Stereochemically (in)active lone pairs in Sb(III) complexes of a soft scorpionate ligand

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Supplementary Information

A. Colour changes

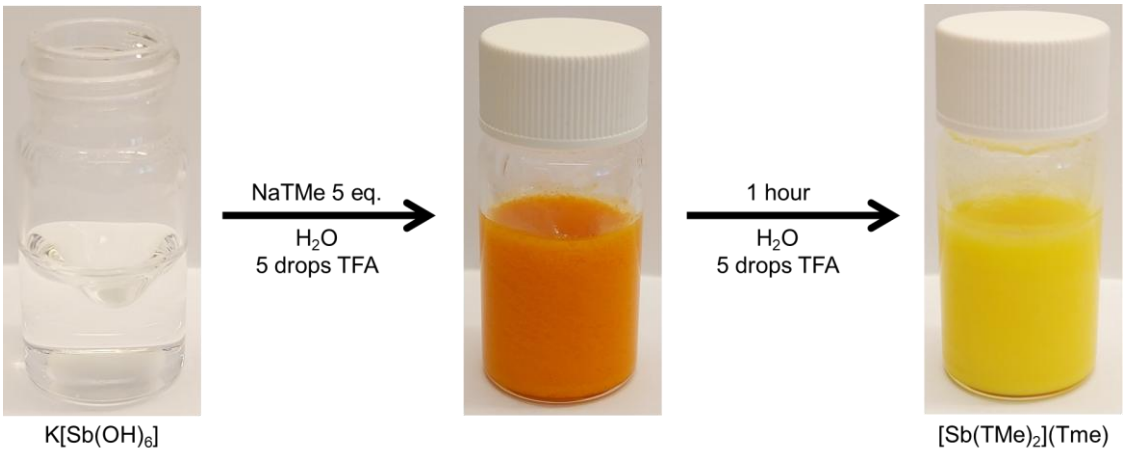

Figure S1. Colour changes during the synthesis of [Sb(TMe)$_2$](TMe).

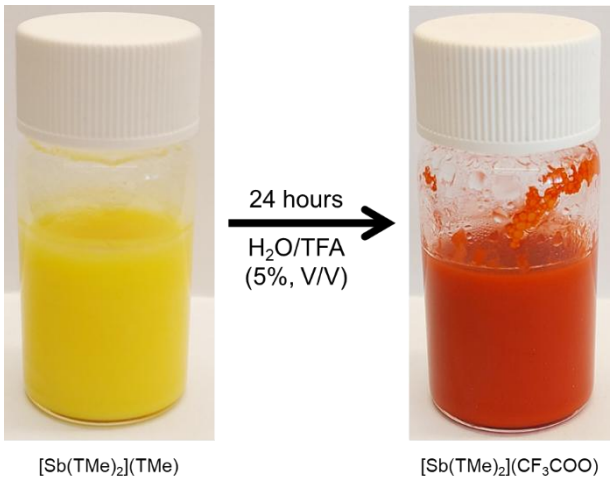

Figure S2. Colour changes during the synthesis of [Sb(TMe)$_2$](CF$_3$COO).

Figure S3. Co-crystallisation of [Sb(TMe)$_2$](PF$_6$)·Me$_2$CO (red) and [Sb$_2$(TMe)$_3$(C$_4$H$_6$N$_2$S)](PF$_6$)$_3$·1.7Me$_2$CO (yellow).

B. Crystallography

Table S1. Crystal data and structure refinements

Complex	$[Sb_4Cl_8(TMe)_4]$ ·4MeOH (**1**)	$[Sb(TMe)_2](TMe)$ ·Me_2CO·$3.6H_2O$ (**2**)	$[Sb(TMe)_2](CF_3COO)$ ·½Me_2CO [1.6 CF_3COOH] (**3a**)	$[Sb(TMe)_2](PF_6)$·Me_2CO (**3b**)	$[Sb_2(TMe)_3(C_4H_6N_2S)](PF_6)_3$ ·$1.7Me_2CO$ (**4**)
Formula	$C_{52}H_{80}N_{24}O_4S_{12}Cl_8Sb_4B_4$	$C_{39}H_{60.8}B_3N_{18}O_{4.4}S_9Sb$	$C_{30.7}H_{36.6}B_2F_{7.8}N_{12}O_{5.7}S_6Sb$	$C_{27}H_{38}B_2N_{12}OF_6PS_6Sb$	$C_{45.1}H_{64.2}B_3F_{18}N_{20}O_{1.7}P_3S_{10}Sb_2$
Formula weight	2303.96	1294.97	1148.85	1027.39	1945.20
Temperature/K	100.01(10)	100.00(12)	100.00(10)	100.00(10)	100.00(10)
Crystal system	monoclinic	triclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P1,^{-}$	I2/a	I2/a	C2/c
a/Å	10.86977(5)	10.5707(2)	10.36050(10)	45.083(3)	32.0046(9)
b/Å	26.79870(10)	14.9955(3)	17.2928(2)	9.2529(5)	14.8912(3)
c/Å	15.13528(6)	19.6610(3)	28.3074(3)	30.1304(17)	34.1458(12)
α/°	90	77.2890(10)	90	90	90
β/°	93.6973(4)	79.4900(10)	91.2010(10)	96.992(5)	114.476(4)
γ/°	90	72.973(2)	90	90	90
Volume/$Å^3$	4399.66(3)	2883.54(10)	5070.50(9)	12475.4(12)	14811.0(8)
Z	2	2	4	12	8
ρ_{calc} g/cm^3	1.739	1.491	1.505	1.641	1.745
μ/mm^{-1}	14.993	7.307	7.327	9.052	9.912
F(000)	2288.0	1332.0	2310.0	6216.0	7779.0
Crystal size/mm^3	0.22 × 0.14 × 0.06	0.172 × 0.064 × 0.018	0.2 × 0.12 × 0.04	0.19 × 0.04 × 0.03	0.111 × 0.095 × 0.011
Reflections collected	111568	69071	55956	15324	46676
Indep. refl [R_{int}, R_σ]	8952 [0.0396, 0.0157]	11622 [0.0357, 0.0236]	5151 [0.0378, 0.0156]	15324 [na*, 0.0799]	11519 [0.0583, 0.0587]
Data/restraints/param.	8952/0/510	11622/64/716	5151/6/276	15324/774/831	11519/1773/948
Goodness-of-fit on F^2	1.072	1.036	1.074	0.944	1.151
R1, wR2 [I>=2σ (I)]	0.0189, 0.0465	0.0394, 0.1057	0.0295, 0.0863	0.0439, 0.1019	0.0658, 0.1353
R1, wR2 [all data]	0.0197, 0.0470	0.0425, 0.1088	0.0319, 0.0886	0.0736, 0.1072	0.0789, 0.1419
Largest diff. peak/hole / e $Å^{-3}$	0.75/-0.68	1.69/-1.37	1.11/-0.57	0.50/-0.81	1.60/-0.97
CCDC number	2388628	2388626	2388627	2388624	2388625

*Two-Component twin refined using HKLF5 data

i) $[Sb(TMe)Cl_2]_4 \cdot 4CH_3OH$ (1):

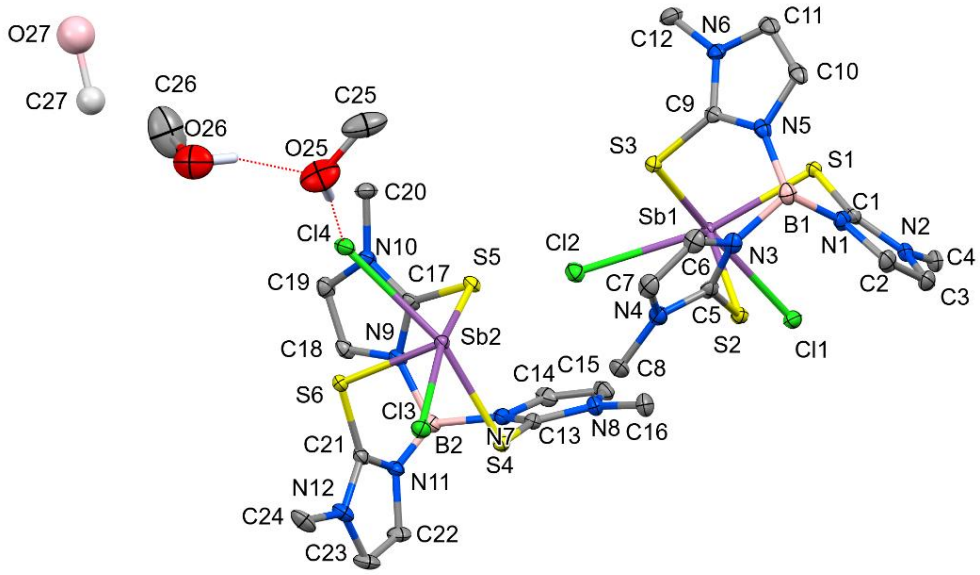

*Figure S4. Asymmetric unit of **1** showing 50% probability ellipsoids with atomic labelling scheme. The minor component disordered MeOH molecule (pale colours) was refined with isotropic displacement parameters. Hydrogen atoms omitted for clarity except those involved in H-bonds (red dashed lines).*

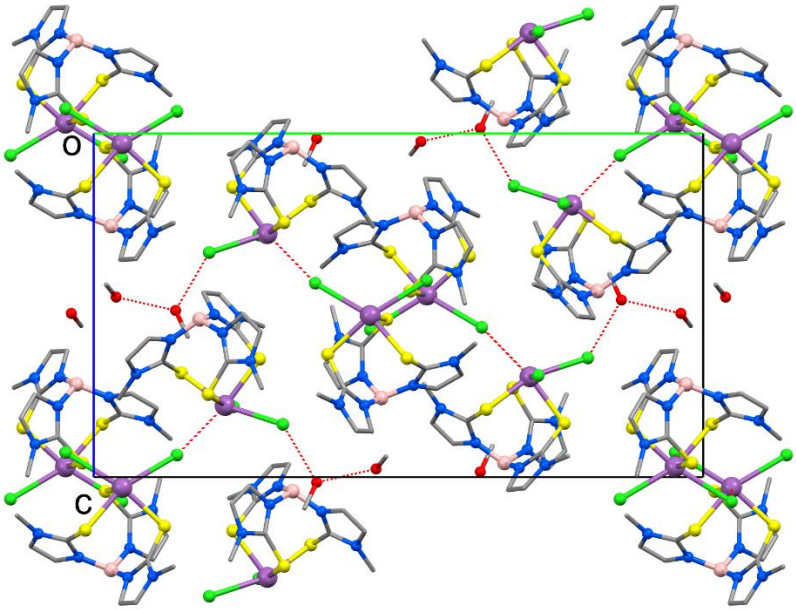

*Figure S5. Unit cell packing of **1** viewed down the a axis. Hydrogen atoms and minor disorder omitted for clarity.*

One of the two independent methanol solvate molecules is disordered (Figure S4), the major component is hydrogen bonded to both a coordinated chloro ligand (O26···Cl4, 3.0573(19) Å) and to the second methanol (O26···O25, 2.679(4) Å). There are no particularly striking interactions between neighbouring $[SbCl_2(TMe)]_4 \cdot 4MeOH$ assemblies (Figure S5), although there are many long C–H···(S, Cl) interactions (Table S2, Figure S5).

*Table S2. Selected geometric parameters (Å, º) for $[Sb(TMe)Cl_2]_4 \cdot 4CH_3OH$ (**1**)*

Sb1—S1	2.5761 (4)	Sb2—S4	2.5640 (5)
Sb1—S2	2.5155 (4)	Sb2—S5	2.6165 (4)
Sb1—S3	2.5590 (4)	Sb2—S6	2.5386 (4)
Sb1—Cl1	2.9268 (5)	Sb2—Cl3	2.7805 (5)
Sb1—Cl2	2.9419 (5)	Sb2—Cl4	2.8800 (5)
Sb1—Cl1^{i}	3.1582 (5)	Sb2—Cl2	3.1684 (5)
Cl1—Sb1—Cl1^{i}	101.116 (11)	Cl3—Sb2—Cl2	110.879 (13)
Cl1—Sb1—Cl2	114.463 (13)	Cl3—Sb2—Cl4	104.179 (14)
Cl2—Sb1—Cl1^{i}	113.524 (13)	Cl4—Sb2—Cl2	106.630 (13)
S1—Sb1—Cl1	82.823 (14)	S4—Sb2—Cl2	89.075 (13)
S1—Sb1—Cl1^{i}	65.616 (13)	S4—Sb2—Cl3	75.871 (14)
S1—Sb1—Cl2	161.855 (14)	S4—Sb2—Cl4	162.732 (14)
S2—Sb1—Cl1	72.309 (14)	S4—Sb2—S5	91.111 (14)
S2—Sb1—Cl1^{i}	156.939 (14)	S5—Sb2—Cl2	70.716 (13)
S2—Sb1—Cl2	88.938 (14)	S5—Sb2—Cl3	166.748 (15)
S2—Sb1—S1	91.434 (14)	S5—Sb2—Cl4	87.496 (14)
S2—Sb1—S3	92.107 (15)	S6—Sb2—Cl2	160.350 (14)
S3—Sb1—Cl1	162.748 (14)	S6—Sb2—Cl3	88.001 (14)
S3—Sb1—Cl1^{i}	90.373 (13)	S6—Sb2—Cl4	72.352 (14)
S3—Sb1—Cl2	71.449 (14)	S6—Sb2—S4	90.435 (15)
S3—Sb1—S1	90.410 (14)	S6—Sb2—S5	89.656 (14)
Sb1—Cl1—Sb1^{i}	78.884 (11)	Sb1—Cl2—Sb2	165.327 (18)

*Table S3. Hydrogen-bond geometry (Å, º) for [Sb(TMe)Cl$_2$]$_4$·4CH$_3$OH (**1**)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O25—H25···Cl4	0.84	2.22	3.0573 (19)	174
O26—H26···O25	0.84	1.87	2.679 (4)	161
C2—H2···S4^{ii}	0.95	2.91	3.515 (2)	123
C3—H3···Cl3^{ii}	0.95	2.65	3.583 (2)	167
C4—H4*A*···Cl1	0.98	2.71	3.497 (2)	138
C7—H7···Cl4^{iii}	0.95	2.91	3.490 (2)	120
C7—H7···S6^{iii}	0.95	2.77	3.712 (2)	170
C8—H8*A*···Cl2	0.98	2.94	3.745 (2)	140
C8—H8*C*···S2^{ii}	0.98	2.91	3.706 (2)	139
C10—H10···O26^{iv}	0.95	2.30	3.238 (3)	168
C12—H12*A*···Cl1^{i}	0.98	2.87	3.751 (2)	149
C12—H12*B*···Cl4^{v}	0.98	2.84	3.596 (2)	135
C12—H12*C*···Cl3^{v}	0.98	2.93	3.884 (2)	166
C14—H14···O25^{vi}	0.95	2.45	3.282 (3)	146
C15—H15···S1^{i}	0.95	2.97	3.543 (2)	120
C16—H16*B*···Cl2	0.98	2.85	3.622 (2)	136
C16—H16*C*···Cl1	0.98	2.70	3.580 (2)	150
C18—H18···Cl3^{vi}	0.95	2.75	3.677 (2)	165
C19—H19···Cl2^{vi}	0.95	2.83	3.723 (2)	158
C20—H20*A*···Cl3^{vii}	0.98	2.93	3.859 (2)	160
C20—H20*C*···S3^{vi}	0.98	2.84	3.732 (2)	151
C23—H23···Cl4^{viii}	0.95	2.55	3.502 (2)	176
C24—H24*B*···Cl3	0.98	2.87	3.769 (2)	154

Symmetry codes: (i) -*x*+1, -*y*+1, -*z*+1; (ii) -*x*+2, -*y*+1, -*z*+1; (iii) *x*+1/2, -*y*+1/2, *z*+1/2; (iv) -*x*+3/2, *y*+1/2, -*z*+3/2; (v) *x*-1/2, -*y*+1/2, *z*+1/2; (vi) *x*-1/2, -*y*+1/2, *z*-1/2; (vii) *x*-1, *y*, *z*; (viii) *x*+1/2, -*y*+1/2, *z*-1/2.

ii) **[Sb(TMe)$_2$](TMe)·(Me)$_2$CO·3.6H$_2$O (2)**

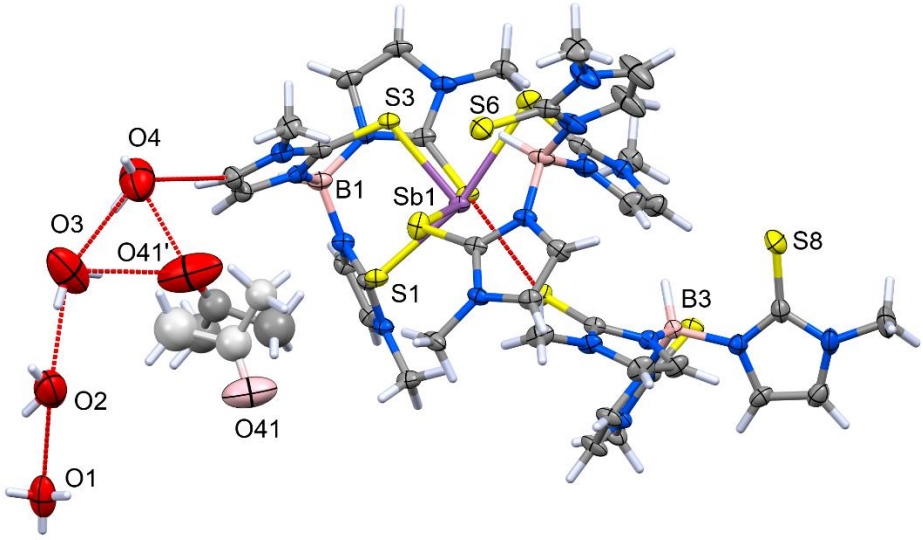

*Figure S6. Asymmetric unit of [Sb(TMe)$_2$](TMe)·(Me)$_2$CO·3.6H$_2$O (**2**) showing 50% probability ellipsoids with hydrogen bonding scheme (red dashed lines). The carbon atoms of the disordered acetone molecule were refined with isotropic displacement parameters.*

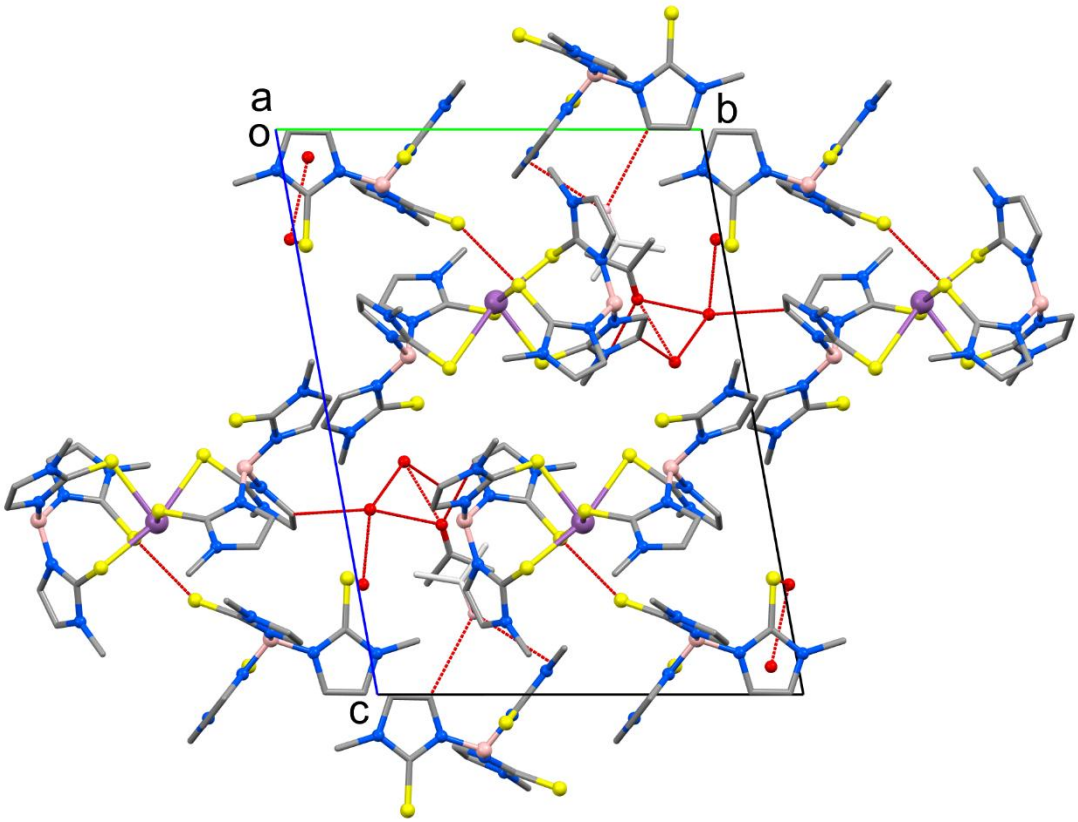

*Figure S7. Unit cell packing of **2** viewed down the a axis. Hydrogen atoms omitted for clarity.*

The solvate molecules are all involved in hydrogen bonding, there is are three H_2O····S bond there are also several C-H····O and C-H····S interactions (Table S5), but no notable specific interactions that could be said to stabilize the [Sb(κ^3-TMe)(κ^2-TMe)](TMe) structure.

*Table S4. Selected geometric parameters (Å, º) for [Sb(TMe)$_2$](TMe)·Me$_2$CO·3.6H$_2$O (**2**)*

Sb1—S1	2.6023 (7)	Sb1—S4	2.8727 (7)
Sb1—S2	2.6301 (7)	Sb1—S5	2.9245 (8)
Sb1—S3	2.5462 (7)	Sb1—S7	3.2579 (7)
S2—S7	3.1043 (10)		
S1—Sb1—S2	89.57 (2)	S3—Sb1—S1	91.54 (2)
S1—Sb1—S4	75.51 (2)	S3—Sb1—S2	91.20 (2)
S1—Sb1—S5	165.53 (2)	S3—Sb1—S4	83.28 (2)
S2—Sb1—S4	163.88 (2)	S3—Sb1—S5	74.09 (2)
S2—Sb1—S5	89.08 (2)	S4—Sb1—S5	103.83 (2)

*Table S5. Hydrogen-bond geometry (Å, º) for [Sb(TMe)$_2$](TMe)·Me$_2$CO·3.6H$_2$O (**2**)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*B*···S9^{viii}	0.85	2.71	3.429 (3)	144
O1—H1*C*···O1^{ix}	0.82	2.49	2.917 (7)	113
O2—H2*B*···S8^{viii}	0.85	2.83	3.332 (5)	119
O2—H2*C*···O1	0.85	2.26	2.859 (7)	128
O3—H3*B*···O41′	0.86 (2)	2.15 (7)	2.938 (18)	152 (12)
O3—H3*C*···O2	0.84 (2)	1.97 (3)	2.800 (8)	168 (10)
O4—H4*D*···O3	0.85 (2)	2.06 (8)	2.812 (11)	148 (13)
O4—H4*E*···S5	0.843	0.843	3.554	130.41
C3—H3···S9^{i}	0.95	2.78	3.636 (3)	151
C4—H4*A*···S7	0.98	2.89	3.746 (3)	147
C7—H7···S5^{ii}	0.95	2.63	3.423 (3)	141
C8—H8*B*···S4^{iii}	0.98	2.79	3.713 (3)	157
C8—H8*C*···S5	0.98	2.98	3.842 (3)	147
C10—H10···S8^{iv}	0.95	2.83	3.762 (3)	166
C11—H11···O4	0.95	2.37	3.257 (9)	156
C12—H12*A*···S4	0.98	2.96	3.820 (4)	147
C27—H27···O1^{v}	0.95	2.59	3.513 (4)	163
C28—H28*B*···S9^{vi}	0.98	2.77	3.691 (3)	156
C30—H30···O41^{vii}	0.95	2.33	3.229 (9)	158
C14—H14···O3^{v}	0.95	2.62	3.513 (7)	157
C16—H16*B*···S2^{vi}	0.98	2.94	3.791 (3)	146
C16—H16*C*···S9^{vi}	0.98	2.81	3.749 (4)	162
C18—H18···O3^{v}	0.95	2.49	3.335 (6)	148
C19—H19···S8	0.95	2.92	3.743 (4)	146
C20—H20*C*···S8	0.98	2.96	3.890 (4)	159

Symmetry codes: (i) -*x*+2, -*y*+1, -*z*+2; (ii) -*x*+2, -*y*+1, -*z*+1; (iii) *x*+1, *y*, *z*; (iv) *x*, *y*-1, *z*; (v) *x*, *y*+1, *z*; (vi) *x*-1, *y*, *z*; (vii) -*x*+1, -*y*+1, -*z*+2; (viii) *x*-1, *y*-1, *z*; (ix) -*x*, -*y*, -*z*+2 (x) -x+1, -y+1, -z+1.

iii) **[Sb(TMe)$_2$]**($F_3C_2O_2$)·½Me_2CO [+1.6CF_3COOH] **(3a)**

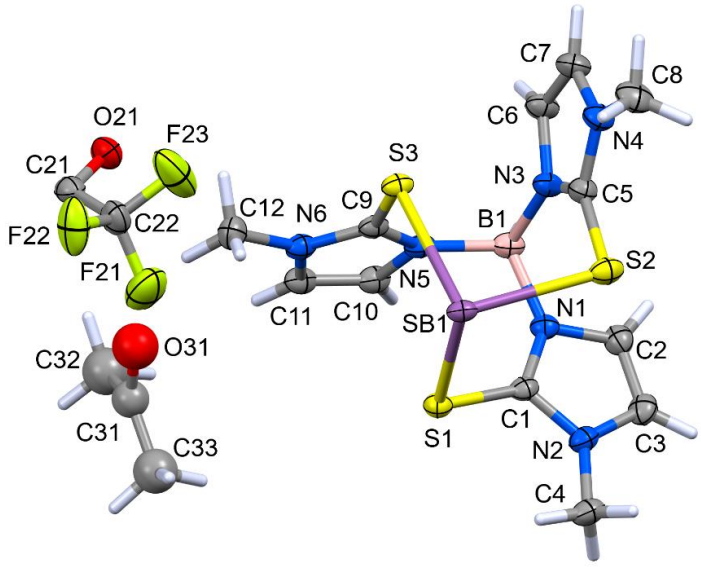

Figure S8. The asymmetric unit of 3a showing 50% ADPs for non-hydrogen atoms except for the 25% occupancy acetone molecule. The trifluoroacetate anion is disordered around a 2-fold axis.

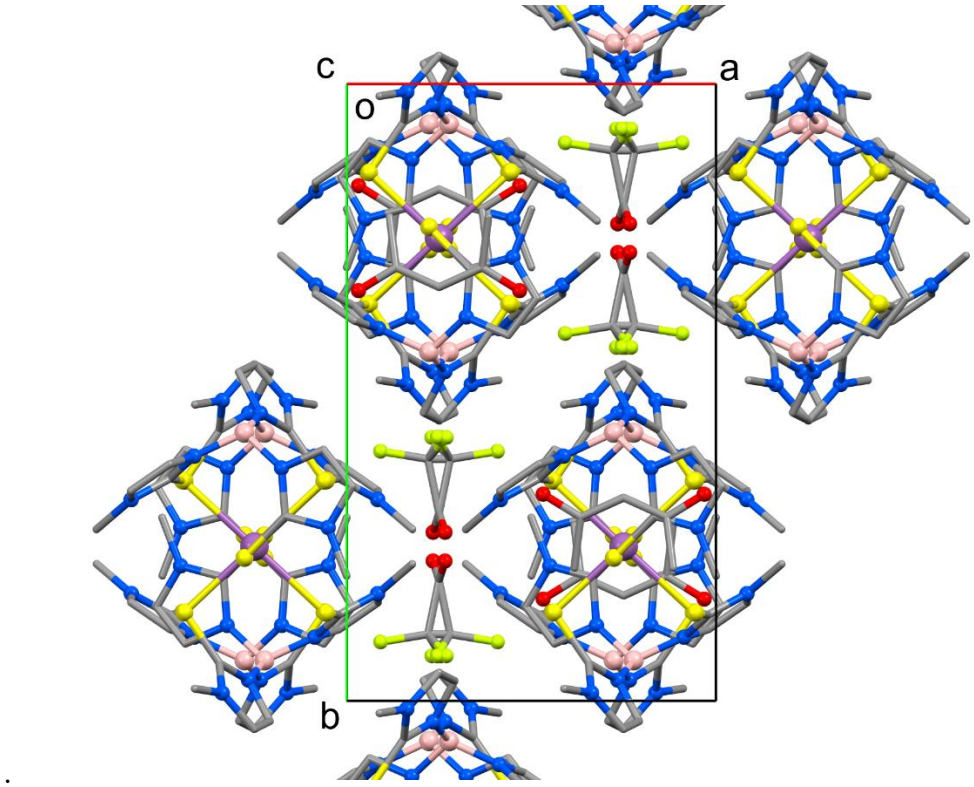

Figure S9. Packing diagram for 3a viewed down the c axis.

Table S6. Selected geometric parameters (Å, º) for ***3a***

Sb1—S1	2.7311 (5)	Sb1—S1^{i}	2.7310 (5)
Sb1—S2	2.7365 (6)	Sb1—S2^{i}	2.7365 (6)
Sb1—S3	2.7108 (5)	Sb1—S3^{i}	2.7108 (5)
S1^{i}—Sb1—S1	180.0	S3—Sb1—S1	94.238 (17)
S1^{i}—Sb1—S2^{i}	92.013 (17)	S3^{i}—Sb1—S1^{i}	94.239 (17)
S1^{i}—Sb1—S2	87.987 (17)	S3^{i}—Sb1—S2^{i}	91.973 (17)
S1—Sb1—S2	92.014 (17)	S3^{i}—Sb1—S2	88.027 (17)
S1—Sb1—S2^{i}	87.986 (17)	S3—Sb1—S2	91.972 (17)
S2—Sb1—S2^{i}	180.0	S3—Sb1—S2^{i}	88.027 (17)
S3—Sb1—S1^{i}	85.763 (18)	S3^{i}—Sb1—S3	180.0
S3^{i}—Sb1—S1	85.761 (18)		

Symmetry codes: (i) -*x*+1/2, -*y*+1/2, -*z*+1/2

iv) **[Sb(TMe)$_2$](PF$_6$)·Me$_2$CO (3b)**

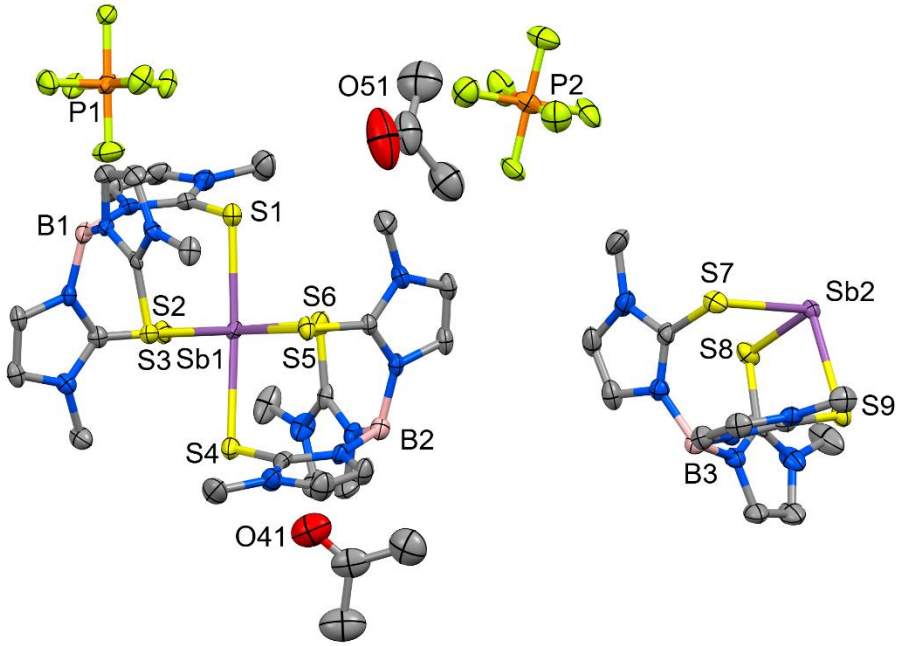

*Figure S20. Asymmetric unit of (**3b**) showing 50% probability ellipsoids (hydrogen atoms omitted).*

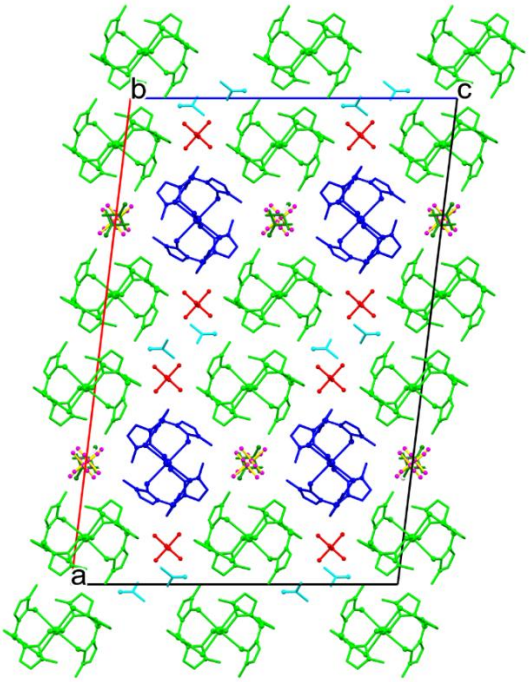

*Figure S11. Unit cell packing of **3** viewed down the b axis. Atoms are coloured by symmetry equivalence, the strictly centrosymmetric cation is shown in blue. Hydrogen atoms omitted for clarity.*

Table S7. Selected geometric parameters (Å, º) for ***3b***

Sb1—S1	2.698 (2)	Sb2—S7	2.7307 (16)
Sb1—S2	2.714 (2)	Sb2—S8	2.7337 (19)
Sb1—S3	2.6825 (16)	Sb2—S9	2.730 (2)
Sb1—S4	2.757 (2)	Sb2—S7^{i}	2.7308 (16)
Sb1—S5	2.7338 (19)	Sb2—S8^{i}	2.7337 (19)
Sb1—S6	2.7692 (18)	Sb2—S9^{i}	2.730 (2)
S1—Sb1—S2	91.71 (6)	S7—Sb2—S7^{i}	180.00 (4)
S1—Sb1—S4	173.95 (6)	S7—Sb2—S8	90.41 (5)
S1—Sb1—S5	88.26 (6)	S7—Sb2—S8^{i}	89.59 (5)
S1—Sb1—S6	88.76 (6)	S7^{i}—Sb2—S8	89.59 (5)
S2—Sb1—S4	90.94 (6)	S7^{i}—Sb2—S8^{i}	90.41 (5)
S2—Sb1—S5	179.64 (5)	S8^{i}—Sb2—S8	180.0
S2—Sb1—S6	84.27 (5)	S9—Sb2—S7	94.43 (5)
S3—Sb1—S1	89.81 (5)	S9—Sb2—S7^{i}	85.57 (5)
S3—Sb1—S2	94.06 (5)	S9^{i}—Sb2—S7^{i}	94.43 (5)
S3—Sb1—S4	84.58 (5)	S9^{i}—Sb2—S7	85.57 (5)
S3—Sb1—S5	86.30 (5)	S9^{i}—Sb2—S8	86.84 (6)
S3—Sb1—S6	177.77 (6)	S9^{i}—Sb2—S8^{i}	93.16 (6)
S4—Sb1—S6	96.91 (6)	S9—Sb2—S8	93.16 (6)
S5—Sb1—S4	89.12 (6)	S9—Sb2—S8^{i}	86.84 (6)
S5—Sb1—S6	95.37 (5)	S9—Sb2—S9^{i}	180.0

v) **[$Sb_2(TMe)_3(C_4H_6N_2S)$]$(PF_6)_3$·1.7Me_2CO (4)**

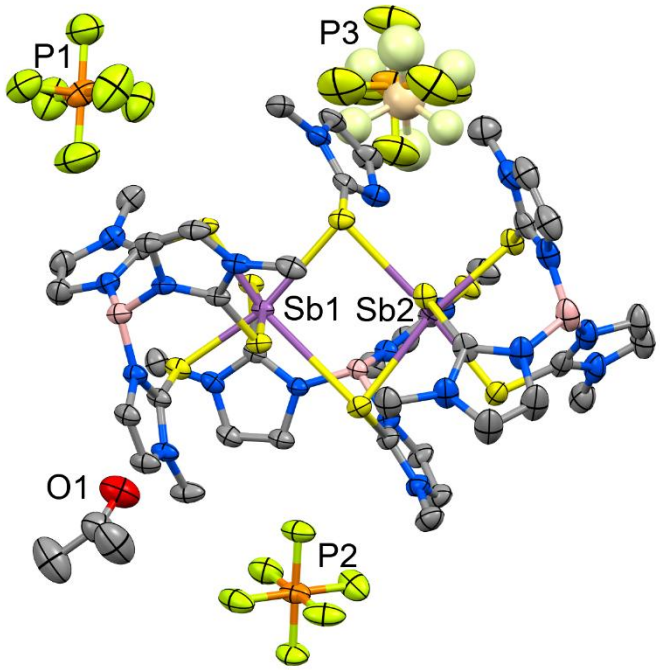

Figure S12. Asymmetric unit of [$Sb_2(TMe)_3(C_4H_6N_2S)$]$(PF_6)_3$·1.7Me_2CO ***(4)*** *showing 50% probability ellipsoids (except for the minor component of disorder); hydrogen atoms omitted.*

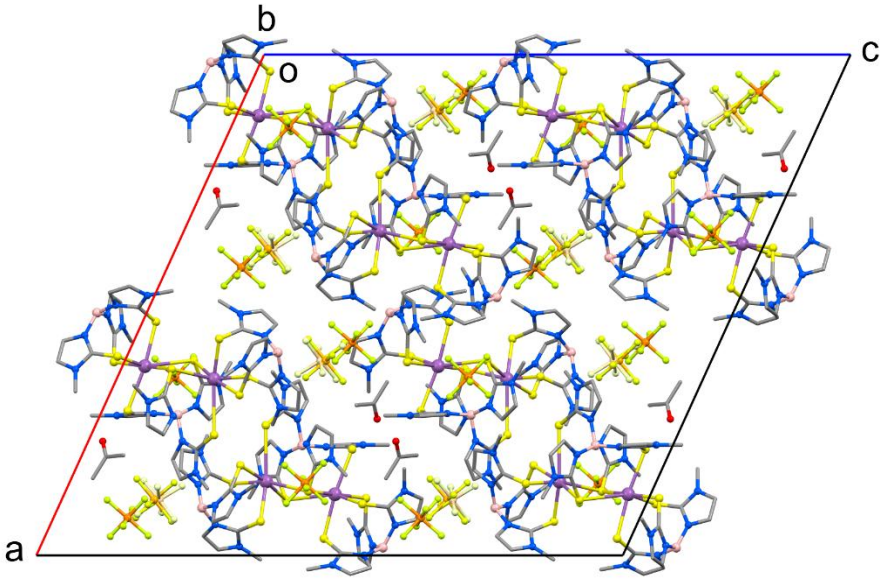

Figure S13. Unit cell packing of ***4*** *viewed down the b axis. Hydrogen atoms omitted for clarity.*

*Table S8. Selected geometric parameters (Å, º) for **4***

Sb1—S1	2.672 (2)	Sb2—S4	2.519 (2)
Sb1—S2	2.507 (2)	Sb2—S5	2.630 (2)
Sb1—S3	2.570 (2)	Sb2—S6	2.515 (2)
Sb1—S7	2.794 (2)	Sb2—S8	2.889 (2)
Sb1—S8	3.385 (2)	Sb2—S9	3.265 (2)
Sb1—S10	3.004 (2)	Sb2—S10	3.191 (2)
S1—Sb1—S7	170.76 (7)	S4—Sb2—S5	89.47 (7)
S1—Sb1—S8	69.37 (6)	S4—Sb2—S8	90.30 (7)
S1—Sb1—S10	90.89 (6)	S4—Sb2—S9	155.93 (7)
S2—Sb1—S1	90.47 (7)	S4—Sb2—S10	73.21 (7)
S2—Sb1—S3	93.15 (7)	S5—Sb2—S8	169.09 (7)
S2—Sb1—S7	89.28 (7)	S5—Sb2—S9	67.65 (6)
S2—Sb1—S8	154.76 (7)	S5—Sb2—S10	92.64 (7)
S2—Sb1—S10	73.20 (7)	S6—Sb2—S4	94.73 (8)
S3—Sb1—S1	90.55 (7)	S6—Sb2—S5	92.69 (8)
S3—Sb1—S7	80.25 (6)	S6—Sb2—S8	76.46 (7)
S3—Sb1—S8	101.77 (7)	S6—Sb2—S9	93.78 (7)
S3—Sb1—S10	166.28 (7)	S6—Sb2—S10	166.76 (7)
S7—Sb1—S8	113.08 (6)	S8—Sb2—S9	113.60 (6)
S7—Sb1—S10	97.87 (6)	S8—Sb2—S10	97.73 (6)
S10—Sb1—S8	91.49 (6)	S10—Sb2—S9	99.45 (6)

C. NMR spectra

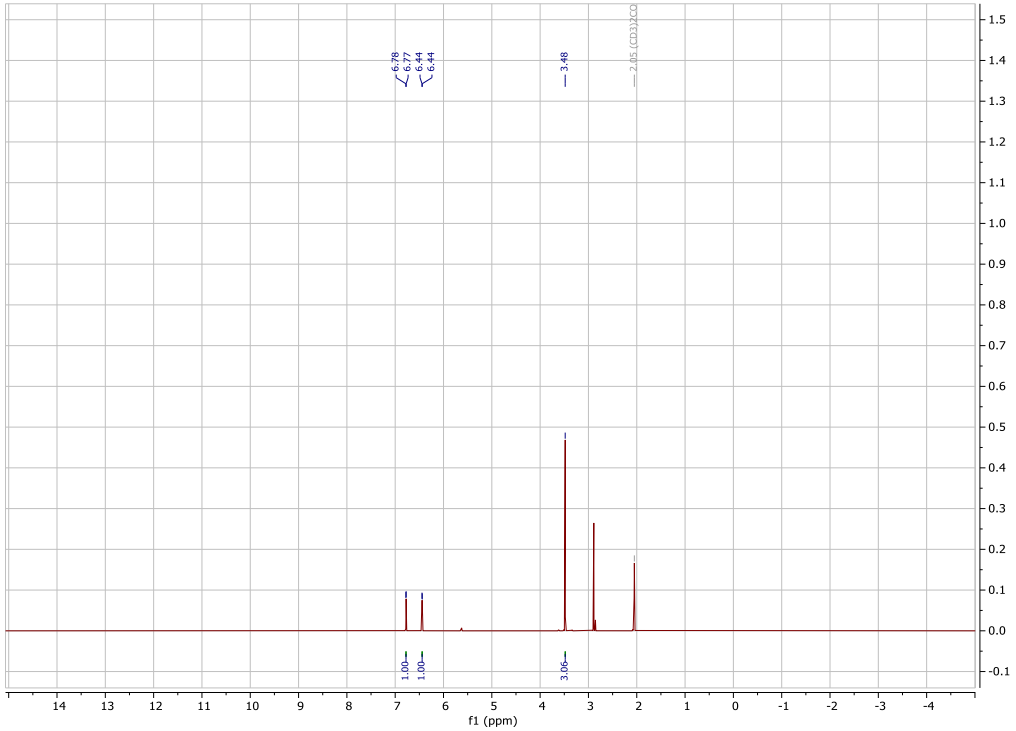

Figure S14. ^{1}H-NMR spectrum of NaTMe in d_6-acetone.

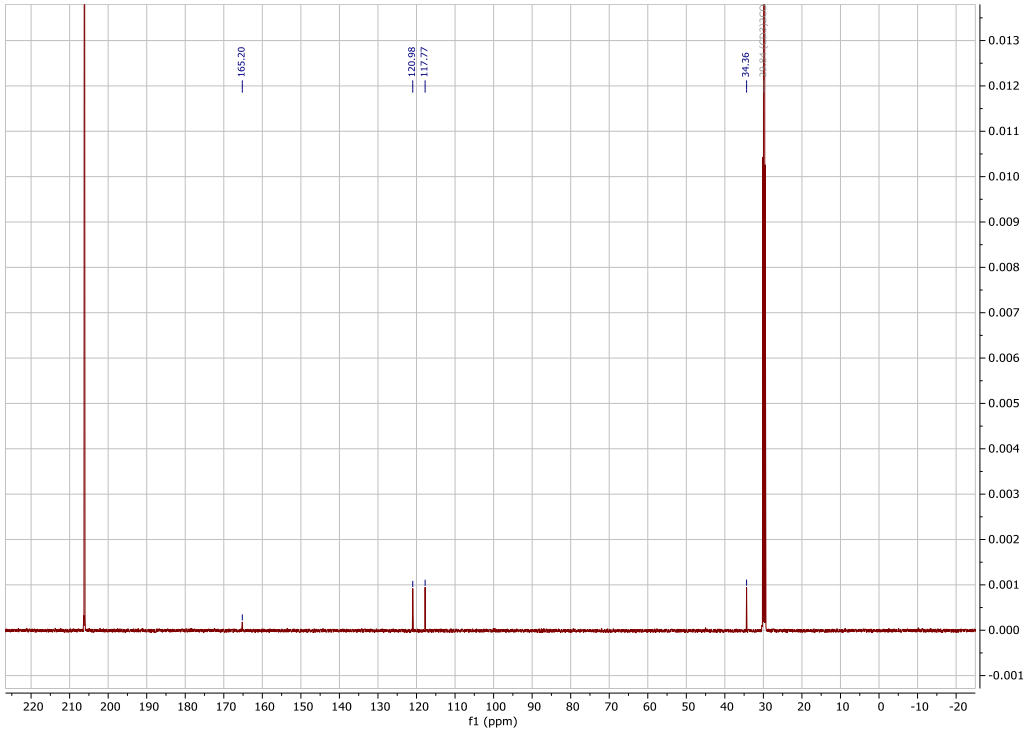

Figure S15. ^{13}C-NMR spectrum of NaTMe in d_6-acetone.

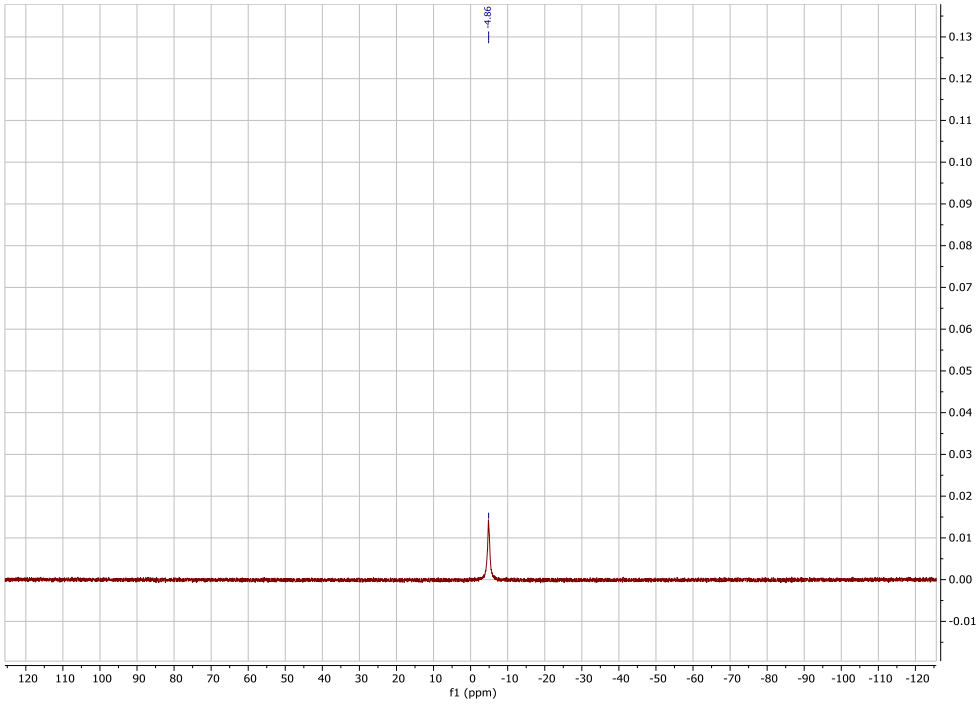

Figure S16. ^{11}B-NMR spectrum of NaTMe in d_6-acetone.

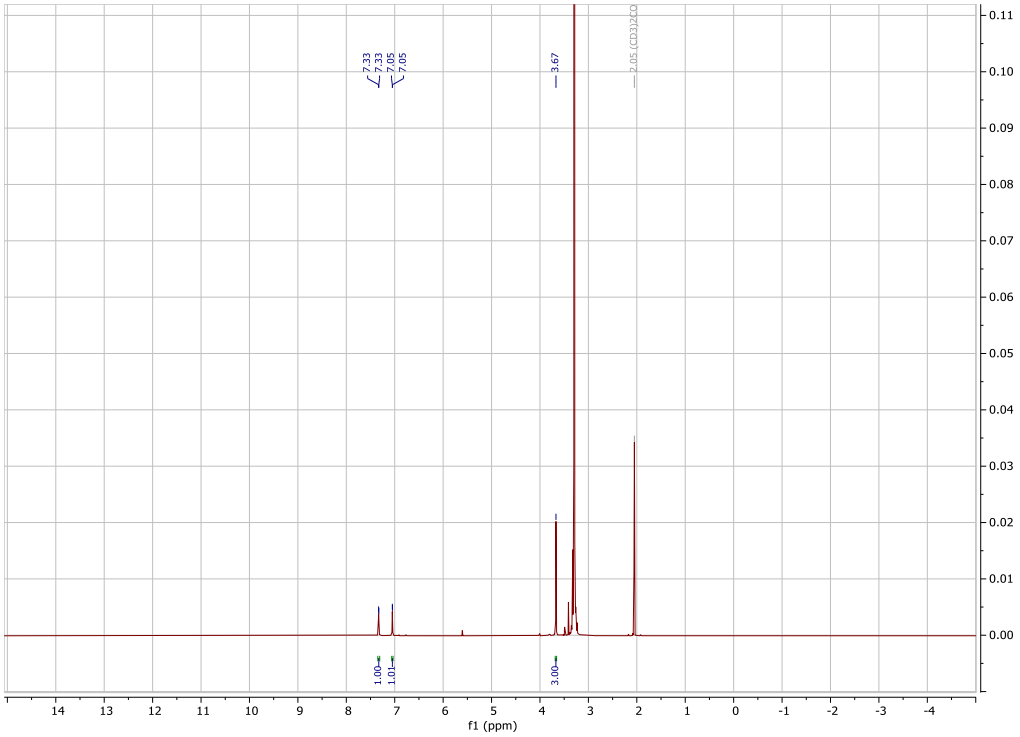

Figure S17. [1]H-NMR spectrum of [Sb(TMe)$_2$](CF$_3$COO) in d$_6$-acetone.

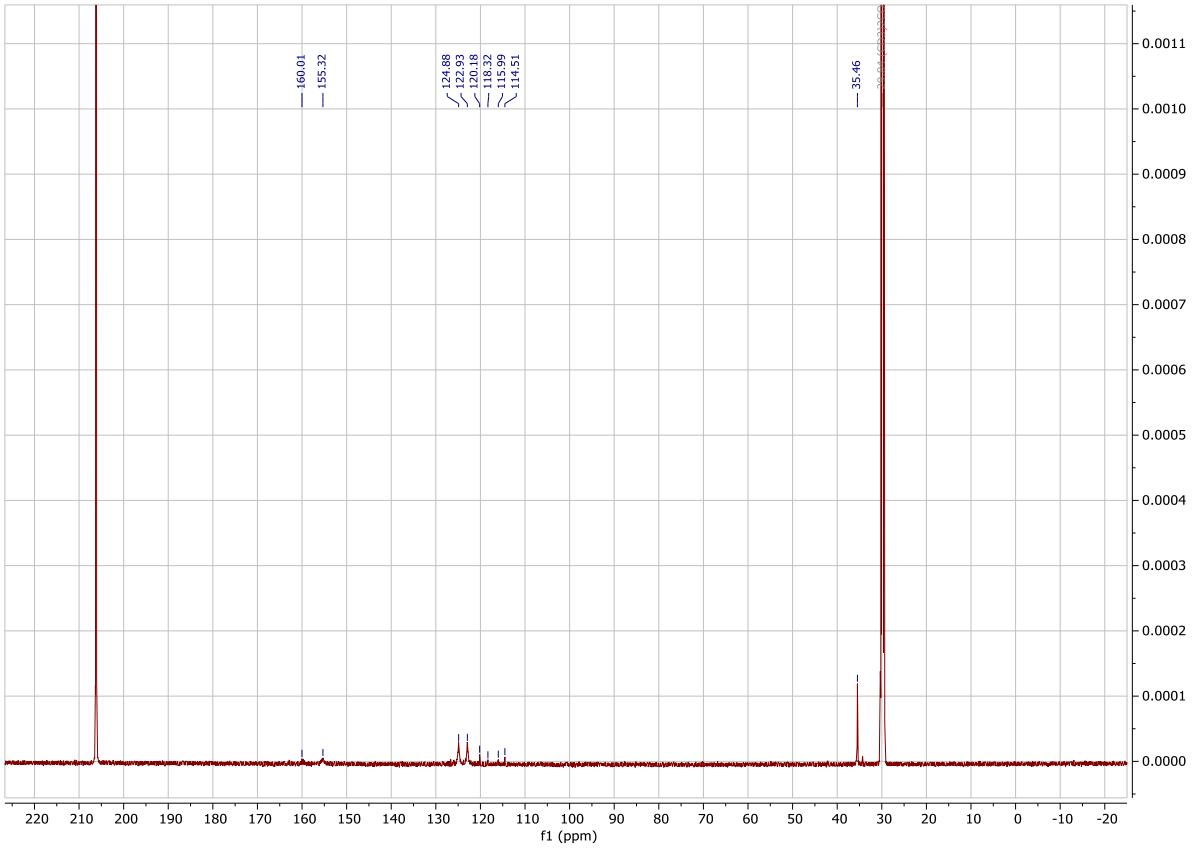

Figure S18. [13]C-NMR spectrum of [Sb(TMe)$_2$](CF$_3$COO) in d$_6$-acetone.

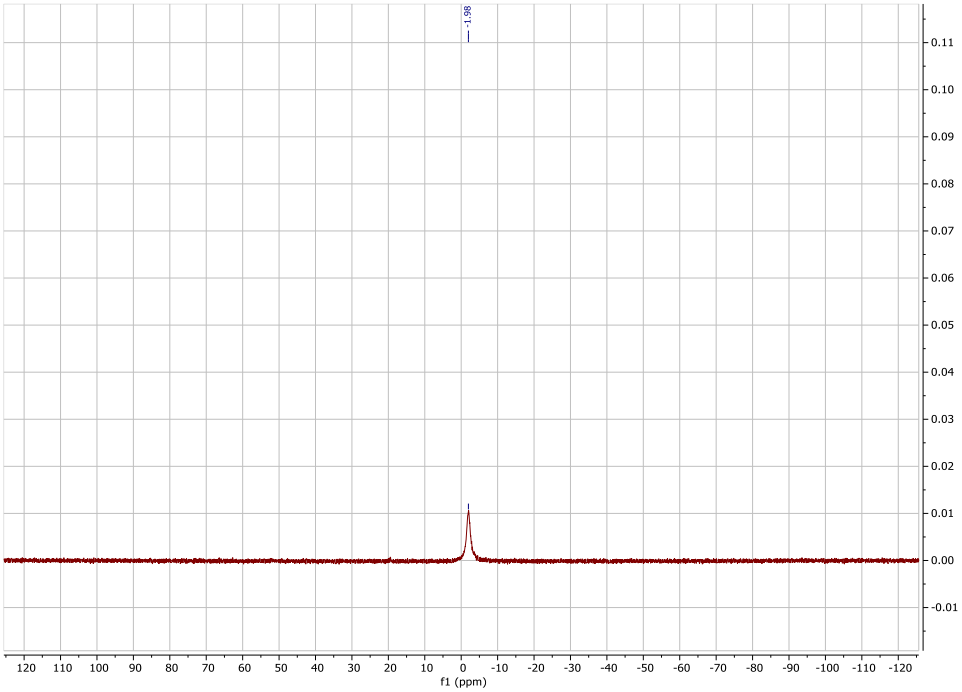

Figure S19. ^{11}B-NMR spectrum of [Sb(TMe)$_2$](CF$_3$COO) in d$_6$-acetone.

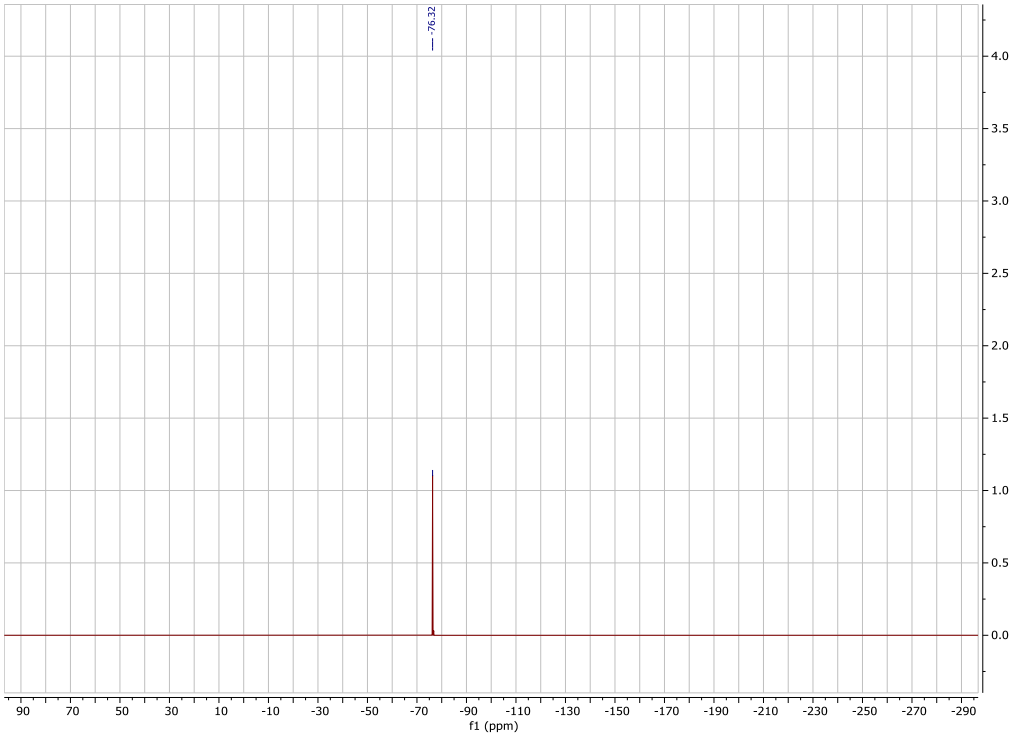

Figure S20. ^{19}F-NMR spectrum of [Sb(TMe)$_2$](CF$_3$COO) in d$_6$-acetone.

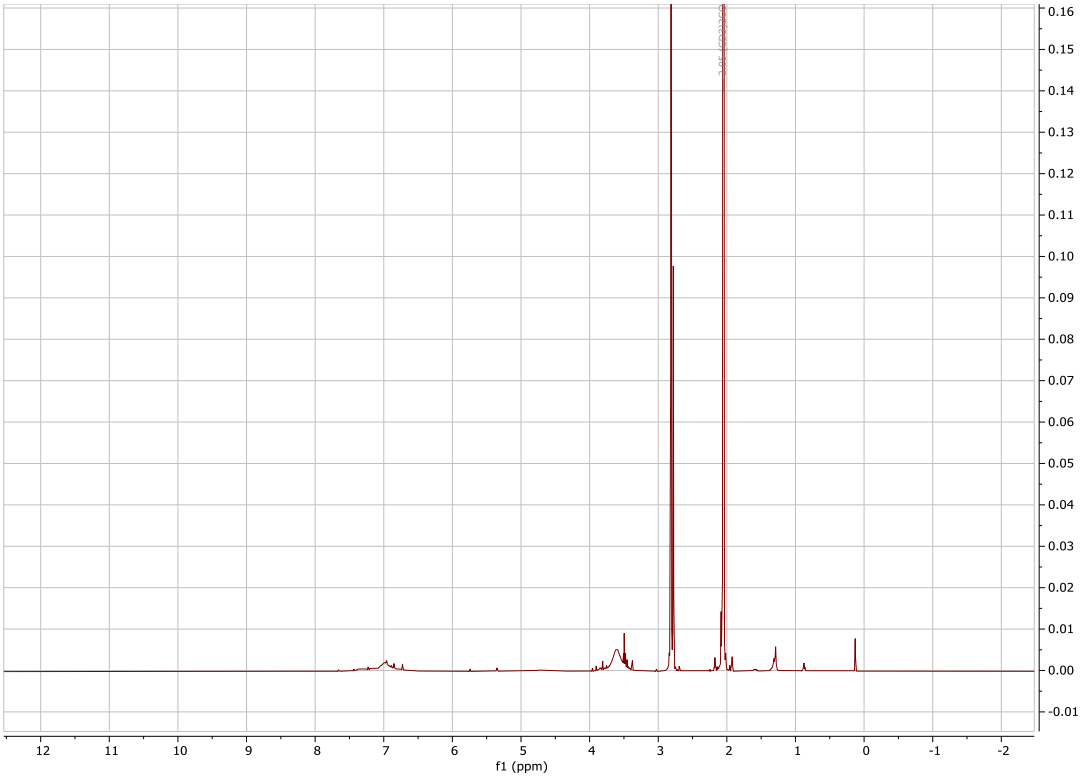

Figure S21. ^{1}H-NMR spectrum of [Sb(TMe)$_2$](TMe) in d$_6$-acetone at 25 °C.

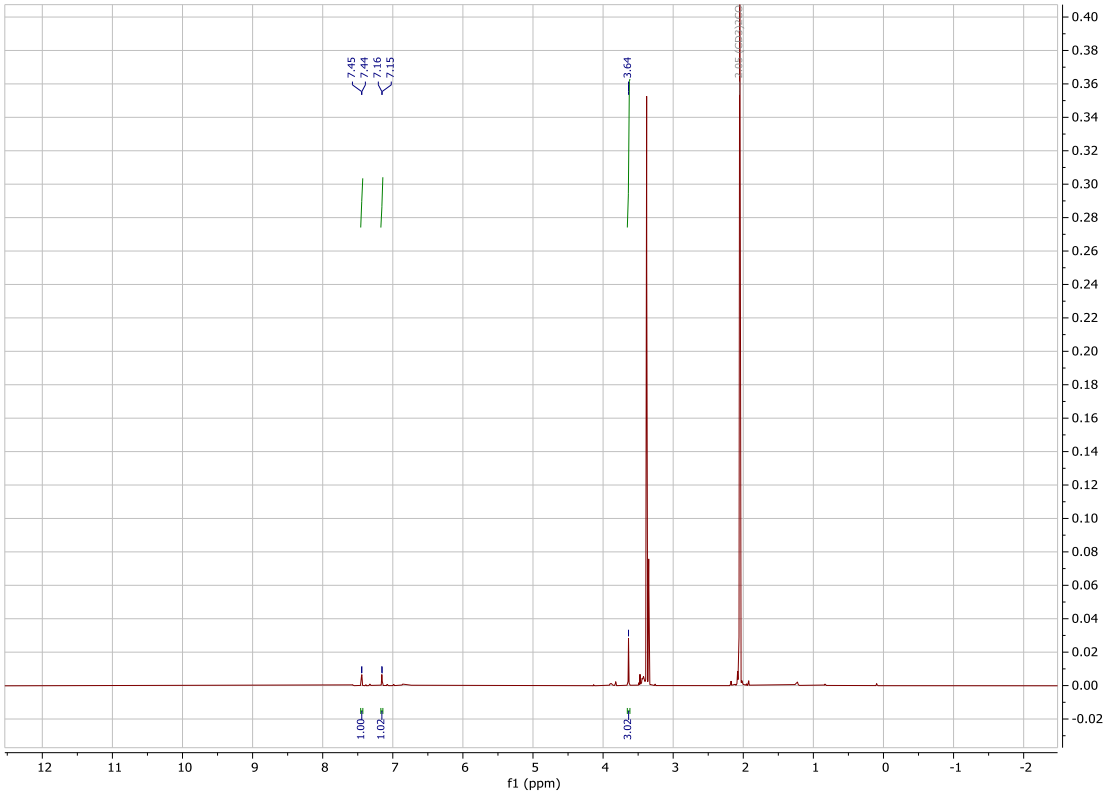

Figure S22. ^{1}H-NMR spectrum of [Sb(TMe)$_2$](TMe) in d$_6$-acetone at -50 °C.

ESI mass spectra

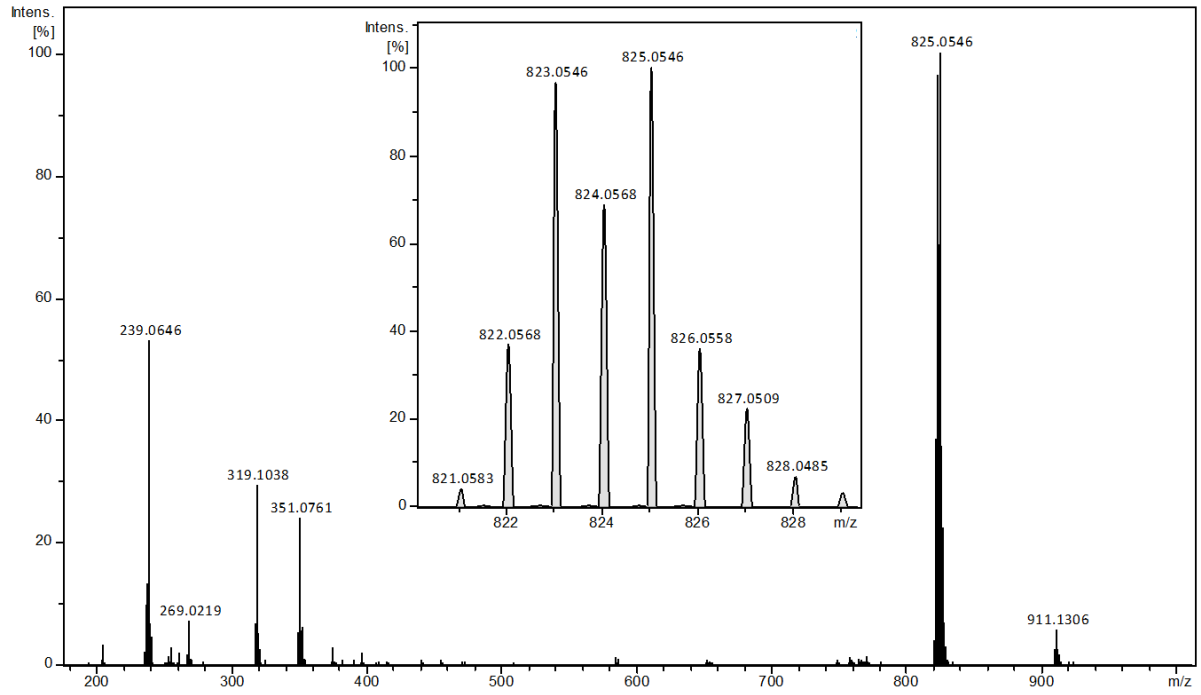

Figure S23. ESI mass spectra of $[Sb(TMe)_2](TMe)$ in acetonitrile recorded in positive mode showing the peaks corresponding to the ligand $[TMe]^+$ (m/z 351.07) and the complex $[Sb(TMe)_2]^+$ (m/z 825.05) (expanded in inset).

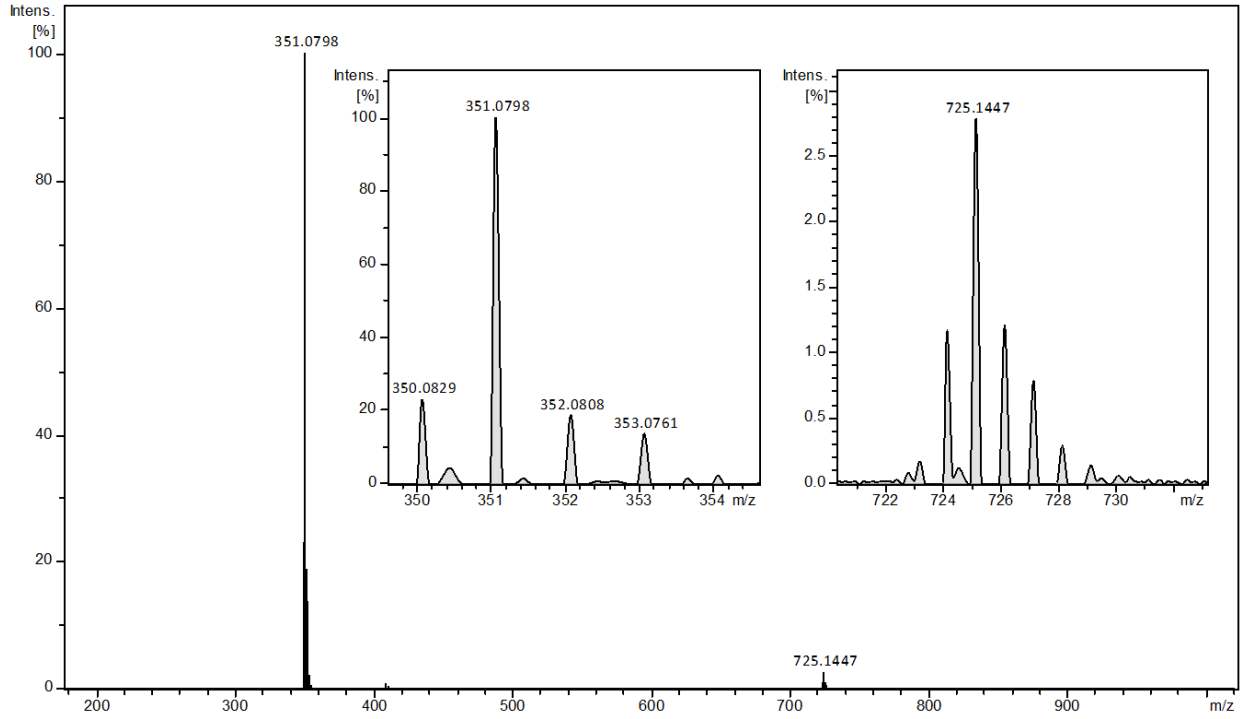

Figure S24. ESI mass spectra of $[Sb(TMe)_2](TMe)$ in acetonitrile recorded in negative mode showing the peaks corresponding to $[TMe]^-$ (m/z 351.07) (expanded in inset) and $[2(TMe)+Na]^-$ (m/z 725.14) (expanded in inset)

D. DFT

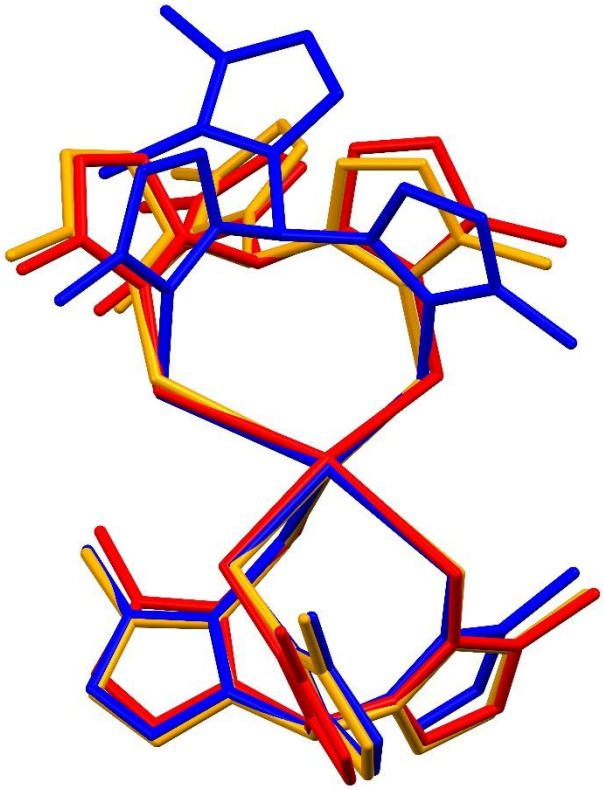

Figure S25. Overlayed structures of [Sb(κ^3–TMe)(κ^2–TMe)]$^+$. Crystal structure (blue), DFT gas phase optimised structure (red) and DFT solution phase optimised structure (orange).

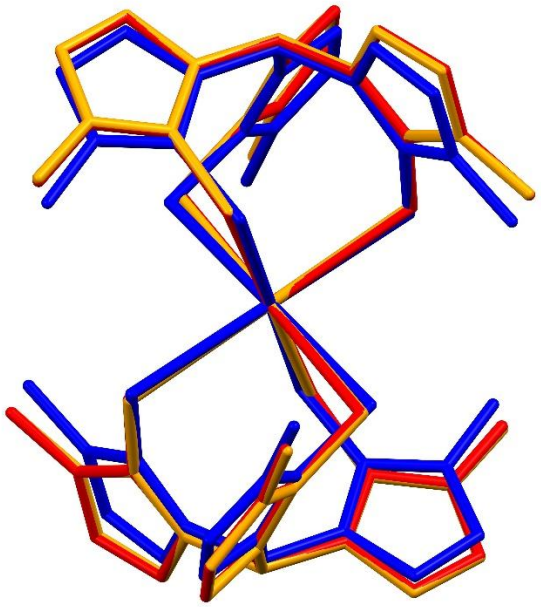

Figure S26. Overlayed structures of [Sb(κ^3–TMe)$_2$]$^+$. Crystal structure (blue), DFT gas phase optimised structure (red) and DFT solution phase optimised structure (orange).

Table S9. Cartesian coordinates of the optimized structures of [Sb(κ^3–TMe)(κ^2–TMe)]$^+$

Gas phase			Solution phase (water)		
Gibbs free energy = -4269.02408396 Eh			Gibbs free energy = -4268.95181031 Eh		
Sb	11.78747874688100	10.51955379253116	13.63788899352125	Sb	11.87696880252036	10.44076715109836	13.48860333289680
S	10.85092044085619	8.38606919912946	15.05856837512066	S	10.97486790676986	8.39217615401922	15.06318381204337
S	14.29180426163680	9.34561834161537	13.80970529061918	S	14.31677965463584	9.37776333677384	13.63163087756977
S	11.44895466328085	9.40025798660145	11.40036599949200	S	11.33966195637927	9.14880208973831	11.37908236272742
N	12.78464969210794	6.50435313571971	14.33476446795562	N	12.95800562825202	6.53946461583247	14.41349768952323
N	12.65522340816899	6.94852229776698	16.47102162283584	N	12.91422872139281	7.16205704250254	16.50827595563146
N	13.78690666109309	7.23473372408439	12.06329082838272	N	13.81207136681754	7.14637604035734	12.04383670055205
N	15.33464632782961	8.63501699855756	11.40984125917816	N	15.23581005924952	8.57598397063202	11.20041306493182
N	11.23410671981837	6.75568511062712	12.26985754122501	N	11.31344703004784	6.55385415530566	12.41626637385949
N	9.38890101819625	7.62764359276877	11.47655170767545	N	9.38238716178279	7.29441135680995	11.70593912455103
C	12.14543083059738	7.26697187418858	15.25338612375419	C	12.32653866663565	7.34387275030579	15.30079927948469
C	13.70192918762884	5.70990043026850	14.99763385898590	C	13.95552992283636	5.85787537228271	15.08689891730750
H	14.33007426432124	5.01572019768665	14.46964554000436	H	14.59618165394434	5.15542716110928	14.58405637117746
C	13.62384707658245	5.97955684957779	16.31952161829180	C	13.92910012336933	6.23781275733597	16.38387016147302
H	14.15692729426607	5.56681913493653	17.15693432850204	H	14.52558271833663	5.93252673620638	17.22521849285048
C	12.22536232880352	7.51163330475520	17.74460296321357	C	12.53003097934748	7.80745138086948	17.75860423246000
H	12.19767639673663	8.59679652546906	17.67797643854757	H	12.51992198863568	8.88815437642403	17.63470964544122
H	12.93680694386045	7.20820792900602	18.50869686280993	H	13.26367657664565	7.53636499777620	18.51298977514840
H	11.23158522656570	7.15045369990942	18.00782788314697	H	11.54447613724319	7.47123539192692	18.07710554265011
C	14.44644028266385	8.37139167905442	12.40231869151845	C	14.43102770381361	8.32911522516178	12.26100017438731
C	14.28152233859782	6.79695265260020	10.84781897821176	C	14.24197734422184	6.65840735458212	10.82502429393908
H	13.91132977639474	5.90311285137374	10.37965782559544	H	13.88618912551517	5.72132536807325	10.43532011780427
C	15.23915985712498	7.65941774761340	10.44083762814319	C	15.12653887624180	7.53886002462010	10.30212793983791
H	15.85901258539131	7.66166656485872	9.56239157939544	H	15.68953974380016	7.51915399428055	9.38591614289405
C	16.26751767886006	9.75508508766413	11.38567518093070	C	16.12415217922563	9.72342674253455	11.03837673115670
H	16.68466812610922	9.82892732157952	10.38433737337298	H	16.51757426015541	9.69894232051198	10.02585205613125
H	17.07119987032554	9.59809371039162	12.10489035677377	H	16.94825793479694	9.67060532398291	11.74821157766402
H	15.74277943466755	10.67456829066298	11.63471288302426	H	15.57110625521192	10.64703171319160	11.19146751826177
C	10.68562756413566	7.88275332182519	11.76344162339934	C	10.68101853696411	7.62220927506756	11.88902226447751
C	10.25415563499483	5.78769462838417	12.29746210026397	C	10.38472175327608	5.54784308508270	12.57012951654140
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C	9.11092570200624	6.32383495289029	11.80472110390465	C	9.18693687518456	6.00156850981734	12.12629052738483
H	8.13737873152529	5.89320786192009	11.65369385216893	H	8.22613566229158	5.52211202341820	12.06394246268779
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H	8.65496373142422	9.57334084369277	11.14787603203437	H	8.33559171365779	9.10792496280839	11.62459827652824
H	7.43738205450081	8.28660485202383	11.18945666716939	H	7.39201293017479	7.64805573630421	11.25951857052150
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S	8.98136736653836	10.81147309934298	14.03880419546558	S	8.87488736988837	10.97043296524991	14.08912046844712
S	12.95040552481306	12.36415712935308	11.82808692551229	S	12.75121892370273	12.26039875946123	11.52663842768679
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N	10.89633062627861	14.14773042849078	12.38973002066791	N	10.76492552708889	13.97093896665613	12.43235125466109
N	12.89646182740950	14.83270329119769	12.96548372300685	N	12.78367471302599	14.49333545960572	13.09626202741090
C	8.25809967092919	12.34632192705977	13.74667953073041	C	8.05539068872259	12.41224156585234	13.64368895843619
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H	7.21068082173488	11.61285962148255	16.18680595763382	H	6.91944871950375	12.00771290145540	16.18682936048762
H	5.93759934609306	11.14375871487371	15.04870015123072	H	5.86094154966223	11.18279693739096	15.02785401242326
H	5.77875096617498	12.64933389108701	15.98180577845013	H	5.40249267786159	12.77270707468541	15.67080755633045
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C	10.77885078515915	15.40101109101387	12.96232844520673	C	10.67854239064568	15.09611817672817	13.23159994478830
H	9.82841436194930	15.88611655371247	13.08599882806085	H	9.74094454486633	15.57798524736982	13.44427364471779
C	12.01199442021679	15.83326053754918	13.31106054026154	C	11.92597225726012	15.42501266240085	13.64048136491344
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C	14.33885465192018	14.88384221720950	13.15521667867331	C	14.22761496351298	14.47279487073921	13.29702643289322
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H	14.68792415045117	13.94181430743674	13.57191321958517	H	14.53199807839624	13.54212302305315	13.77163456524386
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C	8.29834796638653	13.32601403796021	9.65870876228056	C	8.43082353176007	13.59324982241000	9.39624182409517
N	9.24586240277530	13.90539875820776	10.46878451679895	N	9.24042124758702	14.04655951122908	10.40075546773975
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H	9.26808314828021	15.86515558061449	7.84007078356039	H	9.33720422517027	16.50474866593361	8.23102981608435
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C	7.35780501318376	13.83216695988730	7.40926894111030	C	7.67955697567200	14.50089007485665	7.18863319474173
H	7.54293956124415	12.83329408061659	7.01485590778818	H	8.04166014270375	13.67619291684067	6.57475209921516
H	7.54324848724630	14.57569837859769	6.63665410223183	H	7.82587449273885	15.43749567262389	6.65573469200059
H	6.31624180115021	13.88117169684475	7.72761639459767	H	6.61660007708234	14.35369197525959	7.37726275519778
B	9.70938287383776	13.28889926772075	11.80469688003556	B	9.55939158879828	13.27127273943586	11.70861758044218
H	10.07501694457463	12.16908241791277	11.66156858254378	H	9.84463648077727	12.14197818022765	11.47120735209505

Table S10. Cartesian coordinates of the optimized structures of $[Sb(\kappa^3–TMe)_2]^+$

Gas phase			Solution phase (water)		
Gibbs free energy = -4268.97092410 Eh			Gibbs free energy = -4269.02762266 Eh		
Sb	2.44223250227251	4.32344012048253	7.07549898305106	Sb	2.44065442821084	4.32295695847702	7.07524325320397
B	2.20490388074176	7.60481760364469	4.32038326912074	B	2.21193874861312	7.61369913267816	4.31962928305627
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C	0.08735379267391	6.88271775579069	3.12261054910339	C	0.10616267664880	6.87660285951083	3.11628996484737
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C	1.40894728235858	3.32729468145155	10.40173709610449	C	1.40849445686289	3.31842506291387	10.41751844336565
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