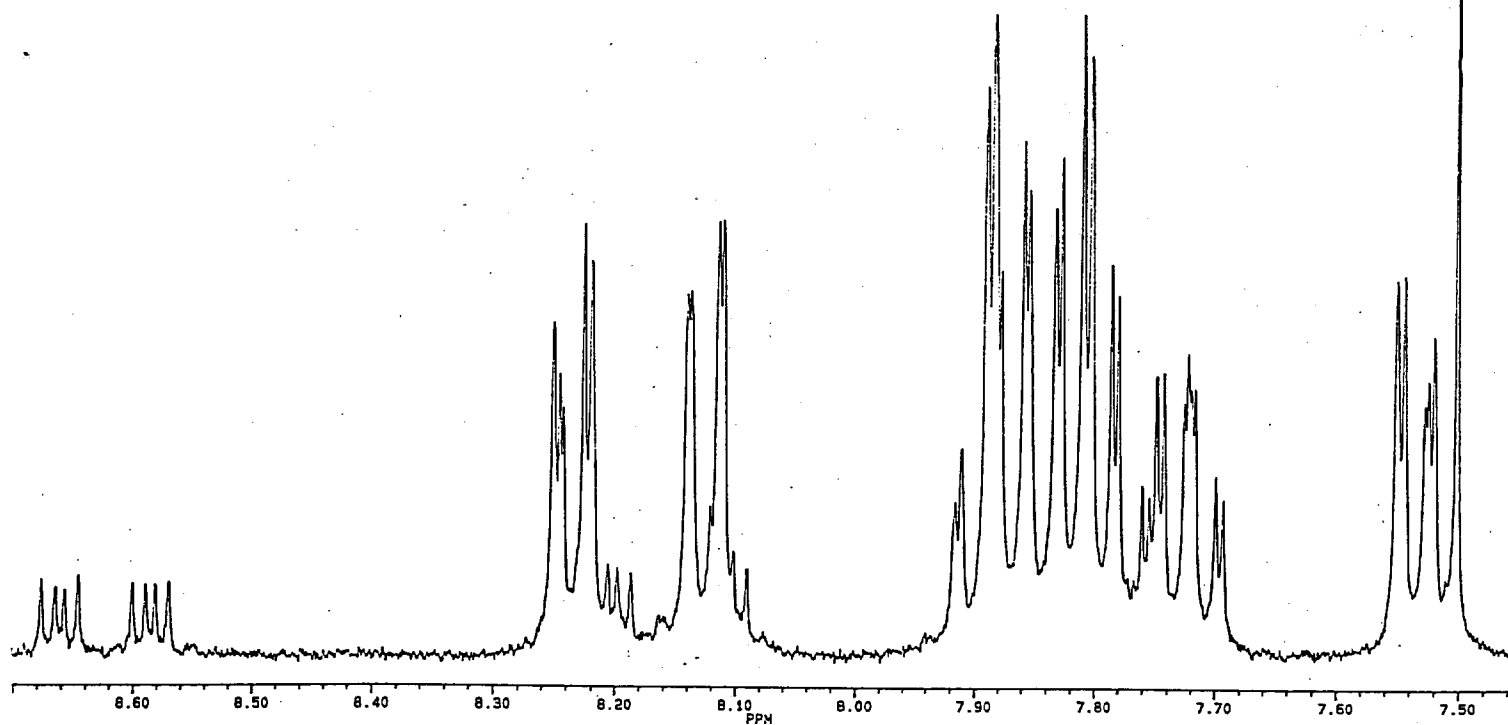


Figure 3. ^1H NMR spectrum (aromatic region) of the mixture of the mono- (8) and bis-adduct (9) of $\text{Th}^+\text{ClO}_4^-$ to cyclopentene.

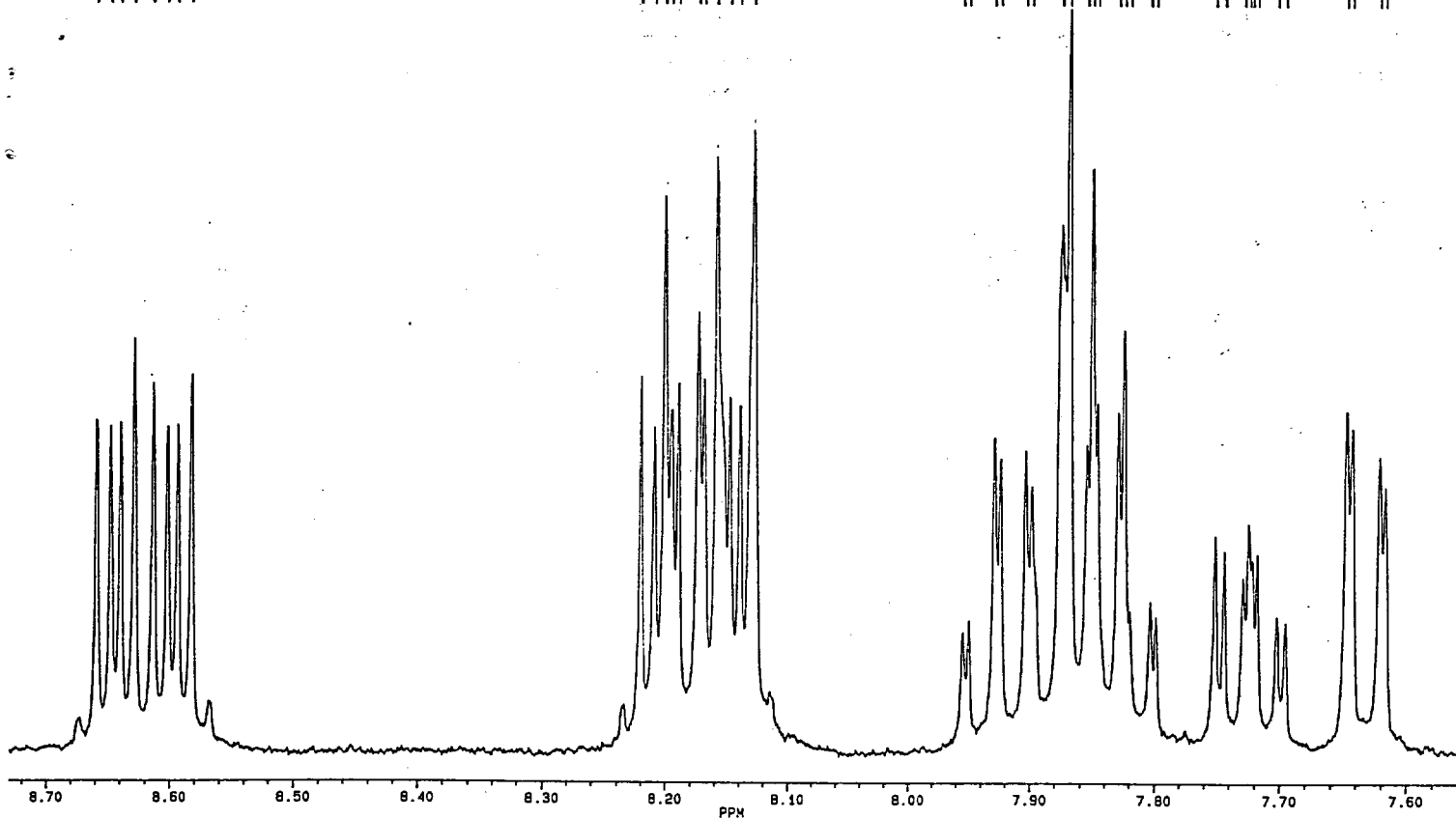


Figure 4. ^1H NMR spectrum (aromatic region) of the mixture of the mono- (10) and bis-adduct (11) of $\text{Th}^+\text{ClO}_4^-$ to cycloheptene.

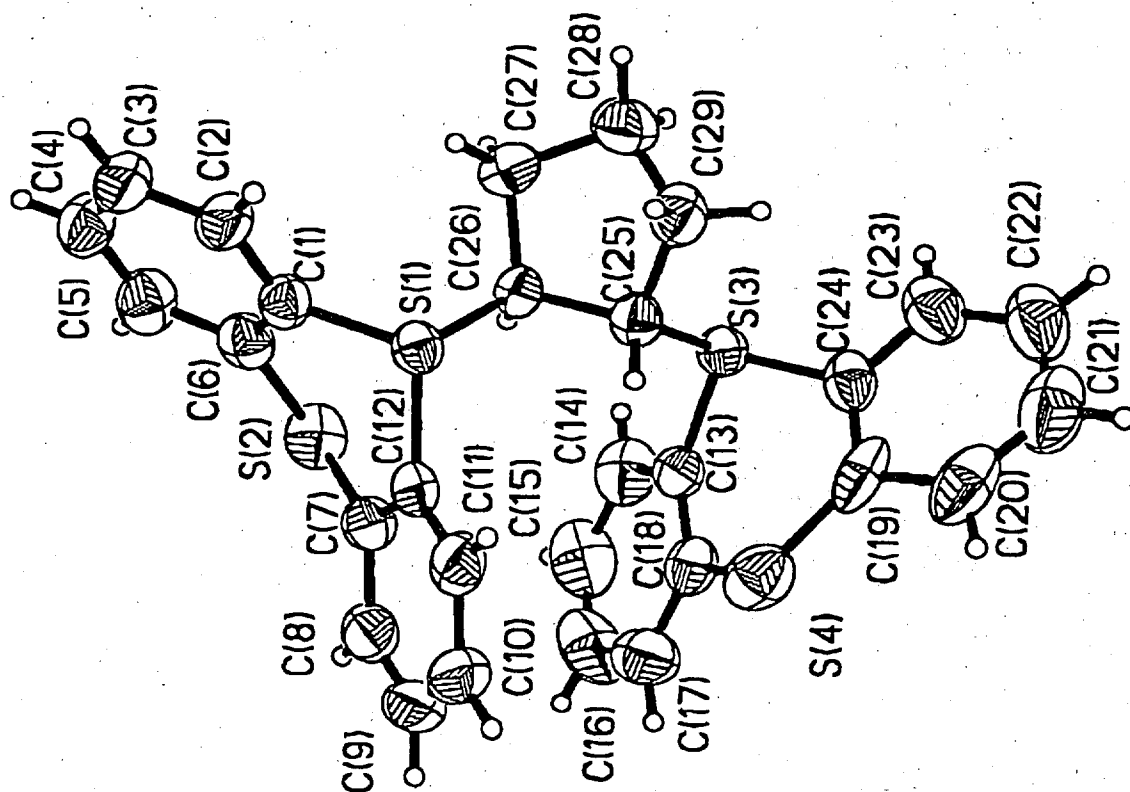


Figure 5. Ortep diagram of the bis-adduct ($C_{29}H_{24}S_4Sb_2F_{12}$) of $Th^+SbF_6^-$ to cyclopentene. The counter ions are not shown.