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Supporting Information of the manuscript entitled:

Synthesis of Polyantimony Ligand Complexes starting from $Cp^*_4Sb_4$

Veronika Heinl, Gábor Balázs, Michael Seidl and Manfred Scheer*

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1. Experimental details

All experiments were performed under an atmosphere of dry nitrogen or argon using Schlenk and glovebox techniques. Solvents were purified, dried and degassed prior use. ^{1}H, ^{13}C{1H} NMR spectra were recorded at room temperature on a Bruker Avance 400 spectrometer (^{1}H: 400,130 MHz, ^{13}C: 100.613 MHz). ^{1}H, ^{13}C NMR chemical shifts are reported in parts per million (ppm) relative to the external standard Me_4Si. Elemental analysis was determined with a Vario micro cube apparatus. For mass spectrometry, a Finnigan MAT 95 (LIFDI MS, FD MS) or a Finnigan MAT SSQ 710 A (ESI MS) device and a Joel AccuTOF GCX spectrometer were used. [Ag][TEF],[1] [Ag][FAL],[2] KCp*,[3] [(Cp'''Co)$_2$tol],[4] [Cp''Fe(CO)$_2$]$_2$[5] and [Cp'''Fe(CO)$_2$]$_2$[6] were prepared according to literature procedures.

Preparation of [Cp*$_4$Sb$_4$] (1):[7]

$SbCl_3$ (1.1 g, 4.9 mmol) in Et_2O is added dropwise to a suspension of KCp* (3.0 g, 17.2 mmol) in 150 mL Et_2O at -78 °C. The colour changes to dark orange. After addition, the reaction solution is stirred for 30 min at -78 °C and thereupon warmed to r.t. A dark orange solution is obtained by filtration and a beige solid remains on the frit. Crystals of **1** are obtained by storing a concentrated Et_2O solution at -30 °C. Crystalline Yield: 984 mg (0.961 mmol, 78%)

X: Analytical data are in agreement with the literature.[7]

Preparation of [Cp*$_2$Sb][TEF] (2a):

A solution of [Cp*$_4$Sb$_4$] (30 mg, 0.029 mmol) in 5 mL DCM is added to a solution of [Ag][TEF] (35 mg, 0.030 mmol) in 5 mL DCM. The colour changes to green and a black solid is formed. After stirring for 1 d at r.t. the reaction mixture is filtered via cannula. The obtained orange solution is concentrated *in vacuo* and stored at -30 °C for crystallization. Crystalline Yield: 26 mg (0.019 mmol, 63%)

2a: **^{1}H NMR** (CD_2Cl_2, 298 K): δ [ppm] = 2.20 (s, 30 H, C*CH*$_3$); **^{13}C{^{1}H} NMR** (CD_2Cl_2, 298 K): δ [ppm] = 10.1 (s, C*C*H$_3$), 127.6 (s, *C*CH$_3$); **FD$^+$ MS** (toluene): *m*/*z* (%): 391.10 ([Cp*$_2$Sb]$^+$); **Elemental analysis** (%): calculated for [$C_{36}H_{30}SbAlO_4F_{36}$] (1358.04 g·mol^{-1}): C, 31.81; H, 2.22; found: C, 32.03; H, 2.27.

Preparation of [Cp*$_2$Sb][FAL] (2b):

A solution of [Cp*$_4$Sb$_4$] (30 mg, 0.029 mmol) in 5 mL DCM is added to a solution of [Ag][FAL] (32 mg, 0.030 mmol) in 5 mL DCM. The colour changes to green and a black solid is formed. After stirring for 1 d at r.t. the reaction mixture is filtered via cannula. An orange solution is

obtained, a black solid remains. Crystals of **2b** suitable for single crystal X-ray diffraction analysis are obtained by storing a concentrated DCM solution at -30 °C Crystalline Yield: 21 mg (0.012 mmol, 40%)

2b: **^{1}H NMR** (CD_2Cl_2, 298 K): *δ* [ppm] = 2.20 (s, 30 H, C*C*H$_3$); **^{13}C{^{1}H} NMR** (CD_2Cl_2, 298 K): *δ* [ppm] = 10.1 (s, C*C*H$_3$), 127.6 (s, *C*CH$_3$); **ESI$^+$ MS** (toluene): *m*/*z* (%): 391.13 ([Cp*$_2$Sb]$^+$); **ESI$^-$ MS** (toluene): *m*/*z* (%): 1380.91 ([FAL]$^-$); **Elemental analysis** (%): calculated for [$C_{56}H_{30}SbAlO_3F_{46}$] (1772.03 g·mol^{-1}): C, 437.93; H, 1.71; found: C, 37.61; H, 1.64.

Preparation of [(Cp*Mo(CO)$_3$)$_3$(μ$_3$-Sb$_3$)] (3) and [Cp*Mo(CO)$_2$(η^3-Sb$_3$)] (4):

A solution of Na[Cp*Mo(CO)$_3$] (51 mg, 0.128 mmol) is dissolved in 15 mL toluene and added to a solution of [Cp*$_4$Sb$_4$] (150 mg, 0.146 mmol) in 15 mL toluene. The reaction solution is refluxed for 1 h. The solvent of the brown suspension is removed *in vacuo* and subsequent column chromatographic workup (SiO_2, *n*-hexane, 18 x 3 cm) yields four fractions. With *n*-hexane a yellow fraction of [Cp*$_4$Sb$_4$] is eluted, followed by an orange fraction of **4**. The third red fraction, eluted with a mixture of *n*-hexane and toluene (1:1), contains a mixture of [Cp*Mo(CO)$_3$]$_2$ and [Cp*Mo(CO)$_2$]$_2$. With toluene as solvent, a red-brown fraction of **3** is obtained. Crystals of **3** and **4** suitable for single crystal X-ray diffraction analysis are obtained by storing a concentrated solution in DCM (**3**) or *n*-hexane (**4**) at -30 °C, respectively. Crystalline Yield: **3**: 17 mg (0.013 μmol, 30%), **4**: 10 mg (0.015 mmol, 12%)

3: **^{1}H NMR** (C_6D_6, 298 K): *δ* [ppm] = 1.78 (s, 45 H, C*C*H$_3$); **^{13}C{^{1}H} NMR** (C_6D_6, 298 K): *δ* [ppm] = 9.8 (s, C*C*H$_3$), 103.2 (s, *C*CH$_3$), 239.5 (s, *C*O); **LIFDI MS** (toluene): *m*/*z* (%): 1310.78 (M$^+$, 100), 968.78 (M$^+$ - [Cp*Mo(CO)$_4$], 40); **ATR-IR** (diamant crystal): v [cm-1] = 1862 (m), 1818 (m); **Elemental analysis** (%): calculated for [$C_{39}H_{45}Mo_3Sb_3O_9$] (1313.73 g mol^{-1}): C, 35.73; H, 3.46; no satisfying elemental analysis could be obtained, even by using Sn capsules.

4: Analytical data are in agreement with the literature.[8]

Preparation of [(Cp'''Ni)$_4$(μ$_3$-Sb)$_4$]/[Cp'''$_2$Ni] (5/5'):

A solution of [Cp*$_4$Sb$_4$] (80 mg, 0.078 mmol) in 5 mL toluene is added to an excess of a freshly prepared solution of [(Cp'''Ni)$_2$tol][9] in 10 mL toluene and stirred for 5 d. The solvent of the green reaction mixture is removed *in vacuo* and subsequent column chromatographic workup (SiO_2, *n*-hexane, 18 x 3 cm) yields four fractions. With *n*-hexane, a yellow fraction of fulvalene is eluted, followed by a brown-violet fraction of **5/5'**. Seamless with *n*-hexane an orange fraction of [Cp*$_4$Sb$_4$] can be observed. The fourth brown fraction, eluted with a mixture of *n*-hexane and toluene (1:1), is still unknown. Crystals of **5/5'** suitable for single crystal X-ray diffraction

analysis are obtained by layering a DCM solution with acetonitrile. Crystalline Yield: 9 mg (4.19 µmol, 13%)

5/5': Analytical data are in agreement with the literature.[10]

Preparation of [(Cp'''Co)$_4$(µ$_3$-Sb$_4$)] (6):

A solution of [Cp*$_4$Sb$_4$] (80 mg, 0.078 mmol) in 5 mL *n*-hexane is added to a solution of [(Cp'''Co)$_2$tol] (54 mg, 0.081 mmol) in 5 mL *n*-hexane and stirred for 5 d. The solvent of the green reaction mixture t is removed *in vacuo* and subsequent column chromatographic workup (SiO_2, *n*-hexane, 18 x 3 cm) yields two fractions. With *n*-hexane, a green fraction of **6** can be obtained. The second fraction containing [Cp*$_4$Sb$_4$] can be eluted with a mixture of *n*-hexane and toluene (1:1). Crystals of **6** suitable for single crystal X-ray diffraction analysis are obtained by layering a DCM solution with acetonitrile. Crystalline Yield: 11 mg (6.66 µmol, 17%)

6: Analytical data are in agreement with the literature.[10]

Preparation of [{Cp''Fe(CO)$_2$}$_4$(µ$_4$-Sb$_4$)] (7a):

A solution of [Cp''Fe(CO)$_2$]$_2$ (169 mg, 0.292 mmol) is dissolved in 15 mL toluene and added to a solution of [Cp*$_4$Sb$_4$] (150 mg, 0.146 mmol) in 15 mL toluene. The reaction solution is refluxed for 1 h. After removing the solvent, the brown residue is extracted with DCM. The red-brown suspension is filtered via cannula. A grey powder remains. Crystals of **7a** suitable for single crystal X-ray structure analysis are obtained by layering the concentrated DCM solution with acetonitrile. Crystalline Yield: 154 mg (0.094 mmol, 64%)

7a: **^{1}H NMR** (thf-d^8, 298 K): *δ* [ppm] = 1.27 (s, 72 H, C(*CH*$_3$)$_3$), 4.44 (d, 8 H, C(*CH*$_3$)$_3$), 4.83 (t, 4 H, C(*CH*$_3$)$_3$); **^{13}C{^{1}H} NMR** (thf-d^8, 298 K): *δ* [ppm] = 31.7 (s, *C*H$_3$), 31.9 (s, *C*(CH$_3$)$_3$), 76.8 (s, *C*H), 82.3 (s, *C*C(CH$_3$)$_3$), 117.1 (s, *C*C(CH$_3$)$_3$), 219.1 (s, *C*O); **LIFDI MS** (toluene): *m*/*z* (%): 1643.89 (M$^+$); **ATR-IR** (diamant crystal): v [cm-1] = 1971 (s), 1947 (s), 1912 (m); **Elemental analysis** (%): calculated for [$C_{60}H_{84}Fe_4Sb_4O_8$] (1639.97 g·mol^{-1}): C, 43.84; H, 5.15; found: C, 43.45; H, 4.81.

Preparation of [{Cp'''Fe(CO)$_2$}$_4$(µ$_4$-Sb$_4$)] (7b):

A solution of [Cp'''Fe(CO)$_2$]$_2$ (135 mg, 0.196 mmol) is dissolved in 15 mL toluene and added to a solution of [Cp*$_4$Sb$_4$] (100 mg, 0.098 mmol) in 15 mL toluene. The reaction solution is refluxed for 1 h. After removing the solvent, the brown residue is extracted with toluene. The red-brown suspension is filtered via cannula. A grey powder remains. Crystals of **7b** suitable for single

crystal X-ray structure analysis are obtained by layering a concentrated toluene solution with acetonitrile. Crystalline Yield: 87 mg (0.047 mmol, 48%)

7b: **^{1}H NMR** (thf-d^{8}, 298 K): δ [ppm] = 1.26 (s, 36 H, C(CH_3)$_3$), 1.43 (s, 72 H, C(CH_3)$_3$), 4.78 (s, 8 H, $C_5H_2{}^t Bu_3$); **^{13}C{^{1}H} NMR** (thf-d^{8}, 298 K): δ [ppm] = 32.2 (s, C(CH$_3$)$_3$), 32.6 (s, CH$_3$), 33.5 (s, C(CH$_3$)$_3$), 34.7 (s, CH$_3$), 84.4 (s, CH), 109.9 (s, CC(CH$_3$)$_3$), 110.5 (s, CC(CH$_3$)$_3$), 219.5 (s, CO); **LIFDI MS** (toluene): *m/z* (%): 1177.93 (M^+ - 2•[$C_{17}H_{29}Fe(CO)_2$]); **ATR-IR** (diamant crystal): v [cm-1] = 1963 (s), 1962 (m), 1899 (s); **Elemental analysis** (%): calculated for [$C_{76}H_{116}Fe_4Sb_4O_8$] (1864.22 g·mol^{-1}): C, 48.86; H, 6.26; found: C, 49.34; H, 5.83.

2. Crystallographic data

Crystals suitable for single crystal X-ray diffraction analysis were obtained as described above. The diffraction intensities were collected either on a Gemini Ultra diffractometer equipped with an Atlas^{S2} CCD detector and with a fine-focus sealed Cu-K_α X-ray tube (**3**), a GV50 diffractometer equipped with a Titan^{S2} CCD detector and a micro-focus Cu-K_α X-ray tube (**7a**), on a XtaLAB Synergy R, DW system diffractometer equipped with a HyPix-Arc 150 detector and a rotating-anode Cu-K_α X-ray tube (**2a**, **2b**) or at a SuperNova diffractometer equipped with a Atlas CCD detector and a micro-focus Cu-K_α X-ray tube (**7b**). Data collection and reduction were performed with **CrysAlisPro** software package.[11] The structures were solved with **Olex2**,[12] using **ShelXT**[13] and a least-square refinement on F^2 was carried out with **ShelXL**.[14] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms at the carbon atoms were located in idealized positions and refined with isotropic displacement parameters according to the riding model.

Using **Olex2**,[12] all pictures of the respective molecular structures were made.

CCDC reference numbers 2120095 (**2a**), 2120096 (**2b**), 2120097 (**3**), 2120098 (**7a**), 2120099 (**7b**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retreving.html (or from the Cambridge Crystallographic Data Center, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: (internat.) + 44-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

[Cp*$_2$Sb][TEF] (2a):

Compound **2a** in a concentrated DCM solution at -30 °C in form of yellow blocks in the monoclinic space group P2$_1$/*c*. The asymmetric unit contains two molecules of **2a**. The [TEF]- anions show some disorders, which can be solved using the restrains SADI, SIMU and DFIX.

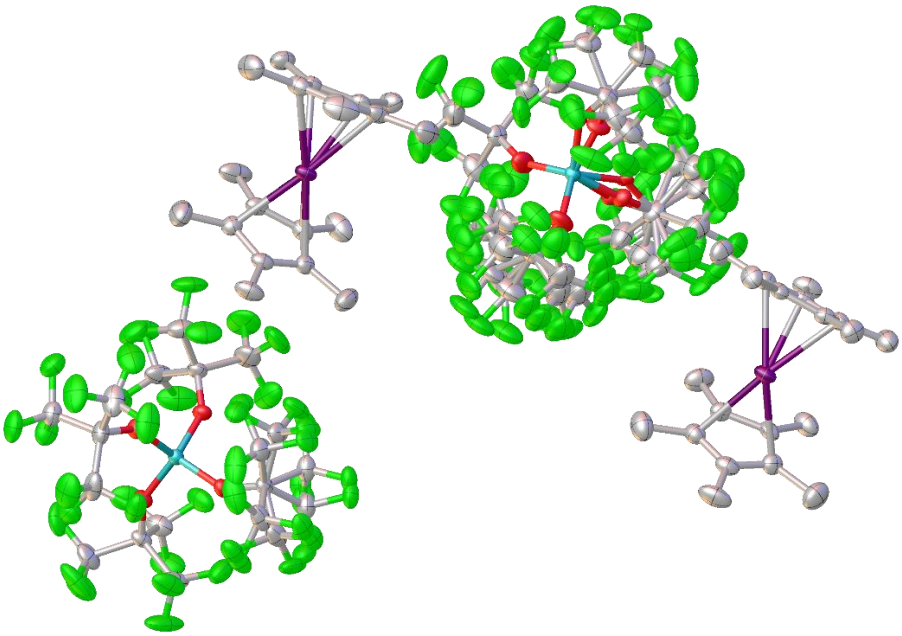

Figure S1: Molecular structure of **2a** in the solid state. Thermal ellipsoids are depicted at 50% probability level. H atoms are omitted for clarity.

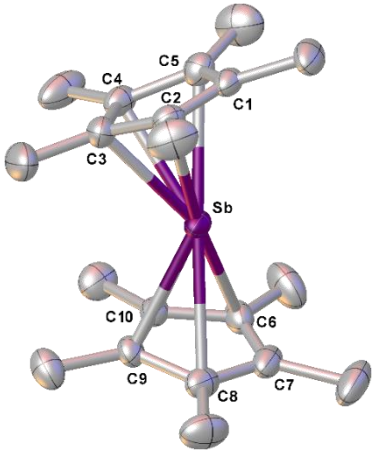

Figure S2: Molecular structure of the cationic part of **2a**. Thermal ellipsoids are depicted at 50% probability level. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Sb-C6 2.599(5), Sb-C8 2.661(5), Sb-C10 2.465(5), Sb-C9 2.494(5), Sb-C2 2.660(5), Sb-C3 2.491(6), Sb-C5 2.596(5), Sb-C4 2.450(5); C2-Sb-C8 132.2(2), C5-Sb-C6 123.9(2), C5-Sb-C2 51.7(2), C8-Sb-C6 52.2(2).

[Cp*$_2$Sb][FAL] (2b):

Compound **2b** crystallizes in a concentrated DCM solution at –30°C in form of orange plates in the triclinic space group $P\bar{1}$. The asymmetric unit contains one molecule of **2b**.

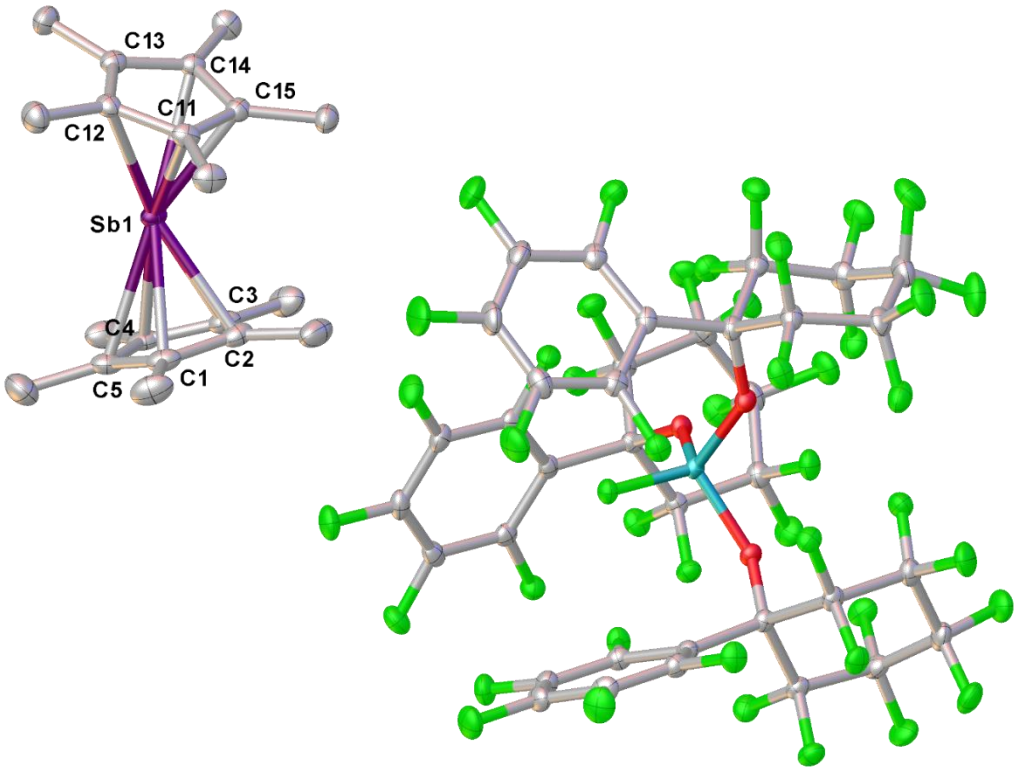

Figure S3: Molecular structure of **2b** in the solid state. Thermal ellipsoids are depicted at 50% probability level. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Sb1-C15 2.479(2), Sb1-C14 2.638(2), Sb1-C4 2.676(2), Sb1-C12 2.631(2), Sb1-C5 2.655(2), Sb1-C11 2.480(2), Sb1-C1 2.512(2), Sb1-C3 2.548(2), Sb1-C2 2.451(2); C15-Sb1-C14 32.19(7), C15-Sb1-C12 53.63(7), C15-Sb1-C11 33.66(7), C12-Sb1-C14 51.68(7), C5-Sb1-C4 30.81(7), C11-Sb1-C14 53.66(7), C11-Sb1-C12 32.44(7), C11-Sb1-C1 109.03(7), C1-Sb1-C4 52.60(7), C1-Sb1-C12 123.70(7), C1-Sb1-C5 31.86(8), C1-Sb1-C3 54.26(7), C3-Sb1-C4 31.46(8), C3-Sb1-C5 52.37(8), C2-Sb1-C15 104.80(8), C2-Sb1-C4 53.49(7).

[(Cp*Mo(CO)$_3$)$_3$(μ$_3$-Sb$_3$)] (3):

Compound **3** crystallizes in a concentrated DCM solution at –30°C in form of red blocks in the monoclinic space group P2$_1$/c. The asymmetric unit contains one molecule of **3** and one DCM molecule. One Cp* ligand is disordered over two positions (occupancy of 0.5 and 0.5). The restrains SADI and SIMU were used to describe the disorder.

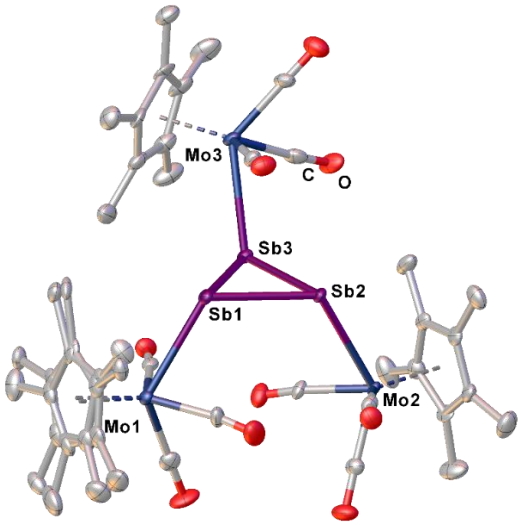

Figure S4: Molecular structure of **3** in the solid state. Thermal ellipsoids are depicted at 50% probability level. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Sb1-Sb2 2.8377(5), Sb1-Sb3 2.8370(5), Sb1-Mo1 2.8930(5), Sb2-Sb3 2.8459(5), Sb2-Mo2 2.8669(6), Sb3-Mo3 2.8885(6); Sb2-Sb1-Mo1 120.904(17), Sb3-Sb1-Sb2 60.200(13), Sb3-Sb1-Mo1 105.463(16), Sb1-Sb2-Sb3 59.888(13), Sb1-Sb2-Mo2 119.245(16), Sb3-Sb2-Mo2 111.694(17), Sb1-Sb3-Sb2 59.912(13), Sb1-Sb3-Mo3 113.202(18), Sb2-Sb3-Mo3 107.283(16).

[Cp''FeSb(CO)$_2$]$_4$ (7a):

Compound **7a** crystallizes by layering a DCM solution with acetonitrile in form of green plates in the triclinic space group $P\bar{1}$. The asymmetric unit contains one molecule of **7a** and one acetonitrile molecule.

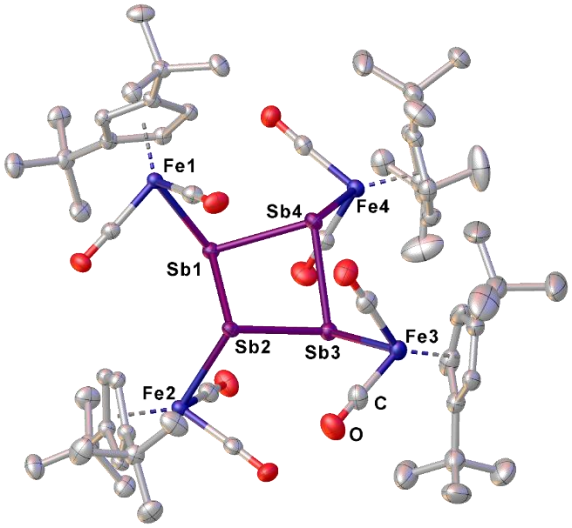

Figure S5: Molecular structure of **7a** in the solid state. Thermal ellipsoids are depicted at 50% probability level. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Sb2-Sb1 2.8521(3), Sb2-Sb3 2.8384(3), Sb2-Fe2 2.6230(6), Sb1-Sb4 2.8445(3), Sb1-Fe1 2.6230(5), Sb3-Sb4 2.8654(3), Sb3-Fe3 2.6144(6), Sb4-Fe4 2.6260(6); Sb3-Sb2-Sb1 81.775(9), Fe2-Sb2-Sb1 105.595(14), Fe2-Sb2-Sb3 102.339(14), Sb4-Sb1-Sb2 81.866(9), Fe1-Sb1-Sb2 101.449(14), Fe1-Sb1-Sb4 104.330(15), Sb2-Sb3-Sb4 81.739(9), Fe3-Sb3-Sb2 105.565(15), Fe3-Sb3-Sb4 104.444(15), Sb1-Sb4-Sb3 81.438(9), Fe4-Sb4-Sb1 106.666(16), Fe4-Sb4-Sb3 105.183(16).

[Cp'''FeSb(CO)$_2$]$_4$ (7b):

Compound **7b** crystallizes by layering a toluene solution with acetonitrile in form of green plates in the orthorhombic space group *Pna*2$_1$. The asymmetric unit contains one molecule of **7b**. One [Cp'''Fe(CO)$_2$] fragment is disordered over two positions (occupancy 0.42 and 0.52). The restrains SADI und SIMU were used during the crystal structure refinement.

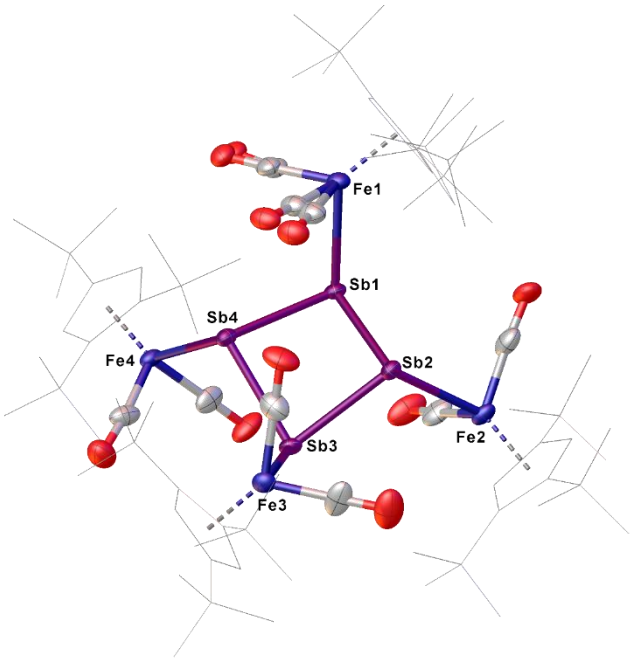

Figure S6: Molecular structure of **7b** in the solid state. Thermal ellipsoids are depicted at 50% probability level. H atoms are omitted and the Cp''' ligands are drawn in the wire frame model for clarity. Selected bond lengths [Å] and angles [°]: Sb2-Sb1 2.8628(11), Sb2-Sb3 2.8552(10), Sb2-Fe2 2.6570(19), Sb1-Sb4 2.8602(9), Sb1-Fe1 2.6501(19), Sb4-Sb3 2.8535(11), Sb4-Fe4 2.6433(19), Sb3-Fe3 2.644(2); Sb3-Sb2-Sb185.74(3), Fe2-Sb2-Sb1 103.91(5), Fe2-Sb2-Sb3 108.22(5), Sb4-Sb1-Sb2 84.15(3), Fe1-Sb1-Sb2 108.89(5), Fe1-Sb1-Sb4 102.89(5), Sb3-Sb4-Sb1 85.82(3), Fe4-Sb4-Sb1 108.61(5), Fe4-Sb4-Sb3 104.95(5), Sb4-Sb3-Sb2 84.42(3), Fe3-Sb3-Sb2 102.39(5), Fe3-Sb3-Sb4 105.02(5).

Table S1: Structure determination summary of the complexes **2a**, **2b** and **4**.

Compound	**2a**	**2b**	**3**
Formula	$C_{36}H_{30}AlF_{36}O_4Sb$	$AlC_{57}Cl_2F_{46}H_{32}O_3Sb$	$C_{40}H_{47}Cl_2Mo_3O_9Sb_3$
CCDC number	2120095	2120096	2120097
$D_{calc.}$/ g cm^{-3}	1.868	1.938	1.948
m/mm^{-1}	6.383	6.039	21.023
Formula Weight	1359.33	1858.45	1395.74
Colour	clear yellow	clear light orange	red
Shape	block-shaped	plate-shaped	block-shaped
Size/mm^3	0.18×0.16×0.12	0.29×0.20×0.06	0.14×0.10×0.09
T/K	123.01(10)	100.00(10)	123.1(1)
Crystal System	monoclinic	triclinic	monoclinic
Space Group	$P2_1/c$	P-1	$P2_1/c$
a/Å	21.9078(2)	13.0472(2)	8.5370(2)
b/Å	20.33870(10)	14.3850(2)	29.4147(5)
c/Å	22.0435(2)	17.8721(4)	19.2872(3)
α/°	90	90.162(2)	90
β/°	100.2420(10)	100.136(2)	100.672(2)
γ/°	90	105.0430(10)	90
V/Å^3	9665.55(14)	3184.65(10)	4759.50(16)
Z	8	2	4
Z'	2	1	1
Wavelength/Å	1.54184	1.54184	1.54184
Radiation type	Cu K$_\alpha$	Cu K$_\alpha$	Cu K$_\alpha$
θ_{min}/°	2.049	2.515	3.804
θ_{max}/°	75.523	74.264	67.075
Measured Refl's.	24123	41998	16875
Ind't Refl's	24123	12196	8391
Refl's with I≥σ(I)	22178	11866	7322
R_{int}	.	0.0318	0.0445
Parameters	2092	974	615
Restraints	1980	0	241
Largest Peak	1.121	0.742	1.707
Deepest Hole	-1.294	-0.556	-1.591
GooF	1.023	1.068	1.040
wR_2 (all data)	0.1463	0.0758	0.1003
wR_2	0.1421	0.0754	0.0956
R_1 (all data)	0.0584	0.0295	0.0479
R_1	0.0540	0.0289	0.0402

Table S2: Structure determination summary of the complexes **7a** and **7b**.

Compound	**7a**	**7b**
Formula	$C_{62}H_{87}Fe_4NO_8Sb_4$	$C_{76}H_{116}Fe_4O_8Sb_4$
CCDC number	2120098	2120099
$D_{calc.}$/ g cm^{-3}	1.650	1.520
m/mm^{-1}	14.588	16.236
Formula Weight	1684.72	1868.08
Colour	black	clear violett
Shape	plate-shaped	block-shaped
Size/mm^3	0.23×0.14×0.10	0.12×0.10×0.07
T/K	123.00(13)	132(13)
Crystal System	triclinic	orthorhombic
Flack Parameter		0.050(12)
Hooft Parameter		0.012(7)
Space Group	*P*-1	*Pna*2$_1$
a/Å	10.2505(2)	27.8565(5)
b/Å	18.2944(5)	13.9634(3)
c/Å	18.7216(4)	20.9861(4)
α/°	88.540(2)	90
β/°	85.7954(18)	90
γ/°	75.637(2)	90
V/Å^3	3391.80(15)	8163.0(3)
Z	2	4
Z'	1	1
Wavelength/Å	1.39222	1.54184
Radiation type	Cu K$_\beta$	Cu K$_\alpha$
θ_{min}/°	3.093	3.802
θ_{max}/°	70.024	66.875
Measured Refl's.	27519	45225
Ind't Refl's	16401	12117
Refl's with I≥σ(I)	15071	10566
R_{int}	0.0280	0.0791
Parameters	737	980
Restraints	0	306
Largest Peak	2.524	1.626
Deepest Hole	-1.838	-1.504
GooF	1.089	1.025
wR_2 (all data)	0.1152	0.1425
wR_2	0.1121	0.1335
R_1 (all data)	0.0456	0.0633
R_1	0.0422	0.0538

3. NMR investigations

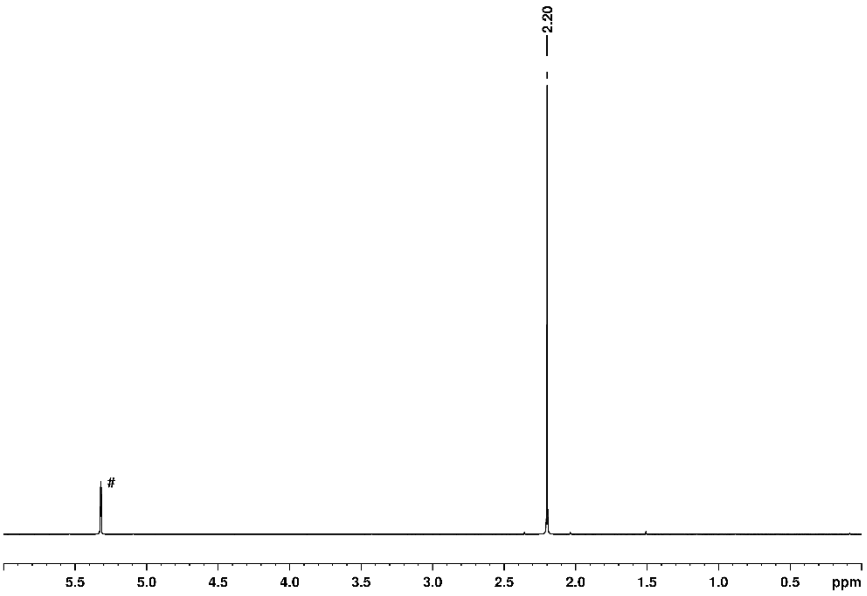

Figure S7: ^{1}H NMR spectrum of **2a** in CD_2Cl_2 (#).

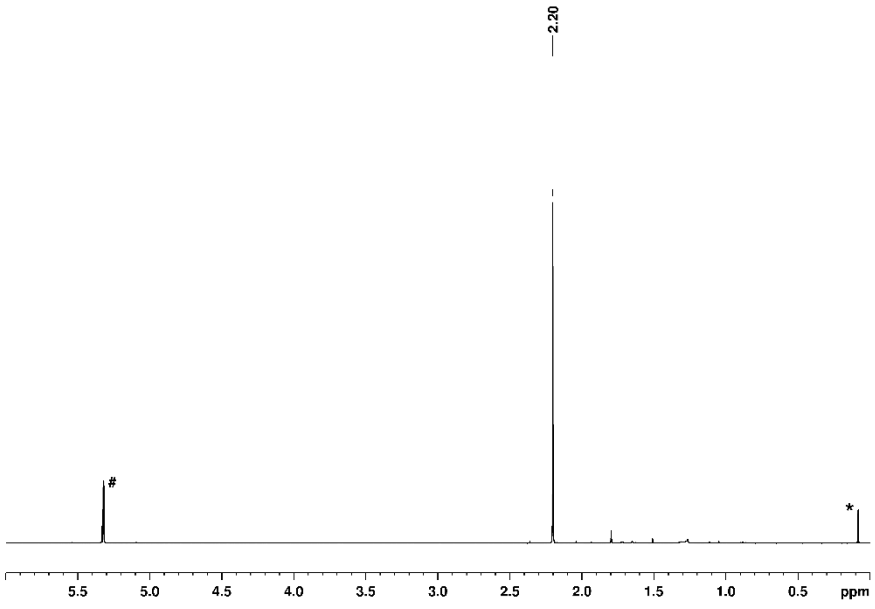

Figure S8: ^{1}H NMR spectrum of **2b** in CD_2Cl_2 (#). The signal marked with * is due to silicon grease.

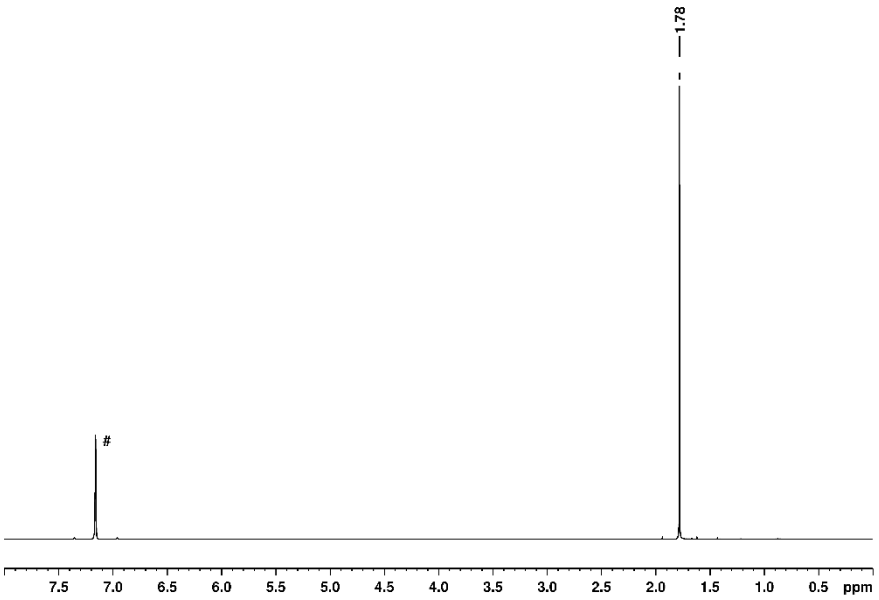

Figure S9: ^{1}H NMR spectrum of **3** in C_6D_6 (#).

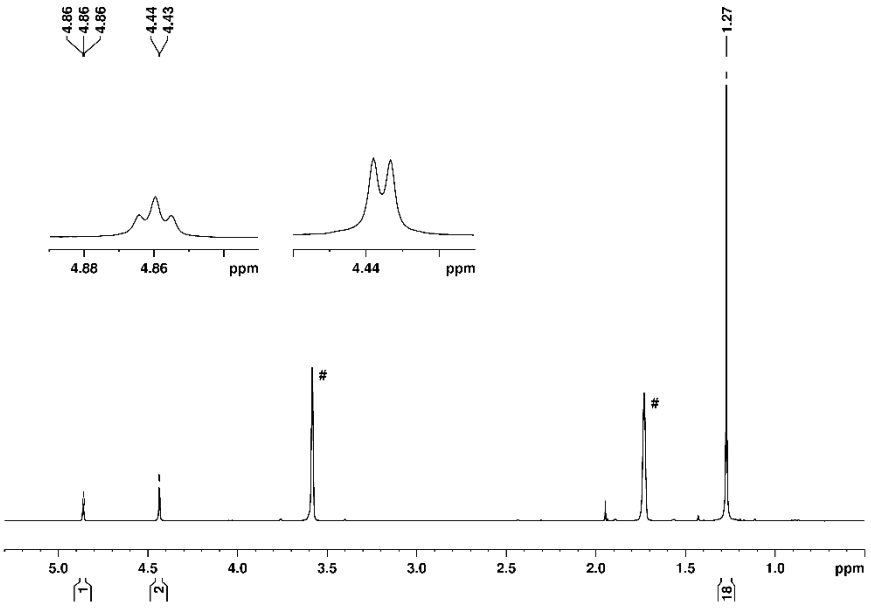

Figure S10: ^{1}H NMR spectrum of **7a** in thf-d_8 (#).

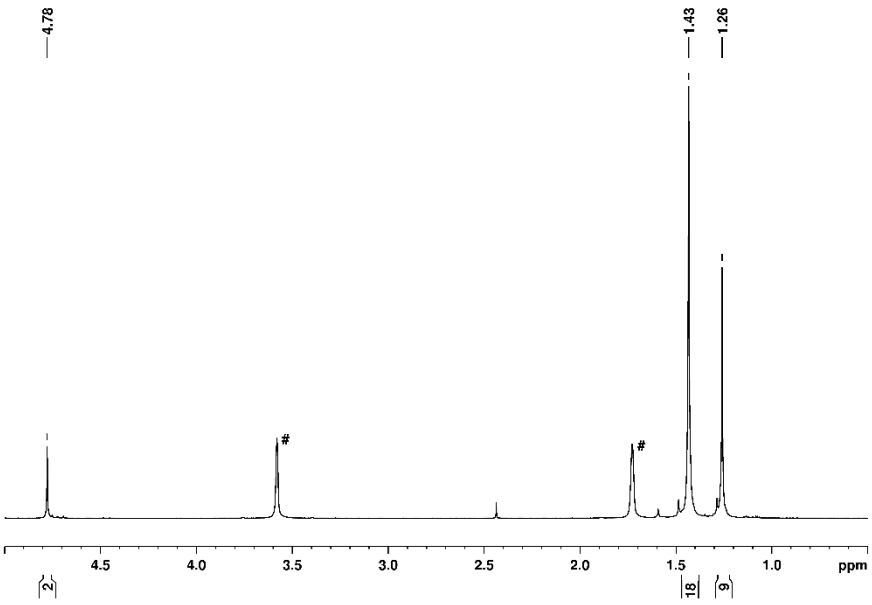

Figure S11: ^{1}H NMR spectrum of **7b** in thf-d_8 (#).

4. Details of DFT calculations

The DFT calculations have been performed with the program Gaussian 16.[15] The geometries have been optimized at the D3(BJ)[16]-BP86[17]/def2TZVP[18] level of theory. The frequency analysis has been performed on the optimized geometries at the D3(BJ)-TPSSh[19]/def2SVP level. For the dispersion corrections the following parameters have been used: s6 = 1.000, a1 = 0.4529, s8 = 2.2382, and a2 = 4.6550.[20] For some complexes imaginary frequencies of low intensity corresponding to the rotation of organic substituents i.e. methyl groups have been observed and they were not considered for the calculation of the thermodynamic parameters. The NBO analysis has been performed with NBO7[21] on the D3(BJ)-BP86/def2TZVP wavefunction.

Table S3: Carteisan coordinates of the optimised geometry of **3**.

Sb	-0.743052000	-1.304981000	1.349614000
Sb	0.269607000	1.332743000	1.000603000
Sb	1.057521000	-0.735677000	-0.792674000
Mo	-3.105196000	-2.196214000	-0.031092000
Mo	-1.293326000	3.356435000	-0.315852000
Mo	3.772153000	-1.321308000	0.090774000
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O	-4.003199000	-1.170660000	2.804167000
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O	2.688075000	-3.742263000	-1.594136000
O	-5.800974000	-0.782556000	-0.754974000
O	5.009185000	-3.741231000	1.638854000
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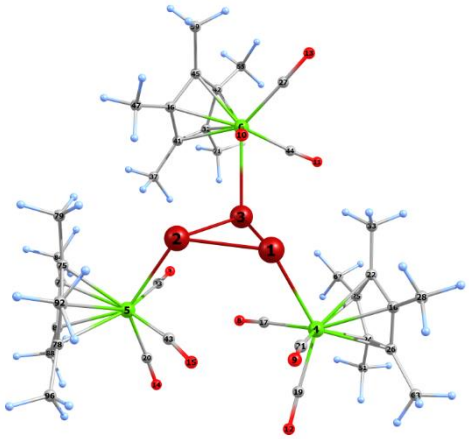

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H	4.736129000	-1.483370000	-3.464844000
H	5.062447000	0.226824000	-3.822427000
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C	0.207886000	4.825263000	0.875154000
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C	0.049505000	5.323090000	-0.460436000
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Zero-point vibrational energy 1958653.8 (Joules/Mol)
468.12949 (Kcal/Mol)

Zero-point correction=	0.746012 (Hartree/Particle)
Thermal correction to Energy=	0.815875
Thermal correction to Enthalpy=	0.816819
Thermal correction to Gibbs Free Energy=	0.635802
Sum of electronic and zero-point Energies=	-3113.963580
Sum of electronic and thermal Energies=	-3113.893718
Sum of electronic and thermal Enthalpies=	-3113.892773
Sum of electronic and thermal Free Energies=	-3114.073790

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	511.969	242.979	380.981
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	47.395
Rotational	0.889	2.981	40.323
Vibrational	510.192	237.017	293.263

********** NBO 7.0 **********

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. Sb	0.0000	0.9323	0.9290	0.4706	0.0302	0.0189	0.0054	0.0455	0.0348
2. Sb	0.9323	0.0000	0.9210	0.0262	0.4657	0.0143	0.0423	0.0021	0.0012
3. Sb	0.9290	0.9210	0.0000	0.0131	0.0182	0.4432	0.0072	0.0085	0.0074
4. Mo	0.4706	0.0262	0.0131	0.0000	0.0084	0.0057	0.0010	0.1240	0.1286
5. Mo	0.0302	0.4657	0.0182	0.0084	0.0000	0.0060	0.1245	0.0042	0.0010
6. Mo	0.0189	0.0143	0.4432	0.0057	0.0060	0.0000	0.0011	0.0028	0.0012

88. (1.94940) LP (1)Sb 1 s(85.37%)p 0.17(14.59%)d 0.00(0.03%)
89. (1.94455) LP (1)Sb 2 s(84.36%)p 0.19(15.61%)d 0.00(0.02%)
90. (1.96567) LP (1)Sb 3 s(86.27%)p 0.16(13.69%)d 0.00(0.04%)

110. (1.91897) BD (1)Sb 1-Sb 2
(48.61%) 0.6972*Sb 1 s(4.93%)p19.18(94.58%)d 0.09(0.45%)
(51.39%) 0.7169*Sb 2 s(5.31%)p17.75(94.31%)d 0.06(0.33%)
111. (1.92892) BD (1)Sb 1-Sb 3
(48.36%) 0.6954*Sb 1 s(4.59%)p20.69(94.93%)d 0.09(0.43%)
(51.64%) 0.7186*Sb 3 s(4.39%)p21.64(95.10%)d 0.11(0.47%)
112. (1.68597) BD (1)Sb 1-Mo 4
(32.04%) 0.5660*Sb 1 s(5.10%)p18.55(94.66%)d 0.04(0.21%)
(67.96%) 0.8244*Mo 4 s(2.15%)p 0.04(0.08%)d45.38(97.76%)
113. (1.92524) BD (1)Sb 2-Sb 3

```
               ( 51.17%)   0.7153*Sb  2 s(  5.19%)p18.18( 94.44%)d 0.06(  0.33%)
               ( 48.83%)   0.6988*Sb  3 s(  4.56%)p20.81( 94.99%)d 0.09(  0.41%)
114. (1.68766) BD ( 1)Sb  2-Mo  5
               ( 37.17%)   0.6097*Sb  2 s(  5.11%)p18.55( 94.70%)d 0.03(  0.17%)
               ( 62.83%)   0.7927*Mo  5 s(  7.74%)p 0.01(  0.06%)d11.92( 92.20%)
115. (1.67239) BD ( 1)Sb  3-Mo  6
               ( 34.97%)   0.5914*Sb  3 s(  4.78%)p19.88( 94.93%)d 0.06(  0.27%)
               ( 65.03%)   0.8064*Mo  6 s(  7.23%)p 0.01(  0.06%)d12.81( 92.70%)
```

Table S4: Carteisan coordinates of the optimised geometry of **7a**.

Sb	-1.765325000	0.918302000	-0.454312000
Sb	-1.174653000	-1.585853000	0.819106000
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Sb	0.926675000	1.467349000	0.310687000
Fe	-2.863324000	2.377342000	1.427770000
Fe	-2.554820000	-3.026154000	-0.874270000
Fe	3.095265000	-2.175288000	1.206385000
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O	-1.128818000	-1.754571000	-3.065410000
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O	0.285741000	4.873406000	-1.437106000
O	1.170096000	-4.224081000	1.947125000
O	-0.507068000	-5.087564000	-0.777704000
O	2.036928000	-0.343770000	3.199479000
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C	-4.039228000	3.845231000	0.426262000
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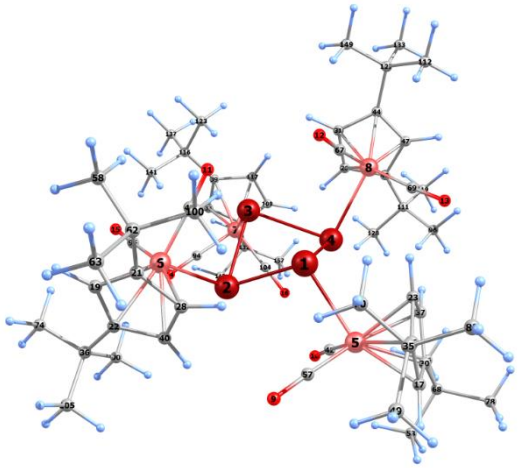

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H	-0.104027000	5.160471000	3.048179000
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C	-1.320773000	-4.252123000	-0.783841000
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H	5.199383000	-0.252504000	1.402619000
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C	2.926119000	4.283405000	-4.813220000
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H	3.027204000	4.518521000	-5.883559000
H	3.137801000	5.202234000	-4.247153000
C	4.171586000	-4.015466000	-1.393570000
C	4.622938000	-1.696278000	-0.209947000
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C	5.453784000	4.594441000	0.677468000
H	6.277764000	3.907219000	0.433903000
H	5.670149000	5.061785000	1.650198000
H	5.434583000	5.386654000	-0.085281000
C	3.908638000	-3.186773000	-2.661126000
H	3.020368000	-2.547187000	-2.542357000
H	3.729109000	-3.857078000	-3.514479000
H	4.770102000	-2.548437000	-2.910754000
C	3.888187000	3.145612000	-4.428864000
C	4.169560000	2.792721000	1.860845000
H	3.237405000	2.211417000	1.927306000
H	4.323161000	3.290919000	2.829259000
H	5.006673000	2.094621000	1.707427000
C	5.534265000	-2.484971000	3.398847000
C	5.341392000	3.573502000	-4.740976000
H	5.610778000	4.486905000	-4.190331000
H	5.458465000	3.772698000	-5.817231000
H	6.052752000	2.783390000	-4.457722000
C	5.448895000	-4.862535000	-1.602103000
H	6.327338000	-4.219037000	-1.760235000
H	5.332653000	-5.511289000	-2.483577000
H	5.647960000	-5.503389000	-0.730553000
C	2.976074000	-4.949628000	-1.141324000
H	3.103757000	-5.534030000	-0.218807000
H	2.864437000	-5.657600000	-1.976228000
H	2.042235000	-4.379144000	-1.051538000
C	4.627262000	-3.397141000	4.243360000
H	3.605441000	-2.996655000	4.287909000
H	5.019321000	-3.475216000	5.268691000
H	4.574261000	-4.413501000	3.826817000
C	3.546616000	1.891643000	-5.249447000
H	4.251077000	1.071705000	-5.044907000
H	3.609368000	2.121173000	-6.323419000
H	2.529069000	1.535785000	-5.038342000
C	6.968726000	-3.063148000	3.378548000
H	6.977851000	-4.081185000	2.962063000
H	7.378168000	-3.104834000	4.399492000
H	7.635543000	-2.438838000	2.765201000
C	5.568460000	-1.080816000	4.023708000
H	6.254180000	-0.414146000	3.479562000
H	5.924977000	-1.144718000	5.062399000
H	4.571587000	-0.619818000	4.036302000

```
Zero-point vibrational energy    3436082.6 (Joules/Mol)
                                  821.24346 (Kcal/Mol)
 Zero-point correction=                           1.308735 (Hartree/Particle)
 Thermal correction to Energy=                    1.404267
 Thermal correction to Enthalpy=                  1.405211
 Thermal correction to Gibbs Free Energy=         1.168843
 Sum of electronic and zero-point Energies=          -8951.529832
 Sum of electronic and thermal Energies=             -8951.434300
 Sum of electronic and thermal Enthalpies=           -8951.433356
 Sum of electronic and thermal Free Energies=        -8951.669724

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                881.191            352.335           497.478
 Electronic             0.000              0.000             0.000
 Translational          0.889              2.981            48.056
 Rotational             0.889              2.981            41.791
 Vibrational          879.413            346.374           407.631


********************************** NBO 7.0 **********************************

Wiberg bond index matrix in the NAO basis:

     Atom    1       2       3       4       5       6       7       8       9
     ---- ------  ------  ------  ------  ------  ------  ------  ------  ------
   1. Sb  0.0000  0.9317  0.0256  0.9338  0.4672  0.0157  0.0130  0.0164  0.0221
   2. Sb  0.9317  0.0000  0.9375  0.0290  0.0151  0.4801  0.0170  0.0135  0.0012
   3. Sb  0.0256  0.9375  0.0000  0.9273  0.0108  0.0168  0.4741  0.0177  0.0011
   4. Sb  0.9338  0.0290  0.9273  0.0000  0.0164  0.0101  0.0198  0.4593  0.0015
   5. Fe  0.4672  0.0151  0.0108  0.0164  0.0000  0.0063  0.0040  0.0058  0.1497
   6. Fe  0.0157  0.4801  0.0168  0.0101  0.0063  0.0000  0.0056  0.0045  0.0004
   7. Fe  0.0130  0.0170  0.4741  0.0198  0.0040  0.0056  0.0000  0.0058  0.0002
   8. Fe  0.0164  0.0135  0.0177  0.4593  0.0058  0.0045  0.0058  0.0000  0.0003

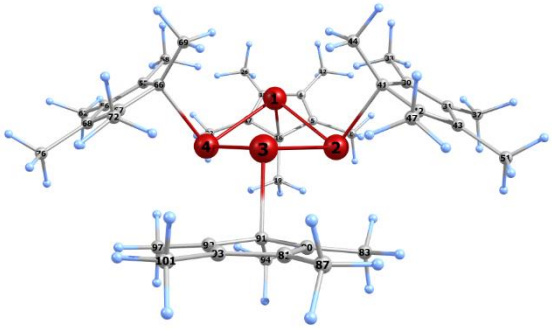


141. (1.96961) LP ( 1)Sb  1            s( 82.44%)p 0.21( 17.51%)d 0.00(  0.04%)
142. (1.97169) LP ( 1)Sb  2            s( 82.69%)p 0.21( 17.27%)d 0.00(  0.05%)
143. (1.96402) LP ( 1)Sb  3            s( 82.61%)p 0.21( 17.35%)d 0.00(  0.03%)
144. (1.96258) LP ( 1)Sb  4            s( 82.52%)p 0.21( 17.45%)d 0.00(  0.03%)

 169. (1.93409) BD ( 1)Sb  1-Sb  2
               ( 50.71%)   0.7121*Sb  1 s(  5.86%)p16.00( 93.70%)d 0.07(  0.41%)
               ( 49.29%)   0.7020*Sb  2 s(  6.00%)p15.57( 93.48%)d 0.08(  0.49%)
170. (1.93725) BD ( 1)Sb  1-Sb  4
               ( 49.53%)   0.7038*Sb  1 s(  6.71%)p13.85( 92.87%)d 0.06(  0.40%)
               ( 50.47%)   0.7104*Sb  4 s(  6.35%)p14.69( 93.30%)d 0.05(  0.32%)
171. (1.68471) BD ( 1)Sb  1-Fe  5
               ( 36.72%)   0.6060*Sb  1 s(  4.98%)p19.00( 94.61%)d 0.08(  0.41%)
               ( 63.28%)   0.7955*Fe  5 s( 22.52%)p 0.01(  0.22%)d 3.43( 77.26%)
172. (1.93664) BD ( 1)Sb  2-Sb  3
               ( 49.00%)   0.7000*Sb  2 s(  6.11%)p15.28( 93.44%)d 0.07(  0.41%)
               ( 51.00%)   0.7142*Sb  3 s(  6.12%)p15.27( 93.50%)d 0.06(  0.34%)
173. (1.69582) BD ( 1)Sb  2-Fe  6
               ( 37.45%)   0.6119*Sb  2 s(  5.18%)p18.20( 94.36%)d 0.09(  0.45%)
               ( 62.55%)   0.7909*Fe  6 s( 22.64%)p 0.01(  0.23%)d 3.41( 77.13%)
174. (1.93558) BD ( 1)Sb  3-Sb  4
               ( 49.79%)   0.7056*Sb  3 s(  6.37%)p14.63( 93.21%)d 0.06(  0.39%)
               ( 50.21%)   0.7086*Sb  4 s(  6.36%)p14.67( 93.28%)d 0.05(  0.34%)
175. (1.68786) BD ( 1)Sb  3-Fe  7
               ( 37.59%)   0.6131*Sb  3 s(  4.88%)p19.44( 94.77%)d 0.07(  0.35%)
               ( 62.41%)   0.7900*Fe  7 s( 23.90%)p 0.01(  0.18%)d 3.18( 75.92%)
176. (1.67930) BD ( 1)Sb  4-Fe  8
               ( 36.37%)   0.6030*Sb  4 s(  4.75%)p19.95( 94.87%)d 0.08(  0.37%)
               ( 63.63%)   0.7977*Fe  8 s( 23.22%)p 0.01(  0.19%)d 3.30( 76.59%)
```

Table S5: Carteisan coordinates of the optimised geometry of **1**.

Sb	-1.942336000	0.000000000	-0.414709000
Sb	0.000000000	-1.942336000	0.414709000
Sb	1.942336000	0.000000000	-0.414709000
Sb	0.000000000	1.942336000	0.414709000
C	-4.042054000	-1.185734000	1.196089000
C	-5.206353000	-0.730209000	0.612815000
H	-1.710314000	0.888410000	2.840000000
C	-3.662445000	-2.585415000	1.555565000
H	-2.643673000	-2.846433000	1.222057000
H	-3.675306000	-2.730902000	2.649936000
H	-4.351770000	-3.318595000	1.116281000
C	-6.314094000	-1.552420000	0.031219000
H	-6.451025000	-1.339604000	-1.042435000
H	-6.120048000	-2.628445000	0.134140000
H	-7.278740000	-1.337573000	0.520284000
C	-3.201389000	0.000000000	1.526779000
C	-4.042054000	1.185734000	1.196089000
C	-5.206353000	0.730209000	0.612815000
C	-2.356283000	0.000000000	2.784117000
H	-3.007962000	0.000000000	3.675260000
H	-1.710314000	-0.888410000	2.840000000
C	-3.662445000	2.585415000	1.555565000
H	-2.643673000	2.846433000	1.222057000
H	-3.675306000	2.730902000	2.649936000
H	-4.351770000	3.318595000	1.116281000
C	-6.314094000	1.552420000	0.031219000
H	-6.451025000	1.339604000	-1.042435000
H	-6.120048000	2.628445000	0.134140000
H	-7.278740000	1.337573000	0.520284000
C	-1.185734000	-4.042054000	-1.196089000
C	-0.730209000	-5.206353000	-0.612815000
H	0.888410000	-1.710314000	-2.840000000
C	-2.585415000	-3.662445000	-1.555565000
H	-2.846433000	-2.643673000	-1.222057000
H	-2.730902000	-3.675306000	-2.649936000
H	-3.318595000	-4.351770000	-1.116281000
C	-1.552420000	-6.314094000	-0.031219000
H	-1.339604000	-6.451025000	1.042435000
H	-2.628445000	-6.120048000	-0.134140000
H	-1.337573000	-7.278740000	-0.520284000
C	0.000000000	-3.201389000	-1.526779000
C	1.185734000	-4.042054000	-1.196089000
C	0.730209000	-5.206353000	-0.612815000
C	0.000000000	-2.356283000	-2.784117000
H	0.000000000	-3.007962000	-3.675260000
H	-0.888410000	-1.710314000	-2.840000000
C	2.585415000	-3.662445000	-1.555565000
H	2.846433000	-2.643673000	-1.222057000
H	2.730902000	-3.675306000	-2.649936000
H	3.318595000	-4.351770000	-1.116281000
C	1.552420000	-6.314094000	-0.031219000
H	1.339604000	-6.451025000	1.042435000
H	2.628445000	-6.120048000	-0.134140000
H	1.337573000	-7.278740000	-0.520284000
C	-1.185734000	4.042054000	-1.196089000
C	-0.730209000	5.206353000	-0.612815000
H	0.888410000	1.710314000	-2.840000000
C	-2.585415000	3.662445000	-1.555565000
H	-2.846433000	2.643673000	-1.222057000
H	-2.730902000	3.675306000	-2.649936000
H	-3.318595000	4.351770000	-1.116281000
C	-1.552420000	6.314094000	-0.031219000
H	-1.339604000	6.451025000	1.042435000
H	-2.628445000	6.120048000	-0.134140000
H	-1.337573000	7.278740000	-0.520284000
C	0.000000000	3.201389000	-1.526779000
C	1.185734000	4.042054000	-1.196089000
C	0.730209000	5.206353000	-0.612815000
C	0.000000000	2.356283000	-2.784117000
H	0.000000000	3.007962000	-3.675260000
H	-0.888410000	1.710314000	-2.840000000
C	2.585415000	3.662445000	-1.555565000
H	2.846433000	2.643673000	-1.222057000
H	2.730902000	3.675306000	-2.649936000
H	3.318595000	4.351770000	-1.116281000
C	1.552420000	6.314094000	-0.031219000
H	1.339604000	6.451025000	1.042435000
H	2.628445000	6.120048000	-0.134140000
H	1.337573000	7.278740000	-0.520284000
C	4.042054000	-1.185734000	1.196089000
C	5.206353000	-0.730209000	0.612815000
H	1.710314000	0.888410000	2.840000000
C	3.662445000	-2.585415000	1.555565000
H	2.643673000	-2.846433000	1.222057000
H	3.675306000	-2.730902000	2.649936000
H	4.351770000	-3.318595000	1.116281000
C	6.314094000	-1.552420000	0.031219000



H	6.451025000	-1.339604000	-1.042435000
H	6.120048000	-2.628445000	0.134140000
H	7.278740000	-1.337573000	0.520284000
C	3.201389000	0.000000000	1.526779000
C	4.042054000	1.185734000	1.196089000
C	5.206353000	0.730209000	0.612815000
C	2.356283000	0.000000000	2.784117000
H	3.007962000	0.000000000	3.675260000
H	1.710314000	-0.888410000	2.840000000
C	3.662445000	2.585415000	1.555565000
H	2.643673000	2.846433000	1.222057000
H	3.675306000	2.730902000	2.649936000
H	4.351770000	3.318595000	1.116281000
C	6.314094000	1.552420000	0.031219000
H	6.451025000	1.339604000	-1.042435000
H	6.120048000	2.628445000	0.134140000
H	7.278740000	1.337573000	0.520284000

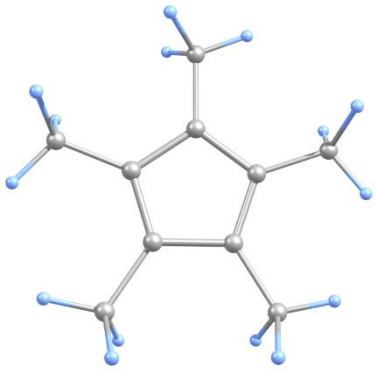
Zero-point vibrational energy 2320550.0 (Joules/Mol)
554.62476 (Kcal/Mol)

Zero-point correction=	0.883851 (Hartree/Particle)
Thermal correction to Energy=	0.945598
Thermal correction to Enthalpy=	0.946542
Thermal correction to Gibbs Free Energy=	0.784258
Sum of electronic and zero-point Energies=	-2519.549287
Sum of electronic and thermal Energies=	-2519.487540
Sum of electronic and thermal Enthalpies=	-2519.486596
Sum of electronic and thermal Free Energies=	-2519.648880

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	593.372	216.913	341.556
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	46.653
Rotational	0.889	2.981	36.359
Vibrational	591.594	210.951	258.544

Table S6: Carteisan coordinates of the optimised geometry of $C_5Me_5^{\bullet}$.

C	0.851623000	0.053528000	-3.701782000
C	0.916638000	-1.140804000	-2.813863000
C	0.276451000	-0.837122000	-1.617663000
C	-0.190885000	0.514750000	-1.724834000
C	0.177850000	1.049187000	-3.029207000
C	-0.147342000	2.434865000	-3.489715000
H	0.294474000	3.202787000	-2.831385000
H	0.226905000	2.621599000	-4.505634000
H	-1.235239000	2.620963000	-3.501845000
C	1.438722000	0.090029000	-5.072084000
H	2.525659000	-0.103155000	-5.055130000
H	0.998831000	-0.684264000	-5.724773000
H	1.281713000	1.062420000	-5.557906000
C	1.575474000	-2.416483000	-3.209450000
H	2.642111000	-2.262461000	-3.450223000
H	1.517006000	-3.174882000	-2.417604000
H	1.116616000	-2.842981000	-4.118827000
C	0.088346000	-1.721210000	-0.421978000
H	-0.977561000	-1.882568000	-0.187950000
H	0.536260000	-2.711617000	-0.582443000
H	0.553986000	-1.298880000	0.484536000
C	-0.935831000	1.274271000	-0.685194000
H	-1.917231000	1.612426000	-1.062758000
H	-1.106756000	0.678772000	0.221129000
H	-0.394060000	2.191965000	-0.394724000



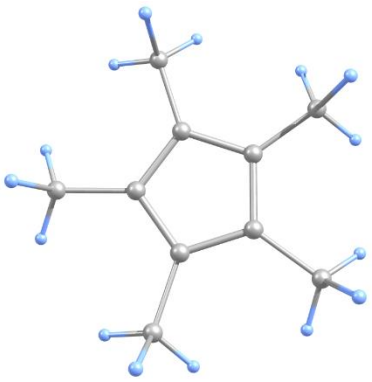
Zero-point vibrational energy 567013.9 (Joules/Mol)
135.51958 (Kcal/Mol)

Zero-point correction=	0.215964 (Hartree/Particle)
Thermal correction to Energy=	0.227626
Thermal correction to Enthalpy=	0.228570
Thermal correction to Gibbs Free Energy=	0.178078
Sum of electronic and zero-point Energies=	-389.637943
Sum of electronic and thermal Energies=	-389.626282
Sum of electronic and thermal Enthalpies=	-389.625337
Sum of electronic and thermal Free Energies=	-389.675829

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	142.837	42.023	106.269
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	40.615
Rotational	0.889	2.981	29.721
Vibrational	141.060	36.061	34.555

Table S7: Carteisan coordinates of the optimised geometry of $C_5Me_5^-$.

C	0.871680000	0.020301000	-3.691723000
C	0.915180000	-1.129434000	-2.853795000
C	0.260677000	-0.807827000	-1.631488000
C	-0.187360000	0.540632000	-1.714005000
C	0.190291000	1.052470000	-2.987281000
C	-0.090841000	2.434048000	-3.501669000
H	-0.131099000	3.176473000	-2.683133000
H	0.690421000	2.777279000	-4.205077000
H	-1.055602000	2.528162000	-4.047197000
C	1.435011000	0.122572000	-5.078984000
H	2.318493000	-0.528997000	-5.212455000
H	0.720316000	-0.163727000	-5.881781000
H	1.760190000	1.152799000	-5.315206000
C	1.532496000	-2.452134000	-3.202742000
H	2.390086000	-2.336310000	-3.891298000
H	1.912033000	-2.977063000	-2.306533000
H	0.835245000	-3.161841000	-3.700112000
C	0.066336000	-1.731522000	-0.464698000
H	-0.876707000	-2.320081000	-0.503362000
H	0.883707000	-2.472240000	-0.386961000
H	0.042007000	-1.181893000	0.494638000
C	-0.936751000	1.287332000	-0.649477000
H	-2.042527000	1.188354000	-0.717996000
H	-0.663307000	0.941416000	0.364718000
H	-0.726216000	2.372366000	-0.683688000



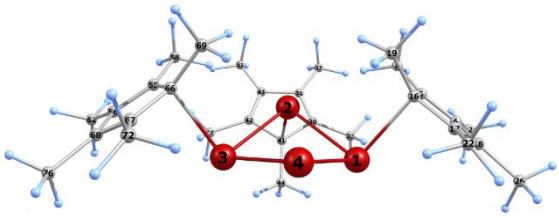
Zero-point vibrational energy 561743.4 (Joules/Mol)
134.25991 (Kcal/Mol)

Zero-point correction=	0.213957 (Hartree/Particle)
Thermal correction to Energy=	0.225600
Thermal correction to Enthalpy=	0.226544
Thermal correction to Gibbs Free Energy=	0.175968
Sum of electronic and zero-point Energies=	-389.676338
Sum of electronic and thermal Energies=	-389.664695
Sum of electronic and thermal Enthalpies=	-389.663751
Sum of electronic and thermal Free Energies=	-389.714327

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	141.566	41.264	106.446
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.615
Rotational	0.889	2.981	29.731
Vibrational	139.789	35.302	36.099

Table S8: Carteisan coordinates of the optimised geometry of $Cp^*_3Sb_4^-$.

Sb	-0.777576000	0.732674000	-1.940987000
Sb	0.986754000	-0.365210000	0.000000000
Sb	-0.777576000	0.732674000	1.940987000
Sb	-2.727338000	0.169207000	0.000000000
C	0.324639000	-1.070249000	-4.041288000
C	0.113060000	-0.284607000	-5.168897000
H	-2.138260000	-2.263674000	-1.848675000
C	1.590220000	-1.723870000	-3.587416000
H	1.834846000	-1.483460000	-2.537509000
H	1.517006000	-2.824701000	-3.642967000
H	2.448416000	-1.417778000	-4.201701000
C	1.150018000	0.247311000	-6.111548000
H	1.192096000	1.350821000	-6.093623000
H	2.154215000	-0.120273000	-5.856269000
H	0.944929000	-0.042733000	-7.157297000
C	-0.966839000	-1.242161000	-3.364093000
C	-1.973161000	-0.600559000	-4.225239000
C	-1.303030000	0.004306000	-5.282055000
C	-1.277175000	-2.444875000	-2.513110000
H	-1.504345000	-3.323484000	-3.144465000
H	-0.427521000	-2.703321000	-1.862464000
C	-3.443466000	-0.642708000	-3.949163000
H	-3.663959000	-0.426415000	-2.889126000
H	-3.870975000	-1.640290000	-4.158509000
H	-3.995423000	0.088104000	-4.558293000
C	-1.890622000	0.877023000	-6.349838000
H	-1.473541000	1.899273000	-6.318112000
H	-2.981811000	0.963739000	-6.246264000
H	-1.684444000	0.485133000	-7.361677000
C	3.449018000	0.714964000	-1.179485000
C	4.434493000	-0.147906000	-0.726852000
H	1.514548000	2.807228000	0.885595000
C	3.150214000	1.144477000	-2.580213000
H	2.082128000	1.033822000	-2.835044000
H	3.397260000	2.210608000	-2.733005000
H	3.724513000	0.563656000	-3.315136000



C	5.332666000	-1.013602000	-1.557342000
H	5.152725000	-2.086577000	-1.367541000
H	5.178167000	-0.841635000	-2.631958000
H	6.399319000	-0.829964000	-1.339246000
C	2.731183000	1.241510000	0.000000000
C	3.449018000	0.714964000	1.179485000
C	4.434493000	-0.147906000	0.726852000
C	2.144414000	2.635518000	0.000000000
H	2.948651000	3.394509000	0.000000000
H	1.514548000	2.807228000	-0.885595000
C	3.150214000	1.144477000	2.580213000
H	2.082128000	1.033822000	2.835044000
H	3.397260000	2.210608000	2.733005000
H	3.724513000	0.563656000	3.315136000
C	5.332666000	-1.013602000	1.557342000
H	5.152725000	-2.086577000	1.367541000
H	5.178167000	-0.841635000	2.631958000
H	6.399319000	-0.829964000	1.339246000
C	0.324639000	-1.070249000	4.041288000
C	0.113060000	-0.284607000	5.168897000
H	-2.138260000	-2.263674000	1.848675000
C	1.590220000	-1.723870000	3.587416000
H	1.834846000	-1.483460000	2.537509000
H	1.517006000	-2.824701000	3.642967000
H	2.448416000	-1.417778000	4.201701000
C	1.150018000	0.247311000	6.111548000
H	1.192096000	1.350821000	6.093623000
H	2.154215000	-0.120273000	5.856269000
H	0.944929000	-0.042733000	7.157297000
C	-0.966839000	-1.242161000	3.364093000
C	-1.973161000	-0.600559000	4.225239000
C	-1.303030000	0.004306000	5.282055000
C	-1.277175000	-2.444875000	2.513110000
H	-1.504345000	-3.323484000	3.144465000
H	-0.427521000	-2.703321000	1.862464000
C	-3.443466000	-0.642708000	3.949163000
H	-3.663959000	-0.426415000	2.889126000
H	-3.870975000	-1.640290000	4.158509000
H	-3.995423000	0.088104000	4.558293000
C	-1.890622000	0.877023000	6.349838000
H	-1.473541000	1.899273000	6.318112000
H	-2.981811000	0.963739000	6.246264000
H	-1.684444000	0.485133000	7.361677000

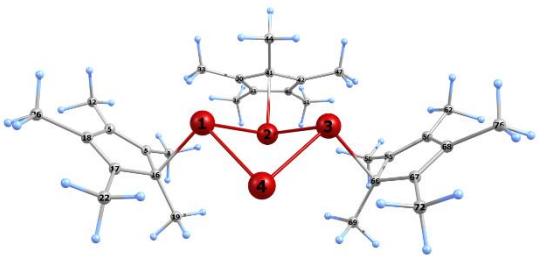
Zero-point vibrational energy 1733752.7 (Joules/Mol)
414.37685 (Kcal/Mol)

Zero-point correction=	0.660352 (Hartree/Particle)
Thermal correction to Energy=	0.709269
Thermal correction to Enthalpy=	0.710214
Thermal correction to Gibbs Free Energy=	0.571375
Sum of electronic and zero-point Energies=	-2129.932171
Sum of electronic and thermal Energies=	-2129.883253
Sum of electronic and thermal Enthalpies=	-2129.882309
Sum of electronic and thermal Free Energies=	-2130.021148

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	445.073	167.772	292.210
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	46.231
Rotational	0.889	2.981	38.200
Vibrational	443.296	161.811	207.780

Table S9: Carteisan coordinates of the optimised geometry of $Cp^*_3Sb_4^\bullet$.

Sb	-0.767464000	-0.691936000	1.899346000
Sb	1.025698000	0.524072000	0.000000000
Sb	-0.767464000	-0.691936000	-1.899346000
Sb	-2.622822000	0.275891000	0.000000000
C	0.277949000	0.889526000	4.125940000
C	0.124430000	0.028214000	5.196720000
H	-2.392743000	2.273111000	2.299993000
C	1.485424000	1.668699000	3.718762000
H	1.748121000	1.515589000	2.657255000
H	1.319017000	2.752314000	3.844275000
H	2.364212000	1.396900000	4.317703000
C	1.191573000	-0.473399000	6.118553000
H	1.294672000	-1.569846000	6.054748000
H	2.170977000	-0.034915000	5.885478000
H	0.960560000	-0.239886000	7.170991000
C	-1.037914000	1.022515000	3.456422000
C	-1.996992000	0.249618000	4.296342000
C	-1.276299000	-0.366799000	5.300265000
C	-1.437178000	2.343384000	2.839598000
H	-1.549065000	3.105578000	3.630431000
H	-0.682371000	2.702901000	2.125430000



C	-3.470329000	0.219371000	4.043143000
H	-3.704747000	-0.012659000	2.989362000
H	-3.936187000	1.196548000	4.258700000
H	-3.973702000	-0.532414000	4.665844000
C	-1.785871000	-1.322843000	6.333686000
H	-1.280237000	-2.300493000	6.262580000
H	-2.865063000	-1.498035000	6.231057000
H	-1.604353000	-0.948254000	7.354812000
C	3.377950000	-0.646880000	1.184236000
C	4.369348000	0.203658000	0.729759000
H	1.432829000	-2.733672000	-0.888040000
C	3.094733000	-1.096691000	2.580210000
H	2.029235000	-0.998039000	2.848548000
H	3.350690000	-2.162480000	2.711189000
H	3.674332000	-0.524813000	3.316533000
C	5.300754000	1.035402000	1.554990000
H	5.170312000	2.110989000	1.347567000
H	5.137608000	0.883177000	2.630340000
H	6.356002000	0.799067000	1.339355000
C	2.646351000	-1.164378000	0.000000000
C	3.377950000	-0.646880000	-1.184236000
C	4.369348000	0.203658000	-0.729759000
C	2.056776000	-2.555504000	0.000000000
H	2.864743000	-3.307919000	0.000000000
H	1.432829000	-2.733672000	0.888040000
C	3.094733000	-1.096691000	-2.580210000
H	2.029235000	-0.998039000	-2.848548000
H	3.350690000	-2.162480000	-2.711189000
H	3.674332000	-0.524813000	-3.316533000
C	5.300754000	1.035402000	-1.554990000
H	5.170312000	2.110989000	-1.347567000
H	5.137608000	0.883177000	-2.630340000
H	6.356002000	0.799067000	-1.339355000
C	0.277949000	0.889526000	-4.125940000
C	0.124430000	0.028214000	-5.196720000
H	-2.392743000	2.273111000	-2.299993000
C	1.485424000	1.668699000	-3.718762000
H	1.748121000	1.515589000	-2.657255000
H	1.319017000	2.752314000	-3.844275000
H	2.364212000	1.396900000	-4.317703000
C	1.191573000	-0.473399000	-6.118553000
H	1.294672000	-1.569846000	-6.054748000
H	2.170977000	-0.034915000	-5.885478000
H	0.960560000	-0.239886000	-7.170991000
C	-1.037914000	1.022515000	-3.456422000
C	-1.996992000	0.249618000	-4.296342000
C	-1.276299000	-0.366799000	-5.300265000
C	-1.437178000	2.343384000	-2.839598000
H	-1.549065000	3.105578000	-3.630431000
H	-0.682371000	2.702901000	-2.125430000
C	-3.470329000	0.219371000	-4.043143000
H	-3.704747000	-0.012659000	-2.989362000
H	-3.936187000	1.196548000	-4.258700000
H	-3.973702000	-0.532414000	-4.665844000
C	-1.785871000	-1.322843000	-6.333686000
H	-1.280237000	-2.300493000	-6.262580000
H	-2.865063000	-1.498035000	-6.231057000
H	-1.604353000	-0.948254000	-7.354812000

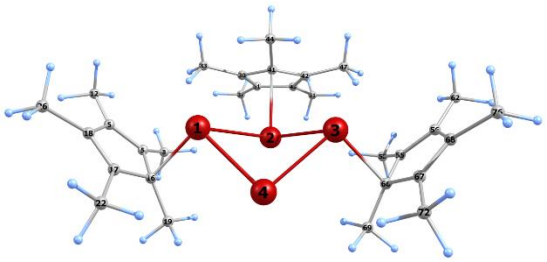
Zero-point vibrational energy 1740400.1 (Joules/Mol)
415.96560 (Kcal/Mol)

Zero-point correction=	0.662883 (Hartree/Particle)
Thermal correction to Energy=	0.710442
Thermal correction to Enthalpy=	0.711386
Thermal correction to Gibbs Free Energy=	0.577136
Sum of electronic and zero-point Energies=	-2129.849174
Sum of electronic and thermal Energies=	-2129.801616
Sum of electronic and thermal Enthalpies=	-2129.800672
Sum of electronic and thermal Free Energies=	-2129.934921

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	445.809	165.308	282.552
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	46.231
Rotational	0.889	2.981	38.184
Vibrational	444.032	159.347	196.760

Table S10: Carteisan coordinates of the optimised geometry of $Cp^*_3Sb_4^+$.

Sb	0.747280000	-0.647899000	-2.064117000
Sb	-0.989391000	0.718631000	0.000000000
Sb	0.747280000	-0.647899000	2.064117000
Sb	2.112649000	0.639550000	0.000000000
C	-0.182070000	0.808351000	-4.297987000
C	-0.061325000	-0.237331000	-5.214891000
H	2.516293000	2.274775000	-2.575821000
C	-1.367369000	1.667955000	-4.009617000
H	-1.590907000	1.704075000	-2.928717000
H	-1.189593000	2.707647000	-4.330430000
H	-2.266709000	1.309759000	-4.525290000
C	-1.145207000	-0.824617000	-6.060535000
H	-1.305848000	-1.889000000	-5.822649000
H	-2.100574000	-0.302082000	-5.926583000
H	-0.884843000	-0.778227000	-7.129727000
C	1.122555000	0.988788000	-3.639365000
C	2.047251000	0.019691000	-4.291400000
C	1.299739000	-0.725176000	-5.208185000
C	1.578263000	2.336371000	-3.144606000
H	1.755180000	3.003774000	-4.004489000
H	0.825158000	2.811612000	-2.501031000
C	3.523431000	0.000588000	-4.059266000
H	3.776239000	0.151740000	-2.997294000
H	4.016123000	0.811605000	-4.621961000
H	3.976034000	-0.946592000	-4.379954000
C	1.782893000	-1.859468000	-6.052885000
H	1.159873000	-2.757443000	-5.915714000
H	2.821475000	-2.128940000	-5.823690000
H	1.733829000	-1.602998000	-7.123700000
C	-3.170232000	-0.672439000	-1.189291000
C	-4.122357000	0.221114000	-0.736175000
H	-1.199218000	-2.738740000	0.891267000
C	-2.934953000	-1.143649000	-2.583553000
H	-1.891166000	-0.998586000	-2.909328000
H	-3.143228000	-2.222427000	-2.674638000
H	-3.581787000	-0.619451000	-3.297729000
C	-5.055476000	1.051575000	-1.553429000
H	-4.959030000	2.120821000	-1.305175000
H	-4.872906000	0.937604000	-2.629238000
H	-6.105943000	0.779682000	-1.359572000
C	-2.456018000	-1.209221000	0.000000000
C	-3.170232000	-0.672439000	1.189291000
C	-4.122357000	0.221114000	0.736175000
C	-1.820099000	-2.570534000	0.000000000
H	-2.610596000	-3.341244000	0.000000000
H	-1.199218000	-2.738740000	-0.891267000
C	-2.934953000	-1.143649000	2.583553000
H	-1.891166000	-0.998586000	2.909328000
H	-3.143228000	-2.222427000	2.674638000
H	-3.581787000	-0.619451000	3.297729000
C	-5.055476000	1.051575000	1.553429000
H	-4.959030000	2.120821000	1.305175000
H	-4.872906000	0.937604000	2.629238000
H	-6.105943000	0.779682000	1.359572000
C	-0.182070000	0.808351000	4.297987000
C	-0.061325000	-0.237331000	5.214891000
H	2.516293000	2.274775000	2.575821000
C	-1.367369000	1.667955000	4.009617000
H	-1.590907000	1.704075000	2.928717000
H	-1.189593000	2.707647000	4.330430000
H	-2.266709000	1.309759000	4.525290000
C	-1.145207000	-0.824617000	6.060535000
H	-1.305848000	-1.889000000	5.822649000
H	-2.100574000	-0.302082000	5.926583000
H	-0.884843000	-0.778227000	7.129727000
C	1.122555000	0.988788000	3.639365000
C	2.047251000	0.019691000	4.291400000
C	1.299739000	-0.725176000	5.208185000
C	1.578263000	2.336371000	3.144606000
H	1.755180000	3.003774000	4.004489000
H	0.825158000	2.811612000	2.501031000
C	3.523431000	0.000588000	4.059266000
H	3.776239000	0.151740000	2.997294000
H	4.016123000	0.811605000	4.621961000
H	3.976034000	-0.946592000	4.379954000
C	1.782893000	-1.859468000	6.052885000
H	1.159873000	-2.757443000	5.915714000
H	2.821475000	-2.128940000	5.823690000
H	1.733829000	-1.602998000	7.123700000



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Zero-point vibrational energy    1738426.9 (Joules/Mol)
                                  415.49400 (Kcal/Mol)
 Zero-point correction=                           0.662132 (Hartree/Particle)
 Thermal correction to Energy=                    0.709829
 Thermal correction to Enthalpy=                  0.710773
 Thermal correction to Gibbs Free Energy=         0.574721
 Sum of electronic and zero-point Energies=          -2129.651100
 Sum of electronic and thermal Energies=             -2129.603403
 Sum of electronic and thermal Enthalpies=           -2129.602459
 Sum of electronic and thermal Free Energies=        -2129.738511

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 445.424            164.279           286.345
 Electronic              0.000              0.000             0.000
 Translational           0.889              2.981            46.231
 Rotational              0.889              2.981            38.118
 Vibrational           443.647            158.317           201.996
```

Table S11: Carteisan coordinates of the optimised geometry of {Cp"Fe(CO)$_2$}$^\bullet$.

```
Fe      -0.047374000     -0.996173000     -0.366629000
O        0.865536000     -2.602806000      1.891595000
O       -2.333955000     -2.739696000     -0.880250000
C       -1.019311000      0.905070000     -0.161124000
C        0.202169000      0.886950000      0.568147000
C        1.311346000      0.641358000     -0.333268000
C        0.748066000      0.525972000     -1.641674000
C       -0.666768000      0.653195000     -1.542109000
C        0.526003000     -1.981702000      0.965705000
C       -1.408423000     -2.057414000     -0.692113000
C       -2.388469000      1.254207000      0.390522000
C       -2.615838000      0.574885000      1.752448000
C       -3.503732000      0.831951000     -0.579320000
C       -2.432736000      2.790282000      0.569433000
C        2.789903000      0.683379000      0.005037000
C        3.318099000      2.075020000     -0.415760000
C        3.553849000     -0.407794000     -0.765856000
C        3.022613000      0.495052000      1.512704000
H        0.294774000      1.021847000      1.641387000
H        1.294505000      0.305412000     -2.555397000
H       -1.364989000      0.581236000     -2.370941000
H       -3.596249000      0.864220000      2.160050000
H       -2.586097000     -0.518860000      1.651267000
H       -1.850115000      0.868718000      2.485007000
H       -3.498884000     -0.252905000     -0.751625000
H       -4.483684000      1.103852000     -0.159945000
H       -3.408452000      1.339501000     -1.550729000
H       -2.257538000      3.302906000     -0.388216000
H       -3.416649000      3.102485000      0.952028000
H       -1.663541000      3.125780000      1.280513000
H        3.192014000      2.234176000     -1.496738000
H        4.388522000      2.166544000     -0.175742000
H        2.777540000      2.875376000      0.111117000
H        3.192739000     -1.407634000     -0.484312000
H        3.434610000     -0.295505000     -1.853381000
H        4.629497000     -0.349246000     -0.540813000
H        4.100445000      0.530647000      1.729774000
H        2.638494000     -0.472718000      1.863213000
H        2.541525000      1.292215000      2.098419000
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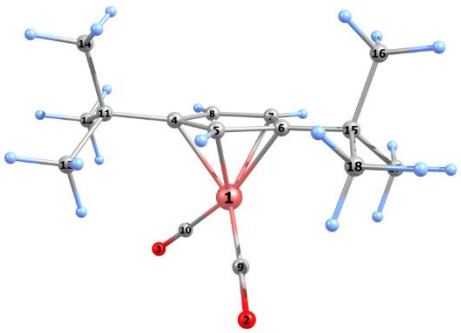

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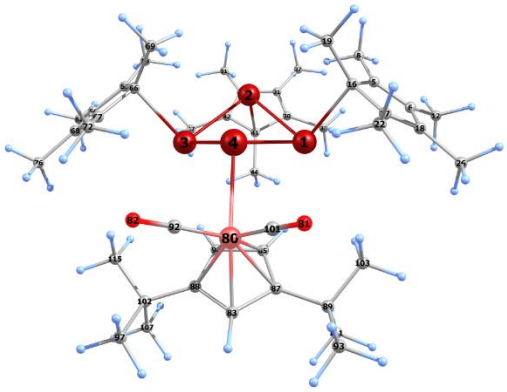
Zero-point vibrational energy     852080.9 (Joules/Mol)
                                  203.65222 (Kcal/Mol)
 Zero-point correction=                           0.324540 (Hartree/Particle)
 Thermal correction to Energy=                    0.345328
 Thermal correction to Enthalpy=                  0.346272
 Thermal correction to Gibbs Free Energy=         0.274783
 Sum of electronic and zero-point Energies=          -1997.614577
 Sum of electronic and thermal Energies=             -1997.593790
 Sum of electronic and thermal Enthalpies=           -1997.592845
 Sum of electronic and thermal Free Energies=        -1997.664335

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 216.697             78.800           150.461
 Electronic              0.000              0.000             1.377
 Translational           0.889              2.981            42.882
 Rotational              0.889              2.981            33.192
 Vibrational           214.919             72.838            73.010
```

Table S12: Carteisan coordinates of the optimised geometry of {Cp"Fe(CO)$_2$}Cp*$_3$Sb$_4$.

Sb	-0.491637000	-1.915958000	-0.035696000
Sb	-2.591536000	0.022387000	-0.278145000
Sb	-0.458068000	1.924110000	-0.035510000
Sb	1.101341000	-0.009457000	-1.464201000
C	-2.139954000	-4.051791000	-1.084375000
C	-1.566400000	-5.172313000	-0.513335000
H	-0.521168000	-1.932413000	-3.390839000
C	-3.578156000	-3.648976000	-1.112848000
H	-3.730074000	-2.603397000	-0.793377000
H	-3.990199000	-3.723171000	-2.134207000
H	-4.190963000	-4.285432000	-0.461065000
C	-2.228657000	-6.177696000	0.376482000
H	-1.750605000	-6.210862000	1.370123000
H	-3.292205000	-5.949820000	0.528177000
H	-2.159717000	-7.196295000	-0.040174000
C	-1.069455000	-3.303746000	-1.794518000
C	0.148979000	-4.154573000	-1.687946000
C	-0.156967000	-5.234517000	-0.884078000
C	-1.375314000	-2.545233000	-3.067409000
H	-1.614145000	-3.252206000	-3.880792000
H	-2.237090000	-1.873738000	-2.939743000
C	1.423794000	-3.844227000	-2.399739000
H	1.685724000	-2.776693000	-2.321305000
H	1.345701000	-4.062220000	-3.479181000
H	2.270401000	-4.422738000	-2.007039000
C	0.777339000	-6.302252000	-0.406000000
H	0.838918000	-6.319733000	0.695415000
H	1.793985000	-6.155259000	-0.794450000
H	0.442423000	-7.305385000	-0.718331000
C	-4.107833000	-1.150025000	1.911901000
C	-5.391998000	-0.684226000	1.723517000
H	-1.366352000	0.902190000	2.751065000
C	-3.646387000	-2.552778000	2.138491000
H	-2.788310000	-2.825622000	1.500922000
H	-3.314287000	-2.696972000	3.181670000
H	-4.446268000	-3.279346000	1.943637000
C	-6.633372000	-1.496064000	1.520367000
H	-7.099798000	-1.279148000	0.544560000
H	-6.425720000	-2.573905000	1.556449000
H	-7.393275000	-1.275287000	2.288349000
C	-3.195932000	0.028333000	1.959215000
C	-4.088179000	1.221603000	1.910407000
C	-5.379870000	0.776910000	1.722498000
C	-2.005901000	0.019022000	2.897214000
H	-2.352576000	0.023311000	3.945456000
H	-1.382369000	-0.875834000	2.753121000
C	-3.603510000	2.616738000	2.135525000
H	-2.740128000	2.874136000	1.498709000
H	-3.270419000	2.756824000	3.178951000
H	-4.390793000	3.356395000	1.938598000
C	-6.607469000	1.609033000	1.517768000
H	-7.077519000	1.397807000	0.542456000
H	-6.381652000	2.683292000	1.551429000
H	-7.370902000	1.402805000	2.286294000
C	-2.071271000	4.087179000	-1.083448000
C	-1.480968000	5.197131000	-0.508723000
H	-0.481910000	1.947743000	-3.391773000
C	-3.515626000	3.707442000	-1.115688000
H	-3.685048000	2.664290000	-0.796955000
H	-3.923841000	3.788459000	-2.138061000
H	-4.119825000	4.353368000	-0.465207000
C	-2.129006000	6.211356000	0.381539000
H	-1.653972000	6.233874000	1.376921000
H	-3.196836000	6.001409000	0.528964000
H	-2.041168000	7.229660000	-0.032263000
C	-1.011585000	3.323735000	-1.793240000
C	0.220108000	4.154556000	-1.682309000
C	-0.069995000	5.237377000	-0.876357000
C	-1.327294000	2.572301000	-3.067870000
H	-1.555073000	3.284241000	-3.880079000
H	-2.198861000	1.913178000	-2.942223000
C	1.491147000	3.826356000	-2.392990000
H	1.729190000	2.752475000	-2.328893000
H	1.422859000	4.061684000	-3.469490000
H	2.348577000	4.380359000	-1.988505000
C	0.880893000	6.288312000	-0.393734000
H	0.940063000	6.302574000	0.707851000
H	1.895857000	6.124983000	-0.780076000
H	0.563778000	7.297591000	-0.704866000
Fe	3.339907000	-0.025236000	-0.055128000
O	4.287562000	-2.034123000	-1.931671000
O	4.311249000	1.965998000	-1.938401000
C	4.633031000	-0.049672000	1.618289000
H	5.715629000	-0.072123000	1.547723000
C	2.432793000	-0.716890000	1.743354000
H	1.538276000	-1.330365000	1.797632000
C	3.776206000	-1.202402000	1.677619000



C	3.824423000	1.136701000	1.674830000
C	4.185479000	-2.653901000	1.832162000
C	2.461883000	0.706806000	1.740969000
H	1.592986000	1.356414000	1.790457000
C	3.882602000	1.193810000	-1.178046000
C	5.600473000	-2.906040000	1.288120000
H	5.667060000	-2.692486000	0.213373000
H	5.874764000	-3.960163000	1.441714000
H	6.347618000	-2.290892000	1.811002000
C	5.706287000	2.771051000	1.259695000
H	6.437392000	2.122502000	1.764519000
H	6.024856000	3.812179000	1.416516000
H	5.745713000	2.563664000	0.182486000
C	3.867873000	-1.253883000	-1.174581000
C	4.292087000	2.570540000	1.826886000
C	3.181278000	-3.594531000	1.141844000
H	2.157570000	-3.452621000	1.516920000
H	3.461764000	-4.641540000	1.329380000
H	3.161252000	-3.436930000	0.056216000
C	4.317912000	2.850441000	3.350090000
H	3.316018000	2.734148000	3.788488000
H	4.660290000	3.879369000	3.538007000
H	5.000396000	2.159475000	3.866732000
C	4.174488000	-2.939836000	3.354341000
H	4.871542000	-2.275102000	3.885774000
H	4.477117000	-3.980812000	3.544110000
H	3.169674000	-2.789912000	3.775458000
C	3.312018000	3.551077000	1.157633000
H	3.261539000	3.394229000	0.072883000
H	3.638596000	4.585889000	1.338039000
H	2.292401000	3.450383000	1.556332000

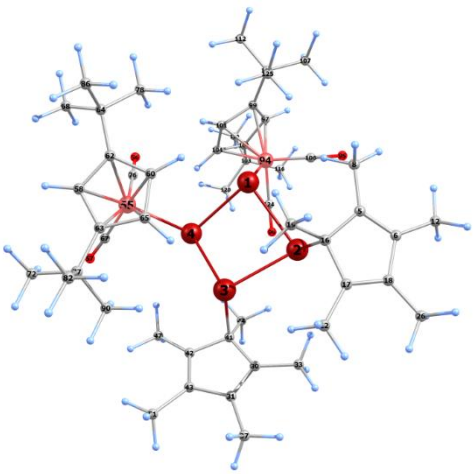
Zero-point vibrational energy 2599460.9 (Joules/Mol)
621.28607 (Kcal/Mol)

Zero-point correction=	0.990082 (Hartree/Particle)
Thermal correction to Energy=	1.059564
Thermal correction to Enthalpy=	1.060508
Thermal correction to Gibbs Free Energy=	0.882006
Sum of electronic and zero-point Energies=	-4127.543821
Sum of electronic and thermal Energies=	-4127.474339
Sum of electronic and thermal Enthalpies=	-4127.473395
Sum of electronic and thermal Free Energies=	-4127.651897

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	664.886	249.014	375.689
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	47.070
Rotational	0.889	2.981	39.876
Vibrational	663.109	243.052	288.744

Table S13: Carteisan coordinates of the optimised geometry of $\{Cp''Fe(CO)_2\}_2Cp^*_2Sb_4$.

Sb	-1.205267000	0.409754000	0.735589000
Sb	0.588940000	2.575429000	0.173065000
Sb	2.494018000	0.457801000	-0.193939000
Sb	0.285255000	-1.086435000	-1.177709000
C	-0.005026000	3.921153000	2.644184000
C	0.404703000	5.218687000	2.411664000
H	2.191790000	1.167166000	2.833396000
C	-1.331182000	3.434848000	3.130490000
H	-1.675542000	2.552029000	2.564529000
H	-1.281760000	3.122997000	4.188767000
H	-2.108641000	4.204588000	3.041441000
C	-0.435100000	6.457534000	2.448984000
H	-0.433054000	6.972674000	1.473722000
H	-1.479546000	6.233663000	2.703323000
H	-0.056802000	7.181950000	3.189561000
C	1.150874000	3.020391000	2.376133000
C	2.298311000	3.924077000	2.088085000
C	1.823068000	5.220602000	2.070796000
C	1.357618000	1.775941000	3.213704000
H	1.591364000	2.054650000	4.256060000
H	0.459030000	1.140583000	3.226954000
C	3.706899000	3.445879000	1.947761000
H	3.804560000	2.623396000	1.218689000
H	4.092055000	3.055986000	2.906356000
H	4.378403000	4.252776000	1.625485000
C	2.585130000	6.463822000	1.730859000
H	2.152298000	6.972366000	0.852932000
H	3.637694000	6.247762000	1.503516000
H	2.563558000	7.191905000	2.558790000
C	4.329833000	2.102679000	-1.695475000
C	5.547674000	1.479525000	-1.502843000
H	1.606194000	0.675929000	-3.423886000
C	3.978602000	3.543861000	-1.516119000
H	3.055131000	3.682272000	-0.927894000



H	3.801185000	4.033117000	-2.489563000
H	4.779590000	4.096888000	-1.007886000
C	6.782981000	2.068193000	-0.895383000
H	7.083134000	1.520778000	0.014186000
H	6.637877000	3.120384000	-0.616231000
H	7.639233000	2.020336000	-1.588632000
C	3.378068000	1.090649000	-2.229145000
C	4.187488000	-0.143718000	-2.438524000
C	5.459882000	0.097286000	-1.960960000
C	2.316868000	1.492638000	-3.231228000
H	2.790155000	1.764998000	-4.190731000
H	1.735058000	2.357996000	-2.883561000
C	3.652069000	-1.367524000	-3.104785000
H	2.704487000	-1.704658000	-2.649464000
H	3.427872000	-1.181086000	-4.169135000
H	4.360048000	-2.205375000	-3.055798000
C	6.593985000	-0.875314000	-1.864440000
H	6.904309000	-1.028289000	-0.816597000
H	6.324591000	-1.856482000	-2.277785000
H	7.484378000	-0.516495000	-2.406893000
Fe	0.426549000	-3.407198000	0.101462000
O	-2.193334000	-3.818877000	-1.091528000
O	1.680983000	-4.440985000	-2.312031000
C	1.041766000	-4.795299000	1.574399000
H	1.134016000	-5.862885000	1.403747000
C	0.180990000	-2.724786000	2.092286000
H	-0.494934000	-1.922682000	2.375669000
C	-0.136024000	-4.124403000	2.030376000
C	2.092043000	-3.828726000	1.380320000
C	-1.407535000	-4.774884000	2.538602000
C	1.539537000	-2.549474000	1.700822000
H	2.070259000	-1.602163000	1.665762000
C	1.194670000	-3.999782000	-1.349213000
C	-1.722349000	-6.072590000	1.776955000
H	-1.892203000	-5.879632000	0.709444000
H	-2.629074000	-6.538449000	2.190752000
H	-0.904398000	-6.801681000	1.868571000
C	3.739621000	-5.518437000	0.486945000
H	3.391442000	-6.302500000	1.175695000
H	4.807651000	-5.698117000	0.294878000
H	3.203273000	-5.628439000	-0.465100000
C	-1.148666000	-3.627896000	-0.603246000
C	3.551631000	-4.115408000	1.086113000
C	-2.606851000	-3.815978000	2.447534000
H	-2.416829000	-2.876149000	2.985817000
H	-3.494152000	-4.283930000	2.898822000
H	-2.847349000	-3.577644000	1.403499000
C	4.289771000	-4.045580000	2.445151000
H	4.204372000	-3.042186000	2.886984000
H	5.357912000	-4.271443000	2.305793000
H	3.873471000	-4.771734000	3.159230000
C	-1.150279000	-5.109463000	4.028578000
H	-0.300378000	-5.799218000	4.135215000
H	-2.039820000	-5.585396000	4.468587000
H	-0.925186000	-4.198804000	4.602918000
C	4.148789000	-3.063869000	0.137773000
H	3.660334000	-3.089708000	-0.844143000
H	5.222413000	-3.254311000	-0.007685000
H	4.043157000	-2.043597000	0.533618000
Fe	-3.259016000	0.967090000	-0.771807000
O	-3.464619000	3.603646000	0.440759000
O	-1.385975000	1.943756000	-2.772122000
C	-5.321845000	0.646701000	-1.024650000
H	-6.057155000	1.443157000	-1.083537000
C	-4.897389000	0.000014000	0.193422000
C	-4.622605000	0.086241000	-2.136088000
C	-3.914461000	-0.968293000	-0.186234000
H	-3.397359000	-1.648679000	0.483906000
C	-4.887845000	0.378036000	-3.600157000
C	-3.735175000	-0.914120000	-1.598883000
H	-3.037309000	-1.523950000	-2.163209000
C	-3.362024000	2.538220000	-0.019604000
C	-6.320325000	1.462998000	1.671168000
H	-5.695102000	2.346868000	1.483429000
H	-6.747400000	1.558957000	2.680307000
H	-7.156403000	1.469454000	0.956357000
C	-5.503127000	0.165101000	1.574098000
C	-6.442223000	-1.044711000	1.795071000
H	-7.216989000	-1.089322000	1.015348000
H	-6.940470000	-0.965960000	2.773485000
H	-5.878576000	-1.988878000	1.769649000
C	-5.050894000	1.888304000	-3.843514000
H	-5.852529000	2.314274000	-3.222780000
H	-5.310009000	2.072765000	-4.896888000
H	-4.121962000	2.427735000	-3.615285000
C	-3.761239000	-0.172357000	-4.489875000
H	-2.791411000	0.281729000	-4.247621000
H	-3.982608000	0.046027000	-5.544977000
H	-3.666763000	-1.263506000	-4.389879000
C	-2.116618000	1.539758000	-1.958426000
C	-4.419481000	0.168131000	2.664414000

H	-3.786256000	-0.729375000	2.612742000
H	-4.887390000	0.193804000	3.660196000
H	-3.764542000	1.044914000	2.566694000
C	-6.208732000	-0.342882000	-3.962547000
H	-6.130713000	-1.424017000	-3.774944000
H	-6.441690000	-0.193822000	-5.027862000
H	-7.047779000	0.047469000	-3.367906000

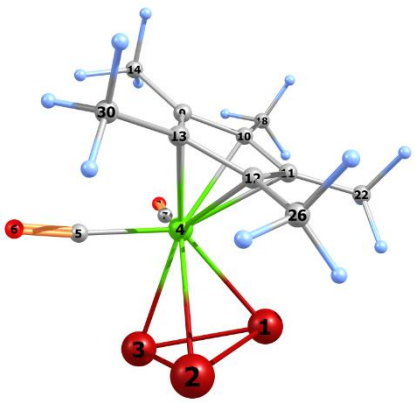
Zero-point vibrational energy 2878579.8 (Joules/Mol)
687.99709 (Kcal/Mol)

Zero-point correction=	1.096393 (Hartree/Particle)
Thermal correction to Energy=	1.175163
Thermal correction to Enthalpy=	1.176107
Thermal correction to Gibbs Free Energy=	0.976623
Sum of electronic and zero-point Energies=	-5735.541333
Sum of electronic and thermal Energies=	-5735.462563
Sum of electronic and thermal Enthalpies=	-5735.461619
Sum of electronic and thermal Free Energies=	-5735.661103

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	737.426	284.734	419.849
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	47.436
Rotational	0.889	2.981	40.591
Vibrational	735.648	278.772	331.822

Table S14: Carteisan coordinates of the optimised geometry of [Cp*Mo(CO)$_2$(η^3-Sb$_3$)].

Sb	-1.367746000	-0.962965000	-1.399457000
Sb	-1.369122000	-0.958097000	1.402180000
Sb	-2.048171000	1.338682000	-0.003132000
Mo	0.748703000	0.395959000	-0.000050000
C	0.648862000	1.804326000	1.379013000
O	0.723216000	2.622285000	2.208138000
C	0.649911000	1.803536000	-1.379946000
O	0.725327000	2.621166000	-2.209347000
C	3.028760000	0.482925000	0.000066000
C	2.636311000	-0.278060000	-1.164250000
C	2.023913000	-1.497937000	-0.717862000
C	2.023580000	-1.497240000	0.719450000
C	2.635937000	-0.277001000	1.164964000
C	3.852746000	1.733820000	-0.000403000
H	4.928378000	1.489508000	-0.000329000
H	3.648469000	2.349835000	0.884860000
H	3.648444000	2.349188000	-0.886111000
C	2.968598000	0.048931000	-2.587492000
H	2.184554000	-0.301699000	-3.271719000
H	3.914988000	-0.435986000	-2.878553000
H	3.084551000	1.128961000	-2.740114000
C	1.682860000	-2.678530000	-1.572483000
H	2.539414000	-3.374220000	-1.610234000
H	1.446012000	-2.380955000	-2.601573000
H	0.822328000	-3.233467000	-1.174282000
C	1.681214000	-2.676778000	1.575002000
H	1.445084000	-2.378099000	2.603937000
H	2.536751000	-3.373696000	1.613012000
H	0.819717000	-3.230719000	1.177476000
C	2.967816000	0.051263000	2.588013000
H	3.083990000	1.131413000	2.739627000
H	3.913981000	-0.433610000	2.879869000
H	2.183440000	-0.298493000	3.272307000



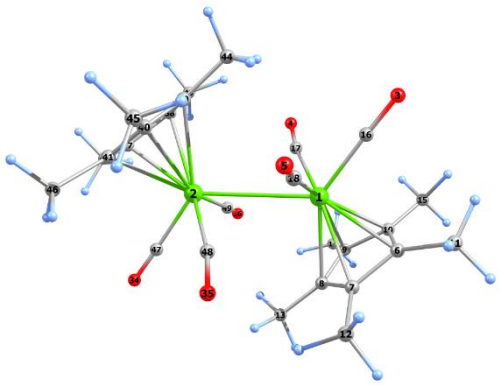
Zero-point vibrational energy 635606.4 (Joules/Mol)
151.91357 (Kcal/Mol)

Zero-point correction=	0.242090 (Hartree/Particle)
Thermal correction to Energy=	0.265804
Thermal correction to Enthalpy=	0.266748
Thermal correction to Gibbs Free Energy=	0.186622
Sum of electronic and zero-point Energies=	-1405.164130
Sum of electronic and thermal Energies=	-1405.140416
Sum of electronic and thermal Enthalpies=	-1405.139471
Sum of electronic and thermal Free Energies=	-1405.219598

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	166.795	81.390	168.640
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	45.305
Rotational	0.889	2.981	35.137
Vibrational	165.017	75.428	88.198

Table S15: Carteisan coordinates of the optimised geometry of $[Cp^*Mo(CO)_3]_2$.

Mo	1.578610000	0.400651000	0.000029000
Mo	-1.578578000	-0.400617000	0.000009000
O	2.650339000	3.324093000	0.003656000
O	0.431694000	1.606027000	-2.653509000
O	0.430044000	1.600065000	2.655518000
C	3.706430000	-0.189152000	0.722686000
C	2.852648000	-1.255577000	1.163913000
C	2.329228000	-1.914624000	-0.001388000
C	2.853329000	-1.253880000	-1.165409000
C	3.706852000	-0.188080000	-0.722118000
C	4.579040000	0.646241000	1.608830000
C	2.723390000	-1.717564000	2.582378000
C	1.515297000	-3.169248000	-0.002580000
C	2.724681000	-1.713633000	-2.584678000
C	4.580040000	0.648640000	-1.606444000
C	2.224510000	2.236818000	0.002253000
C	0.733661000	1.133759000	-1.626849000
C	0.732332000	1.130064000	1.627877000
H	4.823680000	1.611356000	1.146738000
H	5.528271000	0.123910000	1.815339000
H	4.094080000	0.849786000	2.572582000
H	1.825238000	-2.324408000	2.734248000
H	3.599129000	-2.329487000	2.857103000
H	2.675107000	-0.873852000	3.283372000
H	0.874989000	-3.241319000	0.884416000
H	2.183530000	-4.047399000	-0.003778000
H	0.874445000	-3.239322000	-0.889346000
H	2.676975000	-0.868784000	-3.284339000
H	1.826412000	-2.319960000	-2.737941000
H	3.600378000	-2.325370000	-2.859937000
H	4.095780000	0.853522000	-2.570264000
H	4.824257000	1.613112000	-1.142787000
H	5.529473000	0.126692000	-1.813009000
O	-2.650031000	-3.324159000	-0.003617000
O	-0.431620000	-1.605692000	2.653689000
O	-0.430085000	-1.599561000	-2.655700000
C	-3.706306000	0.189089000	-0.722956000
C	-2.852552000	1.255687000	-1.163824000
C	-2.329414000	1.914576000	0.001694000
C	-2.853679000	1.253569000	1.165493000
C	-3.707018000	0.187768000	0.721844000
C	-4.578651000	-0.646234000	-1.609427000
C	-2.723100000	1.717952000	-2.582182000
C	-1.515562000	3.169251000	0.003238000
C	-2.725193000	1.713035000	2.584865000
C	-4.580312000	-0.649196000	1.605837000
C	-2.224214000	-2.236878000	-0.002285000
C	-0.733644000	-1.133546000	1.626992000
C	-0.732299000	-1.129714000	-1.627973000
H	-4.823222000	-1.611489000	-1.147592000
H	-5.527926000	-0.123998000	-1.815976000
H	-4.093500000	-0.849489000	-2.573144000
H	-1.825236000	2.325318000	-2.733666000
H	-3.599089000	2.329439000	-2.857081000
H	-2.674129000	0.874388000	-3.283305000
H	-0.874763000	3.241303000	-0.883407000
H	-2.183848000	4.047363000	0.003998000
H	-0.875218000	3.239428000	0.890361000
H	-2.678482000	0.868029000	3.284404000
H	-1.826456000	2.318561000	2.738555000
H	-3.600471000	2.325477000	2.859889000
H	-4.096225000	-0.854243000	2.569708000
H	-4.824367000	-1.613591000	1.141935000
H	-5.529822000	-0.127358000	1.812322000



Zero-point vibrational energy	1302053.4 (Joules/Mol)	
	311.19823 (Kcal/Mol)	
Zero-point correction=		0.495926 (Hartree/Particle)
Thermal correction to Energy=		0.536455
Thermal correction to Enthalpy=		0.537399
Thermal correction to Gibbs Free Energy=		0.422814
Sum of electronic and zero-point Energies=		-1595.518909
Sum of electronic and thermal Energies=		-1595.478380
Sum of electronic and thermal Enthalpies=		-1595.477436
Sum of electronic and thermal Free Energies=		-1595.592021

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	336.630	145.708	241.165
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	45.223
Rotational	0.889	2.981	36.455
Vibrational	334.853	139.746	159.487

Table S16: Carteisan coordinates of the optimised geometry of CO.

```
O          0.000000000      0.000000000      0.487264000
C          0.000000000      0.000000000     -0.649685000


Zero-point vibrational energy      13136.4 (Joules/Mol)
                                    3.13968 (Kcal/Mol)
 Zero-point correction=                          0.005003 (Hartree/Particle)
 Thermal correction to Energy=                   0.007364
 Thermal correction to Enthalpy=                 0.008308
 Thermal correction to Gibbs Free Energy=       -0.014133
 Sum of electronic and zero-point Energies=          -113.220397
 Sum of electronic and thermal Energies=             -113.218037
 Sum of electronic and thermal Enthalpies=           -113.217092
 Sum of electronic and thermal Free Energies=        -113.239534

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   4.621             4.974            47.232
 Electronic              0.000             0.000             0.000
 Translational           0.889             2.981            35.923
 Rotational              0.592             1.987            11.309
 Vibrational             3.140             0.006             0.001
```

Table S17: Thermodynamic parameters of selected reactions calculated at the D3(BJ)-TPSSh/defSVP level of theory.

Reaction	E^0 ($kJ \cdot mol^{-1}$)	ΔH^0 ($kJ \cdot mol^{-1}$)	ΔG^0_{298} ($kJ \cdot mol^{-1}$)	ΔG^0_{393} ($kJ \cdot mol^{-1}$)	ΔS^0 ($J \cdot mol^{-1} \cdot K^{-1}$)
$Cp^*_4Sb_4 = Cp^*_3Sb_4^{\bullet} + Cp^{*\bullet}$	156.6	159.1	100.1	81.3	197.9
$Cp^*_4Sb_4 = Cp^*_3Sb_4^{+} + Cp^{*-}$	576.1	578.6	514.7	494.3	214.5
$Cp^*_4Sb_4 + \{Cp''Fe(CO)_2\}^{\bullet} = \{Cp''Fe(CO)_2\}Cp^*_3Sb_4 + Cp^{*\bullet}$	−50.6	−50.6	−38.1	−34.1	−42.1
$\{Cp''Fe(CO)_2\}Cp^*_3Sb_4 + \{Cp''Fe(CO)_2\}^{\bullet} = \{Cp''Fe(CO)_2\}_2Cp^*_2Sb_4 + Cp^{*\bullet}$	−54.4	−54.4	−54.3	−54.3	−0.1
$Cp^*_4Sb_4 + \{Cp''Fe(CO)_2\}^{\bullet} = \{Cp''Fe(CO)_2\}_4Sb_4 + 4\ Cp^{*\bullet}$	−201.4	−201.4	−175.4	−167.2	−87.3
$Cp^*_4Sb_4 + [Cp^*Mo(CO)_3]^{-} = \{Cp^*Mo(CO)_3\}Cp^*_3Sb_4 + Cp^{*-}$	48.8	48.8	69.5	76.1	−69.5
$\{Cp^*Mo(CO)_3\}_3Sb_3 = \{Cp^*Mo(CO)_2\}Sb_3 + [Cp^*Mo(CO)_3]_2 + CO$	149.4	154.3	59.4	29.2	318.4

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