Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information of the manuscript entitled:

Transfer of Polyantimony units

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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. The X-band EPR measurements were carried out on a MiniScope MS400 devige (Magnettech GmbH) equipped with rectangular TE102 resonator at a frequency of 9.5 GHz. The compounds were dissolved in a glove box unter argon and placed in tip-sealed Pasteur pipetts. For each sample a spectrum at at room temperature and at 77 K were performed. Elemental analysis were 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 (EI MS) device and a Joel AccuTOF GCX spectrometer were used. [$FeBr_2$·dme], [$NiBr_2$·dme],[1] $KSb(SiMe_3)_2$[2] and [Cp''$_2$$ZrCl_2$][3] were prepared according to literature procedures.

Preparation of NaCp''':[4]

A solution of Cp'''H (19.5 mL, 77.7 mmol) in 40 mL THF is added dropwise to a suspension of $NaNH_2$ (3.03 g, 77.7 mmol) in 100 mL THF. The mixture is refluxed for 20 h, resulting in a white suspension of NaCp'''. After decanting the supernatant THF solution, the white solid is washed with *n*-hexane and dried in vacuo. Yield: 18.7 g (72.9 mmol, 94%).

Preparation of [Cp'''NiBr]$_2$:[5]

A solution of NaCp''' (1.2 g, 4.7 mmol) in DME is added to a suspension of [$NiBr_2$·dme] (1.5 g, 4.9 mmol) in DME at -30°C. The solution is stirred for 2 h at -30 °C and further 2 h at room temperature. After removing the solvent, the red residue is dissolved in *n*-hexane (20 mL) and filtered via canula. The solution is concentrated to approx. 10 mL and stored at -30 °C for crystallization. More product can be obtained by concentrating the mother liquid and further storage at -30°C. Overall yield: 756 mg (1.02 mmol, 43%).

Preparation of [Cp^{Bn}CoCl]$_2$:[6]

A solution of ^{n}BuLi in *n*-hexane (12.1 mL, c = 1.6 mol/L, 19.4 mmol) is added dropwise to a solution of Cp^{Bn}H (516 mg, 0.999 mmol) in THF at -30 °C. The resulting purple solution is stirred for 1 h at -30 °C and additionally for 1 h at room temperature. Then, the reaction mixture is added dropwise to a blue suspension of $CoCl_2$ (2.51 g, 19.4 mmol) in THF at -30 °C. The reaction mixture is stirred for 2 h at -30 °C and further 6 h at room temperature. Meanwhile, a dark brown solution is formed. The solvent is removed in vacuo, the brown residue extracted with warm toluene and the solution filtered via canula. The solution

is concentrated to approx. 10 mL and stored at -30 °C for crystallization. More product can be obtained by concentrating the mother liquid and further storage at -30 °C. Overall yield: 7.24 g (5.94 mmol, 61%).

Preparation of $[(Cp''Zr)_2(\mu,\eta^{1:1:1:1:1:1}\text{-}Sb_6)]$ (1):

All synthetic steps are carried out in the dark. A solution of $[Cp''_2ZrCl_2]$ (100 mg, 0.194 mmol) in THF is added to a solution of $KSb(SiMe_3)_2$ (122 mg, 0.399 mmol) in THF and stirred overnight. The colour changes to brown and a grey precipitate is formed. Subsequently, the solvent is removed *in vacuo*, the residue is dissolved in *n*-pentane and filtered over diatomaceous earth. Crystals suitable for single crystal X-ray structure analysis can be obtained by storing a concentrated solution in *n*-pentane or dichloromethane at -30 °C. **1** is highly air- and light-sensitive and decomposes rapidly. Crystalline yield: 19 mg (0.015 mmol, 21%).

1: **^{1}H NMR** (C_6D_6, 298 K): δ [ppm] = 1.41 (s, 36 H, $C(CH_3)_3$), 5.18 (d, 4 H, $C_5H_3{}^t\text{Bu}_2$), 8.02 (t, 2 H, $C_5H_3{}^t\text{Bu}_2$). **FD MS** (toluene): *m*/*z* (%): 1267.61 (M^+; 33); **Elemental analysis** (%): calculated for $[C_{26}H_{42}Zr_2Sb_6]$ (1259.56 g/mol): C, 24.64; H, 3.34; no satisfying elemental analysis could be obtained, even by using Sn capsules. This is caused by the air and light sensitivity of compound **1**.

Note: Compound **1** is highly light and air sensitive, especially in solution but also in the solid state. Although, it is possible to store it as a solid under inert atmosphere for a few days under rigorous exclusion of light, a partly decomposition is observed. In the presence of light, a fast decomposition occurs. This makes the handling and the use of larger quantities of **1** rather challenging. For this reason, we decided to prepare **1** only in small scale and to use freshly prepared in situ solutions of **1**.

Preparation of $[(Cp'''Ni)_4(\mu_3\text{-}Sb)_4]$/$[Cp'''_2Ni]$ (2/2'):

All synthetic steps are carried out in the dark. A solution of $KSb(SiMe_3)_2$ (525 mg, 1.71 mmol) in THF is added to a solution of $[Cp''_2ZrCl_2]$ (501 mg, 0.974 mmol) in THF and stirred overnight. A solution of $[Cp'''NiBr]_2$ (640 mg, 0.864 mmol) in THF is added to the red-brown solution of **1** and stirred for 3 d. Meanwhile, a grey suspension is formed. The solvent is removed *in vacuo* and subsequent column chromatographic workup (SiO_2, *n*-hexane, 18 x 3 cm) yield two fractions. With *n*-hexane a greenish brown fraction of **2/2'** can be obtained. The second fraction containing $[Cp''_2ZrCl_2]$ can be eluted with a mixture of *n*-hexane and toluene (3:1). Crystals of **2/2'** suitable for single crystal X-ray diffraction analysis can be obtained by layering a toluene solution with acetonitrile. Crystalline yield: **2/2'**: 59 mg (0.0309 mmol, 11%)

2/2': ^{1}H NMR (C_6D_6, 400 MHz, 300 K): δ [ppm] = 1.47 (s, 9 H, $C(CH_3)_3$), 1.60 (s, 18 H, $C(CH_3)_3$), 5.22 (s, 2 H, $C_5H_2t\text{Bu}_3$); **^{13}C{^{1}H} NMR** (C_6D_6, 100 MHz, 300K): δ [ppm] = 32.5 (s, $C_5H_2(C(CH_3)_3)$), 32.5 (s, $C_5H_2(C(CH_3)_3)$), 33.5 (s, $C_5H_2(C(CH_3)_3)$), 34.9 (s, $C_5H_2(C(CH_3)_3)$), 87.1 (s, $C_5H_2(C(CH_3)_3)$), 117.9 (s, $C_5H_2(C(CH_3)_3)$), 119.3 (s, $C_5H_2(C(CH_3)_3)$); **LIFDI MS** (toluene): m/z (%) = 1654.24 ($M^{+\cdot}$,100); **Elemental analysis** (%): calculated for $[C_{85}H_{145}Ni_{4.5}Sb_4]$ (1910.46 g/mol): C, 53.22; H, 7.62; no satisfying elemental

analysis could be obtained, even by using Sn capsules. This is caused by the air and light sensitivity of compound **2/2'**.

Preparation of $[(Cp'''Co)_4(\mu_3\text{-}Sb_4)]$ (3a):

All synthetic steps are carried out in the dark. A solution of $KSb(SiMe_3)_2$ (525 mg, 1.71 mmol) in THF is added to a solution of $[Cp''_2ZrCl_2]$ (500 mg, 0.972 mmol) in THF and stirred overnight. A solution of $[Cp'''CoCl]_2$ (562 mg, 0.859 mmol) in THF is added to the red-brown solution of **1** and stirred for 6 d. The solvent of the grey suspension is removed *in vacuo*. Subsequent column chromatographic workup (SiO_2, *n*-hexane, 3 x 10 cm) afford two fractions. Using toluene as solvent **3a** is eluted as dark green fraction followed by a brown fraction of $[Sb_2(SiMe_3)_4]$. Crystals of **3a** suitable for single crystal X-ray diffraction analysis can be obtained by storing a concentrated *n*-hexane solution at –30 °C. Crystalline yield: **3a**: 54 mg (0.033 mmol, 12%).

3a: ^{1}**H NMR** (C_6D_6, 400 MHz, 300 K): δ [ppm] = 1.53 (s, 9 H, C(C*H*$_3$)$_3$), 1.61 (s, 18 H, C(C*H*$_3$)$_3$); **EVANS NMR** (C_6D_6, 400 MHz, 300K): μ_{eff}: 2.34 μ_B, corresponding to 1.54 unpaired electrons. **LIFDI MS** (toluene): m/z (%) = 1654.24 ($M^{+\cdot}$;100); **Elemental analysis** (%): calculated for $[C_{68}H_{116}Co_4Sb_4 \cdot C_6H_{14}]$ (1738.37 g/mol): C, 51.00; H, 7.52; found: C, 51.15; H, 7,14 (*n*-hexane can also be detected in the ^{1}H NMR)

Preparation of $[(Cp^{Bn}Co)_4(\mu_3\text{-}Sb_4)]$ (3b) and $[(Cp^{Bn}Co)_3(\mu_3\text{-}Sb)_2]$ (4):

All synthetic steps are carried out in the dark. A solution of $KSb(SiMe_3)_2$ (675mg, 2.21 mmol) in THF is added to a solution of $[Cp''_2ZrCl_2]$ (569 mg, 1.11 mmol) in THF and stirred overnight. After addition of a solution of $[Cp^{Bn}CoCl]_2$ (1.19 g, 0.975 mmol) in THF, the reaction mixture is stirred for 3 d. The solvent is removed *in vacuo* and subsequent column chromatographic workup (SiO_2, *n*-hexane, 18 x 3 cm) afforded $[Cp''ZrCl_2]$ as first fraction. A brownish green fraction containing a mixture of **3b** and **4** can be obtained with dichloromethane. Crystals of **3** suitable for single crystal X-ray diffraction analysis can be obtained by layering a toluene solution with acetonitrile and isolate the crystals after a few hours. Overall yield (**3b**+**4**): 320 mg (59%).

NMR spectroscopic investigations revealed a ratio of 4:3b of approximately 2:1. This is in good agreement with the found values of the elemental analysis of the solid ([2·**4**/1·**3b**] calc.: C, 71.49; H, 5.25; found: C, 71.83; H, 5.33).

3b: ^{1}**H NMR** (CD_2Cl_2, 400 MHz, 300 K): δ [ppm] = 4.21 (s, 40 H, $CH_2\{C_6H_5\}$), 6.68 (d, ^{3}J(H,H) = 7.5 Hz, 40 H, $CH_2\{C_6H_5\}$), 6.81-6.91 (m, 60 H, $CH_2\{C_6H_5\}$); ^{13}**C{^{1}H} NMR** (CD_2Cl_2, 100 MHz, 300 K): δ [ppm] = 36.4 (s, $C_5(CH_2\{C_6H_5\})_5$), 99.8 (s, $C_5(CH_2\{C_6H_5\})_5$), 126.0 (s, $C_5(CH_2\{C_6H_5\})_5$), 128.1 (s,

$C_5(CH_2\{C_6H_5\})_5$), 129.6 (s, $C_5(CH_2\{C_6H_5\})_5$), 140.0 (s, $C_5(CH_2\{C_6H_5\})_5$); **FD MS** (toluene): m/z (%) = 2785.26 (M^+).

4: **^{1}H NMR** (CD_2Cl_2, 400 MHz, 300 K): δ [ppm] = 4.20 (s, 30 H, $CH_2\{C_6H_5\}$), 6.55 (d, ^{3}J(H,H) = 7.4 Hz, 30 H, $CH_2\{C_6H_5\}$), 6.82 (m, 30 H, $CH_2\{C_6H_5\}$), 6.90 (m, 15 H, $CH_2\{C_6H_5\}$); **^{13}C{^{1}H} NMR** (CD_2Cl_2, 100 MHz, 300 K): δ [ppm] = 37.1 (s, $C_5(CH_2\{C_6H_5\})_5$), 96.3 (s, $C_5(CH_2\{C_6H_5\})_5$), 126.0 (s, $C_5(CH_2\{C_6H_5\})_5$), 128.1 (s, $C_5(CH_2\{C_6H_5\})_5$), 129.3 (s, $C_5(CH_2\{C_6H_5\})_5$), 140.5 (s, $C_5(CH_2\{C_6H_5\})_5$); **FD MS** (toluene): m/z (%) = 1966.45 (M^+).

Preparation of $[(Cp'''Fe)_3(\mu_3\text{-}Sb)_2]$ (5) and $[(Cp'''Fe)_3(\mu_3, \eta^{4:4:4}\text{-}Sb_6)]$ (6):

A solution of NaCp''' (495 mg, 1.93 mmol) in DME is added to a suspension of $FeBr_2$·dme (591 mg, 1.94 mmol) in DME at -30 °C. The colour changes immidiatly to green. After 2 h of stirring, the solvent is removed *in vacuo* and the green oily residue is extracted with *n*-hexane. The reaction mixture is filtered via canula, all volatiles are removed in vacuo and the orange solid is dissolved in THF.

All further synthetic steps are carried out in der dark. A solution of $KSb(SiMe_3)_2$ (520 mg, 1.69 mmol) in THF is added to a solution of $[Cp''_2ZrCl_2]$ (501 mg, 0.974 mmol) in THF and stirred overnight. The prepared solution of $[Cp'''FeBr]_2$ is added to the red-brown solution of **1**. Immediately, a grey suspension is formed. After stirring for 4 d the solvent is removed *in vacuo*. Subsequent column chromatographic workup (SiO_2, *n*-hexane, 18 x 3 cm) afforded three fractions. With *n*-hexane an unknown pinkish fraction followed by a dark brown fraction of **5** can be obtained. A mixture of *n*-hexane/toluene (1:1) yield a light brown fraction of **6**. Crystals of **5** and **6** suitable for single crystal X-ray diffraction analysis can be obtained by layering a toluene solution with acetonitrile. Crystalline yield: **5**: 38 mg (34.3 µmol, 12%); **6**: 4 mg (2.51 µmol, 1%).

5: **^{1}H NMR** (C_6D_6, 298 K): δ [ppm] = -0.17 (s, 18H, $\omega_{½}$ = 160 Hz, $C(CH_3)_3$), 3.31 (s, 9H, $\omega_{½}$ = 70 Hz, $C(CH_3)_3$); **EVANS NMR** (C_6D_6, 400 MHz, 300K): μ_{eff}: 1.65 μ_B, corresponding to 0.93 electrons. **LIFDI MS** (toluene): m/z (%) = 1111.37 ($M^{+\cdot}$,100); **EPR** (toluene, 77 K): $g_x = g_y = 2.1770$, $g_z = 2.4434$, $g_{iso} = 2.2658$. **elemental analysis** (%): calculated for $[C_{51}H_{87}Fe_3Sb_2]$ (1109.29 g/mol): C, 55.12; H, 7.89; no satisfying elemental analysis could be obtained, even by using Sn capsules. This is caused by the air and light sensitivity of compound **5**.

6: **^{1}H NMR** (C_6D_6, 298 K): δ [ppm] = 0.37 (s, 18H, $\omega_{½}$ = 17 Hz, $C(CH_3)_3$), 0.81 (s, 9H, $\omega_{½}$ = 14 Hz, $C(CH_3)_3$); **LIFDI MS** (toluene): m/z (%) =1596.91 (M^+; 100); Due to the small amount of **6** no elemental analysis could be performed.

2. Crystallographic data

Crystals suitable for single crystal X-ray diffraction analyses were obtained as described above. Single crystal data were acquired using either a Gemini Ultra diffractometer (Rigaku Oxford Diffraction) equipped with an Atlas^{S2} CCD detector using Cu K_α radiation (**3a**, **6**), a GV50 diffractometer (Rigaku Oxford Diffraction) equipped with a Titan^{S2} CCD detector using Cu K_α radiation (**1**, **4**) or respectively Cu K_β radiation (**5**) or a SuperNova diffractometer (Rigaku Oxford Diffraction) equipped with an Atlas CCD detector using Cu K_α radiation (**2/2'**). Data collection and reduction were performed with the **CrysAlisPro** software package (version 1.171.38.43 (**1**, **2/2'**, **4**, **6**); 1.171.39.37b (**3a**); 1.171.40.14a (**5**)).[7] A numerical absorption correction based on gaussian integration over a multifaceted crystal model and an empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm was performed for the compounds (**1**, **4**, **5**).[7] An analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R. C. Clark & J. S. Reid[8] and an empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm was performed for the compounds (**2/2'**, **3a**, **6**). Using **Olex2**,[9] the structures were solved with **ShelXT**[10] and refined by full-matrix least-squares method against $|F|^2$ using **ShelXL**[11]. Hydrogen atoms were refined in calculated positions using the riding model. Using **Olex2**,[9] all pictures of the respective molecular structures were made.

CCDC reference number 2079755 (**1**), 2079756 (**2/2'**)), 2079757 (**3a**), 2079758 (**4**·C_7H_8), 2079759 (**5**) and 2079760 (**6**) contain the supplementary crystallographic data for **1**, **2/2'**, **3a**, **4**, **5** and **6**. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: + 44-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

[(Cp''Zr)$_2$(μ,η$^{1:1:1:1:1:1}$-Sb$_6$)] (1):

Compound **1** crystallizes by storing a concentrated *n*-pentane solution at -30 °C in form of orange plates in the triclinic space group $P\bar{1}$. The asymmetric unit contains half a molecule of **1**.

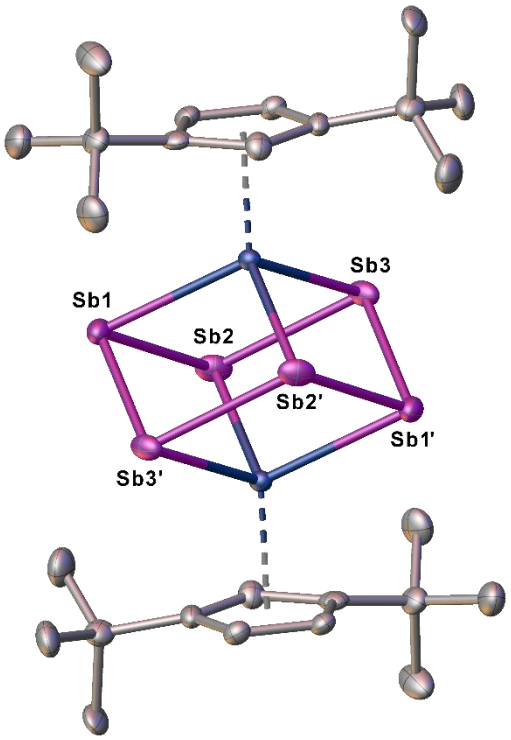


Figure S1: Molecular structure of **1** in the solid state (hydrogen atoms are omitted for clarity). Thermal ellipsoids are depicted at 50% probability level. Selected bond lengths [Å] and angles [°]: Sb1-Sb3$^{'}$ 2.8783(6), Sb1-Sb2 2.8381(7), Sb1-Zr1 2.8340(7), Sb3-Sb2 2.8414(7), Sb3-Zr1 2.8332(7), Sb2-Zr1$^{'}$ 2.8360(6), Zr1··Zr1$^{'}$ 3.6763(10); Sb2-Sb1-Sb3$^{'}$ 103.108(19), Zr1-Sb1-Sb3$^{'}$ 77.792(17), Zr1-Sb1-Sb2 77.841(19), Sb2-Sb3-Sb1$^{'}$ 101.303(17), Zr1-Sb3-Sb1$^{'}$ 75.986(18), Zr1-Sb3-Sb2 77.800(19), Sb1-Sb2-Sb3 102.015(19), Zr1$^{'}$-Sb2-Sb1 76.581(19), Zr1$^{'}$-Sb2-Sb3 78.364(17), Sb1-Zr1-Sb2$^{'}$ 102.54(2), Sb1-Zr1-Zr1$^{'}$ 63.846(17), Sb3-Zr1-Sb1 102.33(2), Sb3-Zr1-Sb2$^{'}$ 104.32(2), Sb3-Zr1-Zr1$^{'}$ 65.387(19), Sb2$^{'}$-Zr1-Zr1$^{'}$ 64.855(18

[(Cp'''Ni)$_4$(μ$_3$-Sb)$_4$]/[Cp'''$_2$Ni] (2/2'):

Compound **2/2'** crystallizes by layering a toluene solution with CH_3CN in form of violet blocks in the monoclinic space group *C*2/*c*. Compound **2** co-crystallizes with **2'** in the composition **(2)$_2$2'**. The asymmetric unit contains one molecule of **2** and half a molecule of **2'**.

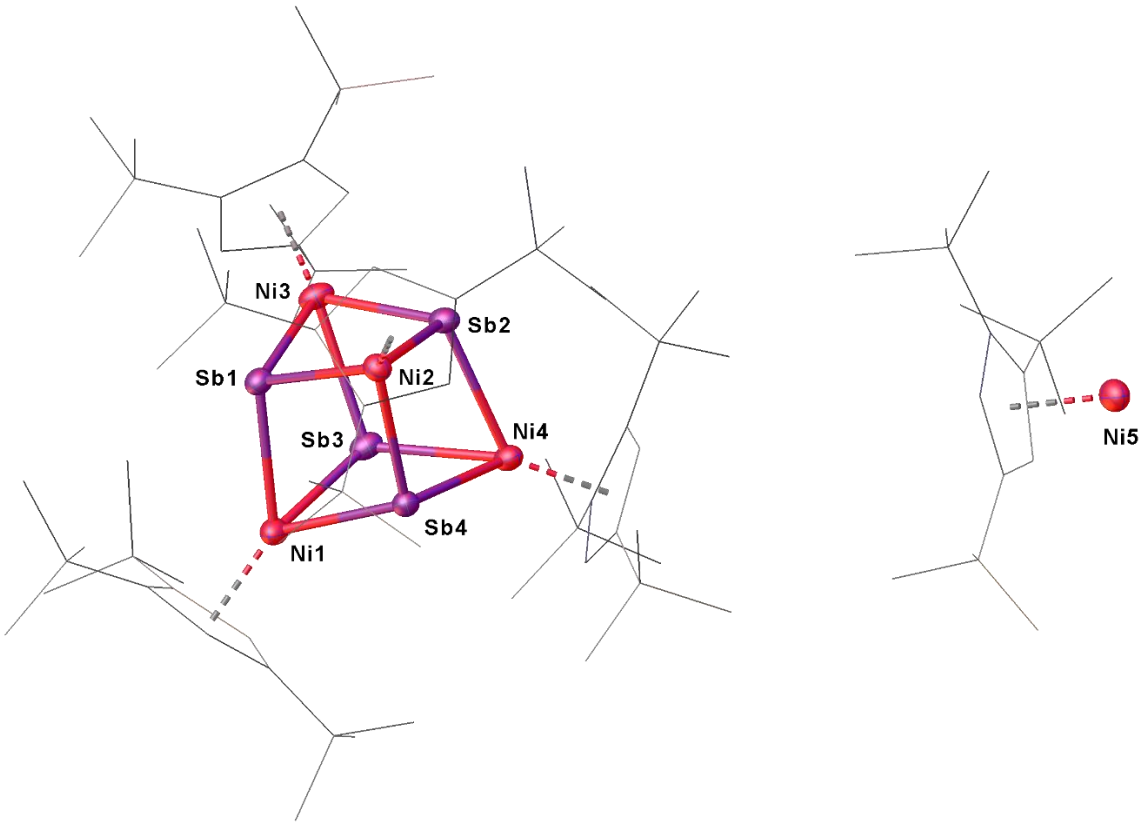


Figure S2: Molecular structure of **2/2'** in the solid state. Cp''' ligands are drawn in the wire frame model and hydrogen atoms are omitted for clarity. Thermal ellipsoids are depicted at 50% probability level. Selected bond lengths [Å] and angles [°]: Sb4-Ni2 2.5309(7) Sb4-Ni4 2.5201(7), Sb4-Ni1 2.5367(7), Sb1-Ni2 2.5565(7), Sb1-Ni1 2.5566(7), Sb1-Ni3 2.5565(7), Sb2-Ni2 2.5405(7), Sb2-Ni4 2.5548(7), Sb2-Ni3 2.5533(7), Sb3-Ni4 2.5541(7), Sb3-Ni1 2.5484(7), Sb3-Ni3 2.5602(7); Ni2-Sb4-Ni1 105.01(2), Ni4-Sb4-Sb1 101.537(17), Ni4-Sb4-Ni2 102.03(2), Ni4-Sb4-Ni1 102.19(2), Ni2-Sb1-Ni1 103.69(2), Ni2-Sb1-Ni3 101.59(2), Ni3-Sb1-Ni1 101.51(2), Ni2-Sb2-Sb1 52.071(15), Ni2-Sb2-Sb3 100.850(17), Ni2-Sb2-Ni4 100.81(2), Ni2-Sb2-Ni3 102.12(2), Ni3-Sb2-Ni4 105.17(2), Ni4-Sb3-Sb4 51.306(16), Ni4-Sb3-Ni3 104.99(2), Ni1-Sb3-Sb4 51.720(16), Ni1-Sb3-Ni4 100.93(2), Ni1-Sb3-Ni3 101.63(2), Sb4-Ni2-Sb1 74.726(18), Sb4-Ni2-Sb2 76.387(19), Sb2-Ni2-Sb1 76.313(19), Sb4-Ni1-Sb1 74.624(19), Sb4-Ni1-Sb3 76.225(19), Sb3-Ni1-Sb1 76.52(2), Sb1-Ni3-Sb3 76.32(2), Sb2-Ni3-Sb1 76.09(2), Sb2-Ni3-Sb3 73.980(19)

[(Cp'''Co)$_4$(μ$_3$-Sb)$_4$] (3a):

Compound **3a** crystallizes out of a *n*-hexane solution in form of dark violet blocks in the hexagonal space group *P*6$_2$22. The asymmetric unit contains a fourth of a molecule of **3a**. To describe the disorder of a tertbutyl-group of the Cp ligands the restrains SADI and SIMU were applied.

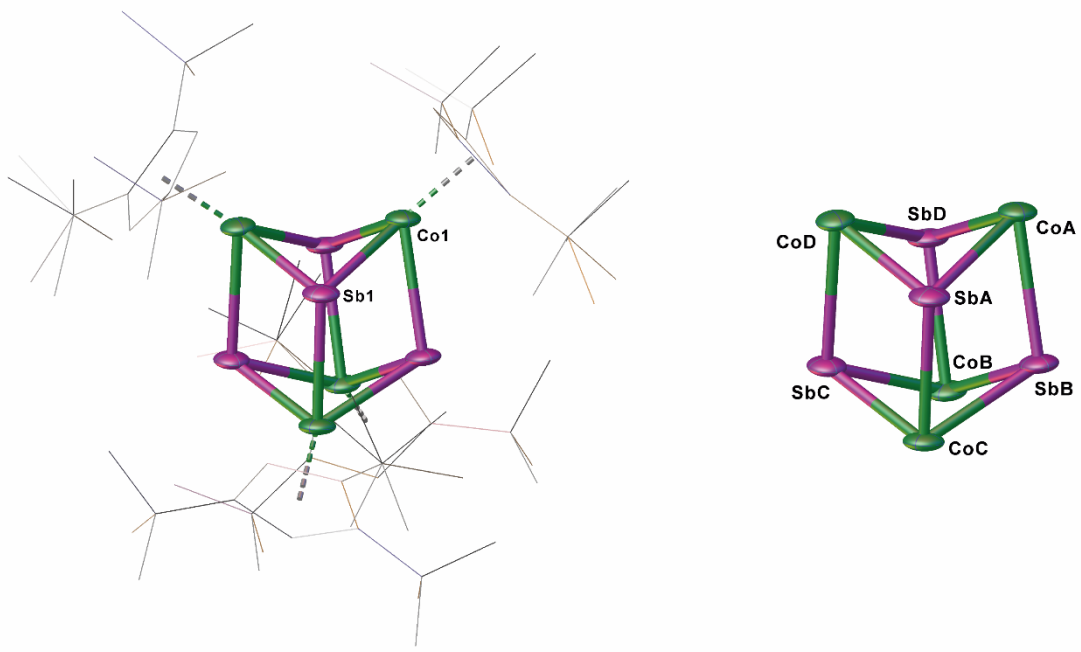


Figure S3: Molecular structure of **3a** in the solid state (left). Cp''' ligands are drawn in the wire frame model and hydrogen atoms are omitted for clarity. Thermal ellipsoids are depicted at 50% probability level. Closer few to the framework with a specific naming (right). Selected bond lengths [Å] and bond angles [°]: CoA-SbD 2.5023(19), CoA-SbA: 2.5528(19), CoA-SbB 2.6305(14); Selected angles CoA-SbA-CoD 74.80(7), SbA-CoD-SbD 90.58(6), SbA-CoA-SbB 69.23(4), CoC-SbA-CoA 108.67(5), SbC-CoD-SbA 76.41(5), CoC-SbA-CoD 103.57(5).

$[(Cp^{Bn}Co)_3(\mu_3\text{-}Sb)_2]$ (4):

Compound **4** crystallizes by layering a toluene solution with CH_3CN in form of brown blocks in the monoclinic space group $P2_1/n$. The asymmetric unit contains one molecule of **4** and one toluene molecule.

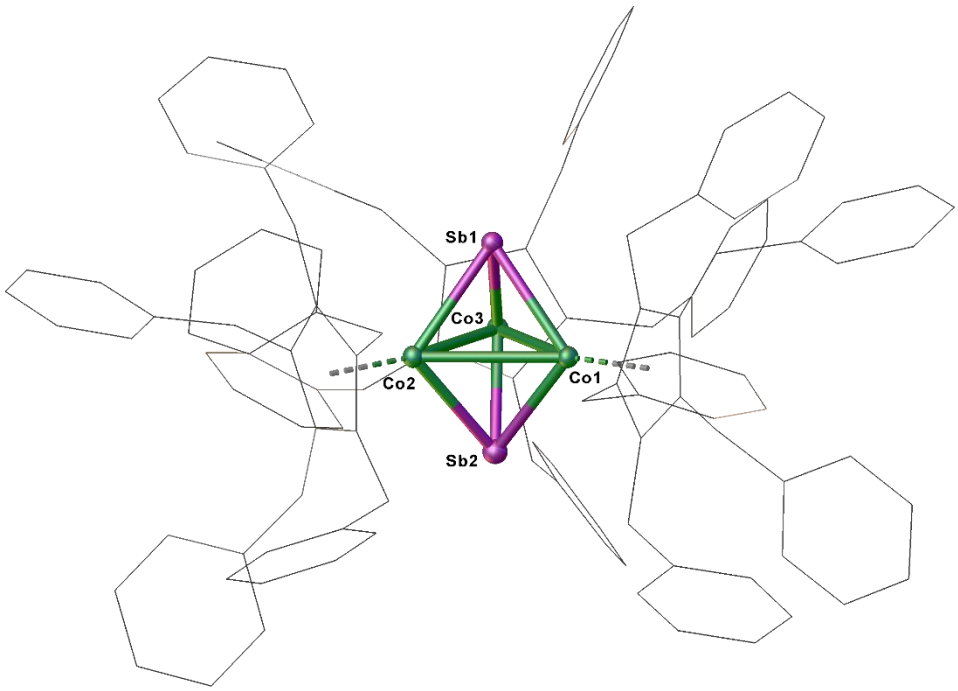


Figure S4 Molecular structure of **4** in the solid state. Cp^{Bn} ligands are drawn in the wire frame model and hydrogen atoms are omitted for clarity. Thermal ellipsoids are depicted at 50% probability level. Selected bond lengths [Å] and angles [°]: Sb1-Co2 2.4495(4), Sb1-Co3 2.4523(4), Sb1-Co1 2.4455(4), Sb2-Co2 2.4547(4), Sb2-Co3 2.4469(4), Sb2-Co1 2.4362(4), Co2-Co3 2.7304(5), Co2-Co1 2.7284(6), Co3-Co1 2.7331(5); Co1-Co2-Co3 60.090(14), Co2-Co1-Co3 59.992(14), Co2-Sb1-Co3 67.700(14), Co1-Sb1-Co2 67.748(14), Co1-Sb1-Co3 67.839(14), Co3-Sb2-Co2 67.704(14), Co1-Sb2-Co2 67.814(14), Co1-Sb2-Co3 68.072(14), Sb1-Co2-Sb2 99.543(15), Sb1-Co2-Co3 56.198(12), Sb1-Co2-Co1 56.057(12), Sb2-Co2-Co3 56.013(12), Sb2-Co2-Co1 55.771(13), Sb1-Co3-Co2 56.101(12), Sb1-Co3-Co1 55.963(12), Sb2-Co3-Sb1 99.680(14), Sb2-Co3-Co2 56.283(12), Sb2-Co3-Co1 55.777(12), Sb1-Co1-Co2 56.195(13), Sb1-Co1-Co3 56.198(12), Sb2-Co1-Sb1 100.168(15), Sb2-Co1-Co2 56.416(13), Sb2-Co1-Co3 56.151(12).

[(Cp'''Fe)$_3$(μ$_3$-Sb)$_2$] (5):

Compound **5** crystallizes by layering a toluene solution with CH_3CN in form of violet blocks in the triclinic space group $P\bar{1}$. The asymmetric unit contains two molecules of **5**.

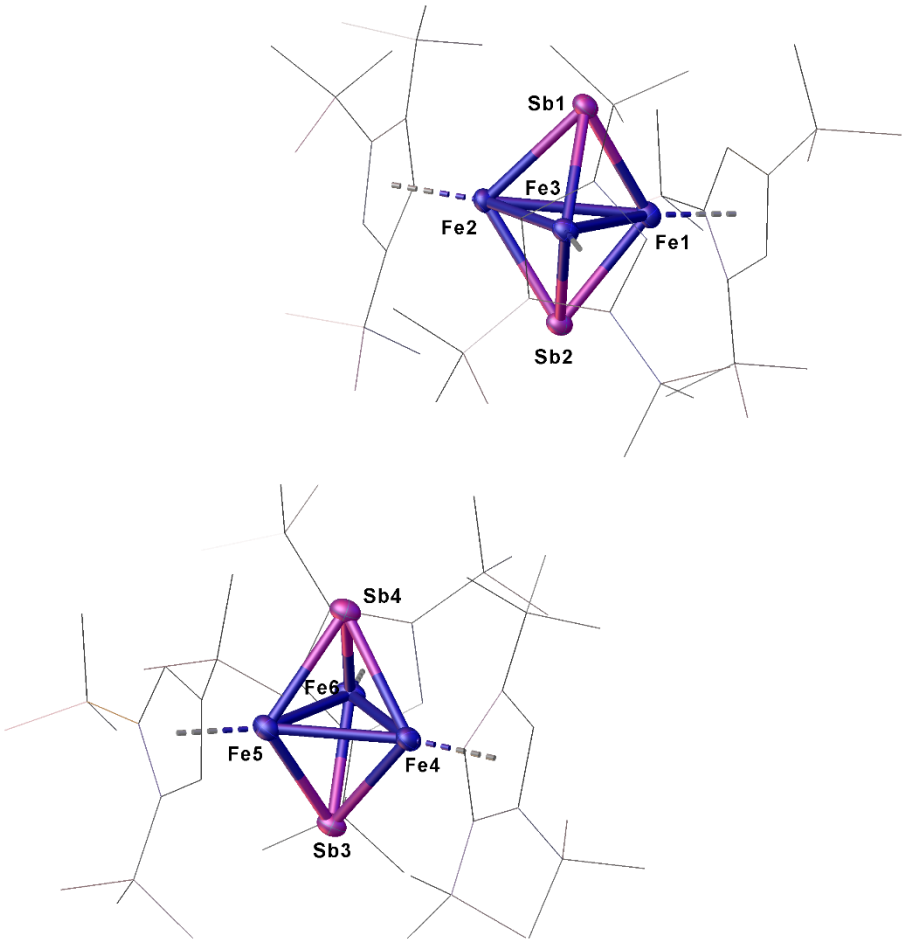


Figure S5: Molecular structure of **5** in the solid state. Cp''' ligands are drawn in the wire frame model and hydrogen atoms are omitted for clarity. Thermal ellipsoids are depicted at 50% probability level. Selected bond lengths [Å] and angles [°]: Sb1-Fe2 2.5007(5), Sb1-Fe3 2.5341(5), Sb1-Fe1 2.5211(5), Sb2-Fe2 2.5089(5), Sb2-Fe3 2.5169(5), Sb2-Fe1 2.5230(5), Sb3-Fe4 2.5144(5), Sb3-Fe6 2.5107(5), Sb3-Fe5 2.4920(5), Sb4-Fe4 2.5342(5), Sb4-Fe6 2.5037(5), Sb4-Fe5 2.4943(5), Fe2-Fe3 2.4489(6), Fe2-Fe1 2.9230(6), Fe3-Fe1 2.9161(7), Fe4-Fe6 2.8079(6), Fe4-Fe5 2.4895(6); Fe3-Fe1-Fe2 49.593(14), Fe3-Fe2-Fe1 65.057(17), Fe4-Fe6-Fe5 51.836(15), Fe5-Fe4-Fe6 65.690(18), Fe2-Sb1-Fe3 58.204(14), Fe2-Sb1-Fe1 71.191(15), Fe1-Sb1-Fe3 70.458(16), Fe2-Sb2-Fe3 58.323(15), Fe2-Sb2-Fe1 71.026(15), Fe3-Sb2-Fe1 70.705(16), Fe6-Sb3-Fe4 67.943(16), Fe5-Sb3-Fe4 59.637(16), Fe5-Sb3-Fe6 70.452(16), Fe6-Sb4-Fe4 67.743(16), Fe5-Sb4-Fe4 59.344(15), Fe5-Sb4-Fe6 70.528(16), Sb1-Fe2-Sb2 101.331(16), Sb1-Fe2-Fe1 54.730(13), Sb2-Fe2-Fe1 54.712(13), Fe3-Fe2-Sb1 61.583(15), Fe3-Fe2-Sb2 61.002(15), Sb1-Fe3-Fe1 54.562(13), Sb2-Fe3-Sb1 100.190(17), Sb2-Fe3-Fe1 54.746(14), Fe2-Fe3-Sb1 60.214(14), Fe2-Fe3-Sb2 60.675(15), Sb3-Fe4-Sb4 100.771(17), Sb3-Fe4-Fe6 55.967(14), Sb4-Fe4-Fe6 55.612(14), Fe5-Fe4-Sb3 59.735(15), Fe5-Fe4-Sb4 59.531(15), Sb3-Fe6-Fe4 56.090(13), Sb3-Fe6-Fe5 54.471(13), Sb4-Fe6-Sb3 101.718(17), Sb4-Fe6-Fe4 56.645(14), Sb4-Fe6-Fe5 54.584(14), Sb4-Fe5-Fe6 54.888(13), Fe4-Fe5-Sb3 60.628(16), Fe4-Fe5-Sb4 61.125(15), Sb1-Fe1-Sb2 100.379(17), Sb1-Fe1-Fe2 54.079(13), Sb1-Fe1-Fe3 54.981(14), Sb2-Fe1-Fe2 54.262(13), Sb2-Fe1-Fe3 54.550(13).

$[(Cp'''Fe)_3(\mu_3, \eta^{4:4:4}\text{-}Sb_6)]$ (6):

Compound **6** crystallizes by layering a toluene solution with CH_3CN in form of green needles in the triclinic space group $P\bar{1}$. The asymmetric unit contains one molecule of **6**.

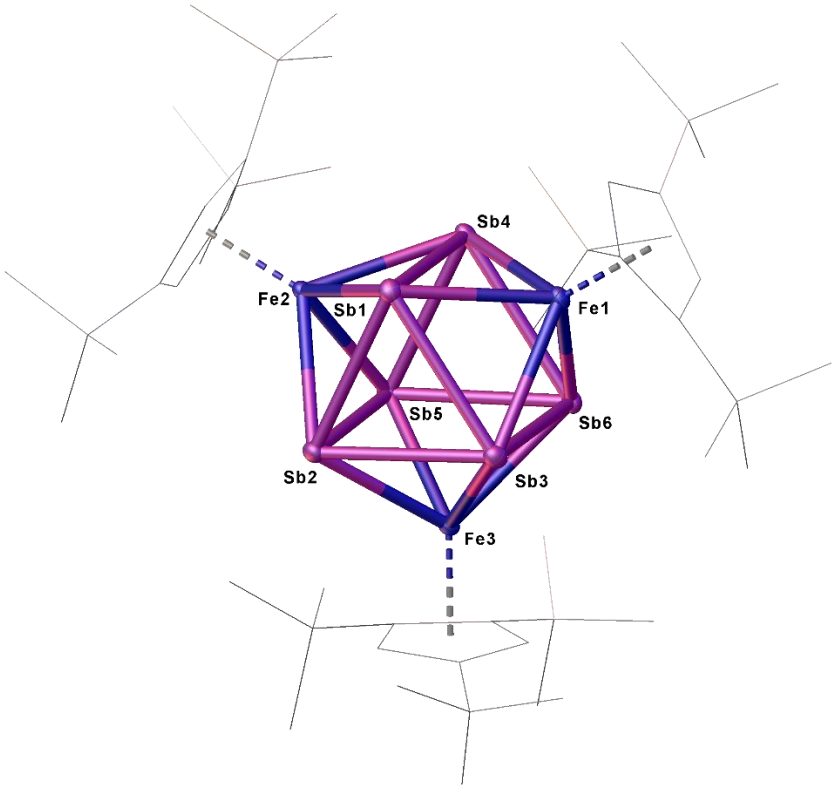


Figure S6: Molecular structure of **6** in the solid state. Cp''' ligands are drawn in the wire frame model and hydrogen atoms are omitted for clarity. Thermal ellipsoids are depicted at 50% probability level. Selected bond lengths [Å] and angles [°]: Sb6-Sb3 3.0286(3), Sb6-Sb4 2.9359(3), Sb6-Sb5 2.9367(3), Sb6-Fe3 2.6147(5), Sb6-Fe1 2.6287(5), Sb3-Sb2 2.9127(3), Sb3-Sb1 2.9236(3), Sb3-Fe3 2.6328(5), Sb3-Fe1 2.6055(5), Sb2-Sb1 2.9322(3), Sb2-Sb5 3.0648(3), Sb2-Fe2 2.6127(4), Sb2-Fe3 2.6030(5), Sb4-Sb1 3.0554(3), Sb4-Sb5 2.9033(3), Sb4-Fe2 2.6068(5), Sb4-Fe1 2.6099(5), Sb1-Fe2 2.6153(5), Sb1-Fe1 2.6231(5), Sb5-Fe2 2.6099(5), Sb5-Fe3 2.6146(5); Sb4-Sb6-Sb3 89.451(7), Sb4-Sb6-Sb5 59.257(6), Sb5-Sb6-Sb3 90.171(7), Sb2-Sb3-Sb6 90.530(7), Sb2-Sb3-Sb1 60.317(6), Sb1-Sb3-Sb6 91.076(7), Sb3-Sb2-Sb1 60.025(6), Sb3-Sb2-Sb5 89.913(7), Sb1-Sb2-Sb5 90.014(7), Sb6-Sb4-Sb1 90.312(7), Sb5-Sb4-Sb6 60.386(6), Sb5-Sb4-Sb1 90.744(7), Sb3-Sb1-Sb2 59.658(6), Sb3-Sb1-Sb4 89.161(7), Sb2-Sb1-Sb4 89.441(7), Sb6-Sb5-Sb2 89.372(7), Sb4-Sb5-Sb6 60.357(6), Sb4-Sb5-Sb2 89.796(7), Sb2-Fe2-Sb1 68.230(12), Sb4-Fe2-Sb2 107.681(16), Sb4-Fe2-Sb1 71.619(12), Sb4-Fe2-Sb5 67.634(12), Sb5-Fe2-Sb2 71.865(12), Sb5-Fe2-Sb1 108.552(16), Sb6-Fe3-Sb3 70.500(13), Sb6-Fe3-Sb5 68.332(12), Sb2-Fe3-Sb6 108.005(16), Sb2-Fe3-Sb3 67.599(13), Sb2-Fe3-Sb5 71.943(12), Sb5-Fe3-Sb3 107.246(16), Sb3-Fe1-Sb6 70.705(13), Sb3-Fe1-Sb4 107.198(16), Sb3-Fe1-Sb1 67.993(12), Sb4-Fe1-Sb6 68.171(12), Sb4-Fe1-Sb1 71.446(12), Sb1-Fe1-Sb6 108.000(16).

Table S1: Structure determination summary of complexes **1**, **2/2'** and **4**.

Compound	**1**	**2 · 0.5 (2')**	**4 · C_7H_8**
CCDC number	2079755	2079756	2079757
Formula	$C_{26}H_{42}Sb_6Zr_2$	$C_{85}H_{145}Ni_{4.5}Sb_4$	$C_{127}H_{113}Co_3Sb_2$
$D_{calc.}$/ g cm^{-3}	2.416	1.475	1.411
Formula Weight	1267.53	1918.20	2059.46
Colour	orange brown	violet	brown
Shape	plate	block	block
Size/mm^3	0.05×0.02×0.02	0.08×0.05×0.04	0.11×0.06×0.04
T/K	123.01(10)	122.97(13)	128.5(3)
Crystal System	triclinic	monoclinic	monoclinic
Space Group	$P\bar{1}$	*C*2/*c*	$P2_1/n$
a/Å	7.7940(6)	46.3369(13)	16.0588(2)
b/Å	10.9301(11)	19.0535(5)	19.7981(2)
c/Å	11.6145(7)	19.5836(6)	30.5084(4)
α/°	105.899(7)	90	90
β/°	96.387(6)	92.226(3)	91.1760(10)
γ/°	109.955(8)	90	90
V/Å^3	871.21(13)	17276.9(8)	9697.6(2)
Z	1	8	4
Z'	0.5	1	1
Wavelength/Å	1.54184	1.54184	1.54184
Radiation type	Cu K_α	Cu K_α	Cu K_α
μ/mm^{-1}	41.088	11.074	8.690
θ_{min}/°	4.063	3.350	2.661
θ_{max}/°	67.079	67.077	67.073
Measured Refl's.	6598	47158	34451
Ind't Refl's	3080	15359	17148
Refl's I≥2 σ(I)	2672	12426	15212
R_{int}	0.0465	0.0569	0.0252
Parameters	160	888	1190
Restraints	0	0	0
Largest Peak	1.624	0.754	0.443
Deepest Hole	-1.603	-0.795	-1.506
GooF	1.061	1.000	1.034
wR_2 (all data)	0.1036	0.0755	0.0771
wR_2	0.0981	0.0690	0.0742
R_1 (all data)	0.0422	0.0471	0.0370
R_1	0.0367	0.0326	0.0306

Table S2: Structure determination summary of complexes **3a**, **5** and **6**.

Compound	**3a**	**5**	**6**
CCDC number	2079758	2079759	2079760
Formula	$C_{68}H_{116}Co_4Sb_4$	$C_{51}H_{87}Fe_3Sb_2$	$C_{51}H_{87}Fe_3Sb_6$
$D_{calc.}$/ g cm^{-3}	1.543	1.422	1.862
Formula Weight	1656.32	1111.25	1598.25
Colour	dark violet	dark violet	dark green
Shape	block	block	needle
Size/mm^3	0.15×0.09×0.07	0.25×0.08×0.06	0.17×0.07×0.04
T/K	123(1)	123.0(2)	123(1)
Crystal System	hexagonal	triclinic	triclinic
Space Group	$P6_222$	$P\bar{1}$	$P\bar{1}$
Flack Parameter	-0.041(6)		
Hooft Parameter	-0.053(6)		
a/Å	13.0892(8)	12.3188(2)	10.4528(3)
b/Å	13.0892(8)	20.5303(4)	14.3499(4)
c/Å	36.0383(18)	20.5490(4)	20.1596(5)
α/°	90	87.329(2)	93.653(2)
β/°	90	89.4550(10)	101.854(2)
γ/°	120	88.3190(10)	104.007(2)
V/Å^3	5347.1(7)	5188.97(17)	2850.83(14)
Z	3	4	2
Z'	0.25	2	1
Wavelength/Å	1.54184	1.39222	1.54184
Radiation type	Cu K_α	Cu K_β	Cu K_α
μ/mm^{-1}	19.176	11.336	28.318
θ_{min}/°	3.679	3.733	3.687
θ_{max}/°	72.933	63.180	66.775
Measured Refl's.	19596	52581	29637
Ind't Refl's	3543	22736	10011
Refl's I≥2 *σ*(I)	3117	20653	9103
R_{int}	0.0545	0.0521	0.0277
Parameters	211	1063	568
Restraints	75	0	0
Largest Peak	0.722	1.114	0.955
Deepest Hole	-1.474	-1.346	-0.654
GooF	1.094	1.050	1.086
wR_2 (all data)	0.1153	0.1160	0.0495
wR_2	0.1063	0.1101	0.0482
R_1 (all data)	0.0572	0.0453	0.0263
R_1	0.0468	0.0411	0.0223

3. NMR investigations

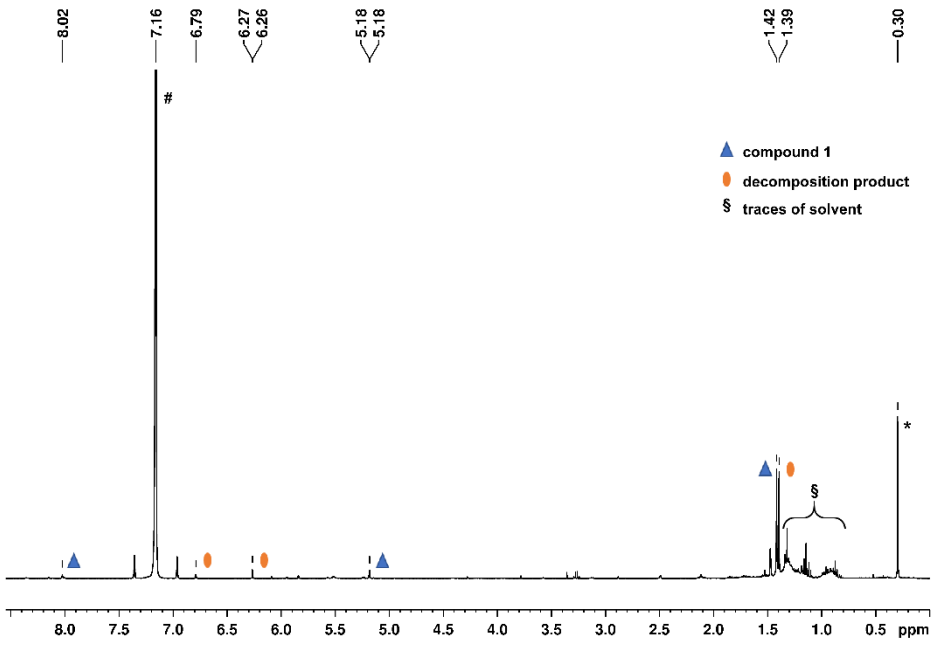


Figure S7: ^{1}H NMR spectrum of the reaction solution of **1** at 293 K in C_6D_6 (#). The signal marked with * is due to silicon grease.

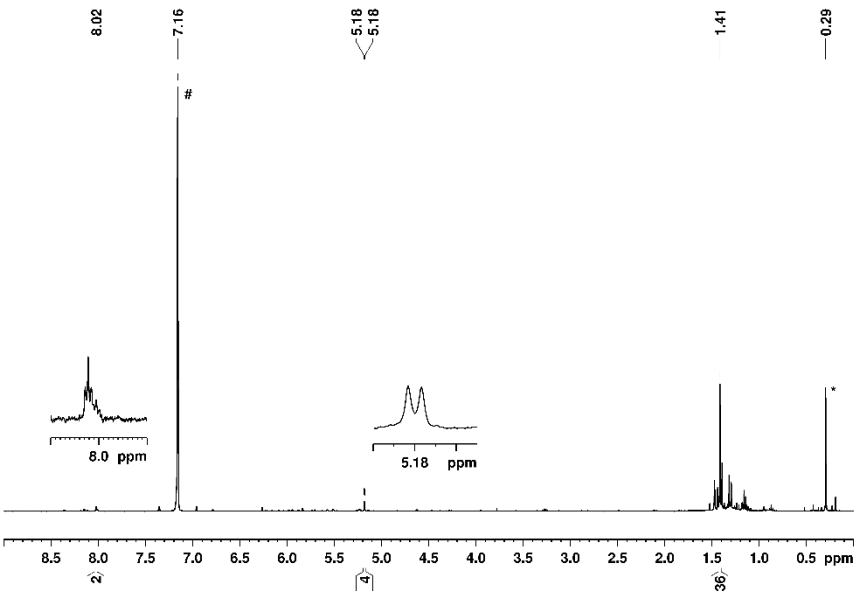


Figure S8: ^{1}H NMR spectrum of **1** at 293 K in C_6D_6 (#). The signal marked with * is due to silicon grease.

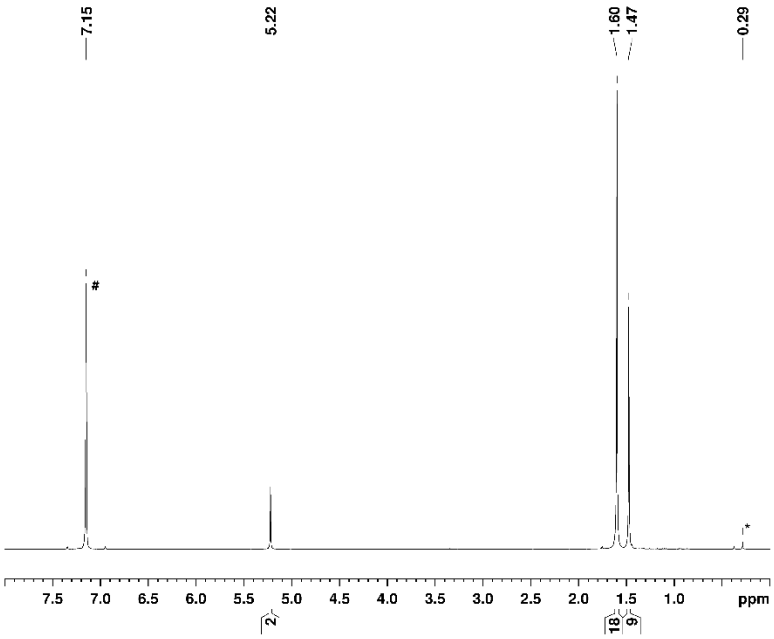


Figure S9: ^{1}H NMR spectrum of **2** at 293 K in C_6D_6 (#). The signal marked with * is due to silicon grease.

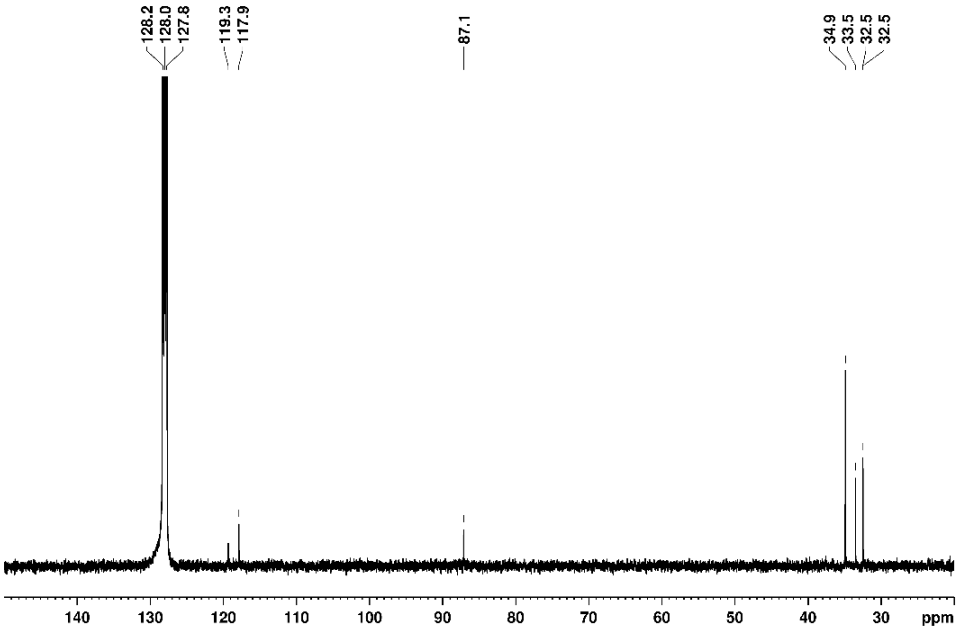


Figure S10: $^{13}C\{^{1}H\}$ NMR spectrum of **2** at 293 K in C_6D_6.

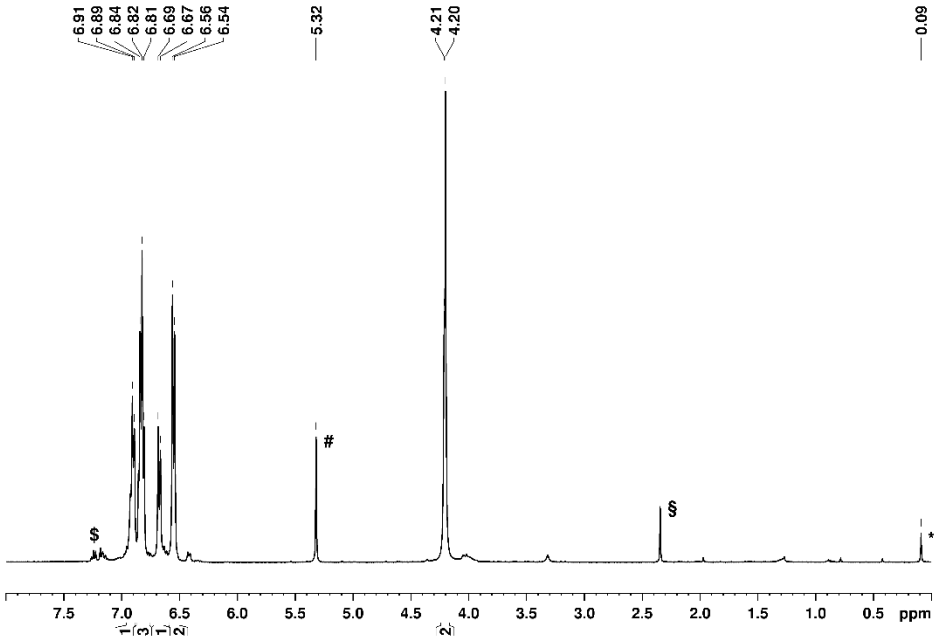


Figure S11: ^{1}H NMR spectrum of the mixture of **3b** and **4** at 273 K in CD_2Cl_2 (#). The signal marked with * is due to silicon grease, the signal marked with § is due to toluene.

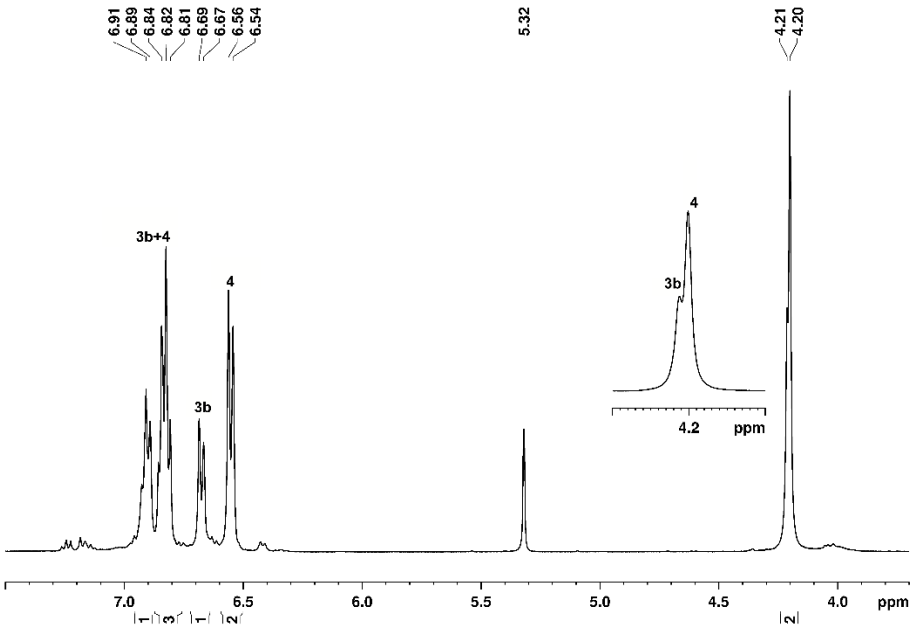


Figure S12: ^{1}H NMR spectrum of the mixture of **3b** and **4** at 273 K in CD_2Cl_2. The signals for the meta and para H atoms aof the phenyl rings of the Cp^{Bn} ligands are superimposed.

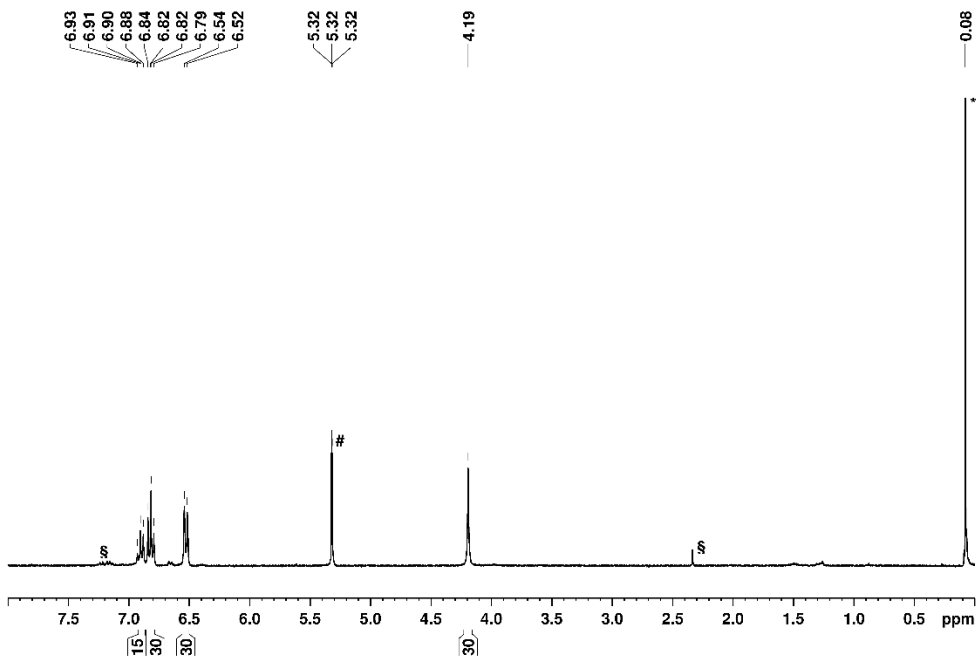


Figure S13: ^{1}H NMR spectrum of **4** at 273 K in CD_2Cl_2 (#). The signal marked with * is due to silicon grease, the signal marked with § is due to toluene.

4. EPR investigations

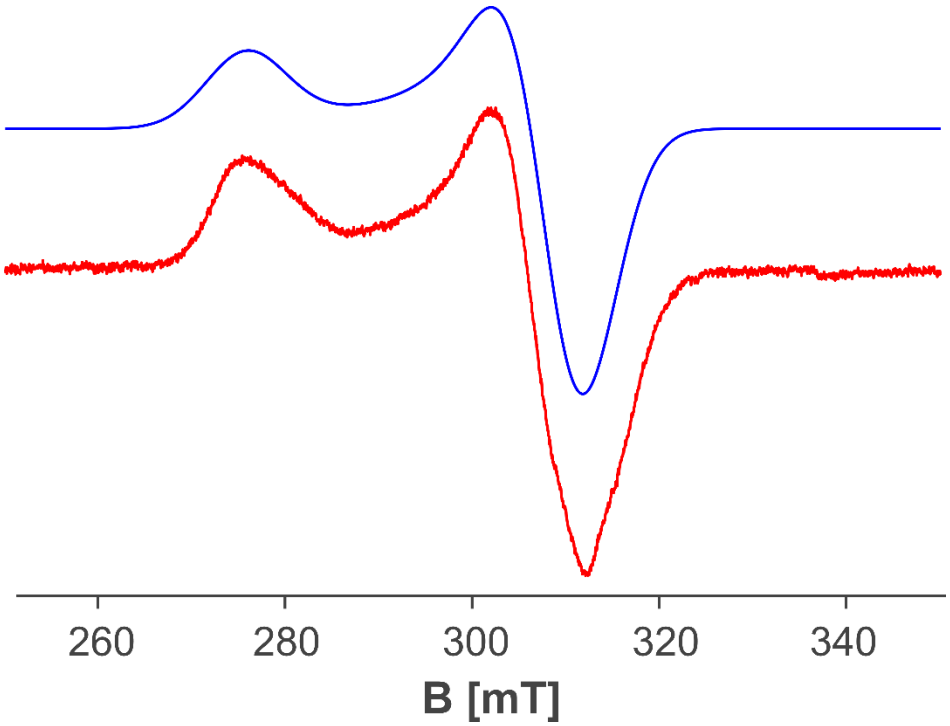


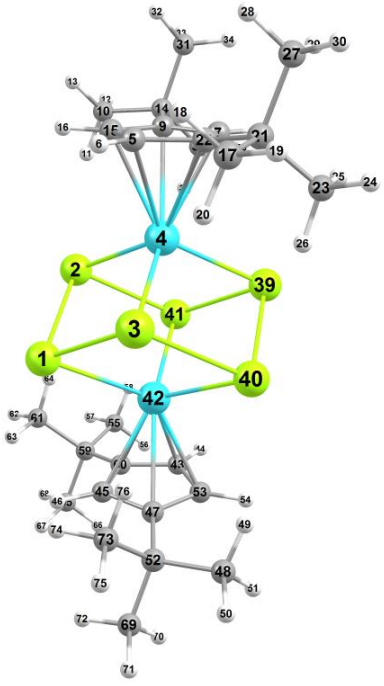
Figure S14: Red: X-band EPR spectrum of compound **5** in toluene at 77 K: $g_x = g_y = 2.1770$ and $g_z = 2.4434$ ($g_{iso} = 2.2658$). Blue: simulated spectrum using the EasySpin program.[12]

5. Computational details

The DFT calculations for [{Cp"Zr}$_2$Sb$_6$] have been performed with the TURBOMOLE program package[13] at the RI[14]-B3LYP[15]/def2-TZVP[16] level of theory. To speed up the geometry optimization the Multipole Accelerated Resolution-of-Identity (MARI-*J*)[17] approximation has been used. The dispersion effects have been incorporated by using the dispersion correction scheme introduced by *Grimme et al.*[18] together with the BJ-damping[19] as implemented in TURBOMOLE. The final energy was determined by single point calculations without using the RI formalism. The DFT calculations for all other compounds have been performed with the ORCA program.[20] The OPBE[21] and/or B3LYP functional together with the TZVP basis set have been used. During the geometry optimisation cycles the RIJCOSX[22] approximation has been used. For the compounds **3a** and **6** the geometry has been optimised at the OPBE/def2-SVP level.

Table S3: Selected Wiberg Bond Indices for [{Cp"Zr}$_2$Sb$_6$] (**1**) calculated at the B3LYP/def2-TZVP level of theory.

Bond	Wiberg Bond Index
Sb 2 - Sb 1	0.84
Sb 3 - Sb 1	0.84
Sb 3 - Sb 2	0.04
Zr 4 - Sb 1	0.22
Zr 4 - Sb 2	0.97
Zr 4 - Sb 3	0.96
Sb 39 - Zr 4	0.93
Sb 40 - Sb 3	0.83
Sb 40 - Zr 4	0.18
Sb 40 - Sb 39	0.84
Sb 41 - Sb 1	0.04
Sb 41 - Sb 2	0.83
Sb 41 - Zr 4	0.18
Sb 41 - Sb 39	0.84
Sb 41 - Sb 40	0.04
Zr 42 - Sb 1	0.93
Zr 42 - Sb 2	0.18
Zr 42 - Sb 3	0.18
Zr 42 - Zr 4	0.13
Zr 42 - Sb 39	0.22
Zr 42 - Sb 40	0.97
Zr 42 - Sb 41	0.96



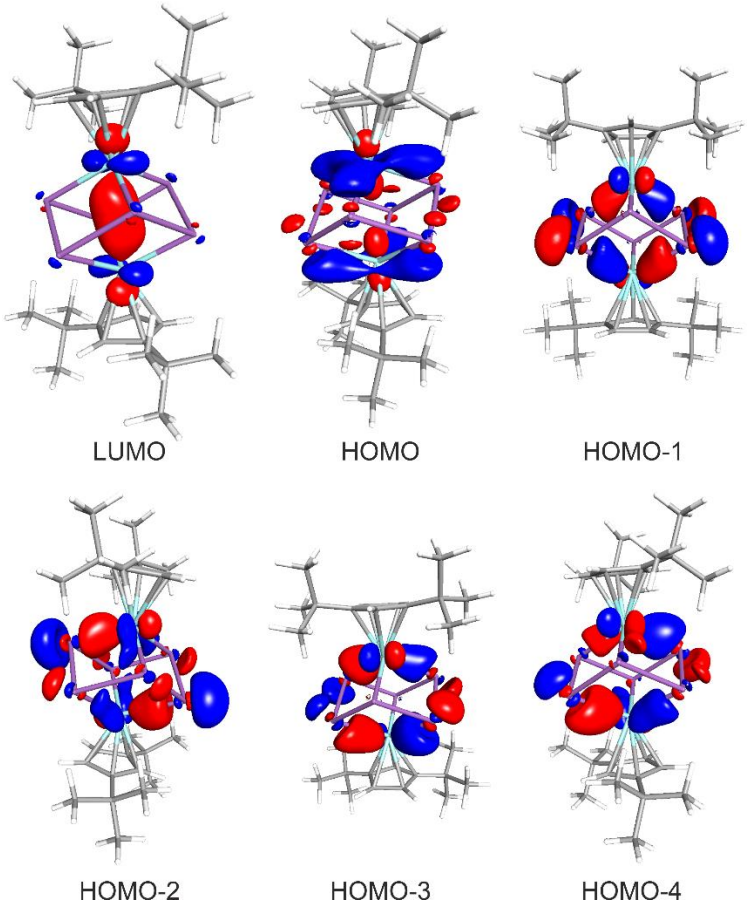


Figure S15: Selected frontier Molecular Orbitals of [(Cp"Zr)$_2$(Sb$_6$)] (**1**) calculated at the B3LYP/def2-TZVP level of theory.

Table S4: Relative energies (single point calculations) of different spin multiplicities of [(Cp'''Fe)$_3$(μ_3-Sb)$_2$] (geometry optimised at the OPBE/def2-TZVP level with spin multiplicity 2), calculated at the OPBE/TZVP and B3LYP/TZVP levels of theory.

		Relative energy (kJ·mol^{-1})		Total energy (hartree)	
Total spin, *S*	Spin multiplicity	OPBE	B3LYP	OPBE	B3LYP
1/2	2	0.0	0.0	-6268.99040020	-6266.63853261
3/2	4	53.5	43.8	-6268.97000908	-6266.62186285
5/2	6	48.8	82.2	-6268.97182153	-6266.60723195
7/2	8	83.6	213.1	-6268.95857707	-6266.55738429
9/2	10	178.2	393.0	-6268.92253529	-6266.48883142

Table S5: Relative energies of the different spin multiplicities of [(Cp'''Fe)$_3$(μ_3-Sb)$_2$]. The geometries have been optimised at the OPBE/TZVP level in different spin multiplicities. The B3LYP/TZVP energies have been calculated as single point calculations on the OPBE/TZVP optimised geometries in the corresponding spin states.

		Relative energy (kJ·mol^{-1})		Total energy (hartree)	
Total spin, *S*	Spin multiplicity	OPBE	B3LYP	OPBE	B3LYP
1/2	2	23.6	116.3	-6268.99040020	-6266.63853261
3/2	4	34.6	186.7	-6268.98620935	-6266.61171208
5/2	6	19.4	123.5	-6268.99199884	-6266.63577402
7/2	8	7.5	77.6	-6268.99653586	-6266.65325000
9/2	10	0.0	0.0	-6268.99938975	-6266.68281727

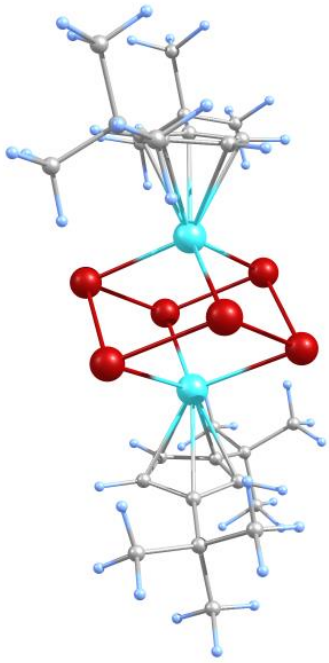
Table S6: Selected distances (Å) from X-ray diffractions as well as from the OPBE/def2-TZVP optimised geometries of [(Cp'''Fe)$_3$(μ_3-Sb)$_2$] in different spin states.

			Spin multiplicity				
Distance	Exp. molec. 1	Exp. molec. 2	2	4	6	8	10
Fe3-Fe5	2.490	2.4489	2.424	2.562	2.630	2.415	3.861
Fe3-Fe4	2.808	2.9161	2.991	2.545	3.536	4.157	3.957
Fe4-Fe5	2.886	2.923	3.022	2.989	2.724	4.203	4.031
Sb-Sb	3.889	3.875	3.806	3.824	3.597	2.800	2.777

Table S7: Total and relative energy of [(Cp'''Fe)$_3$(μ_3-Sb)$_2$] in different spin multiplicities calculated with the double hybrid functional B2PLYP[23]/TZVP, as single point calculations on the OPBE/TZVP optimised geometry in doublet spin sate.

Total spin, *S*	Spin multiplicity	Relative energy (kJ·mol^{-1})	total energy (Hartree)
1/2	2	89.7	-4850.99254455
3/2	4	97.4	-4850.98961574
5/2	6	64.1	-4851.00229258
7/2	8	0.0	-4851.02671511
9/2	10	71.3	-4850.99955754

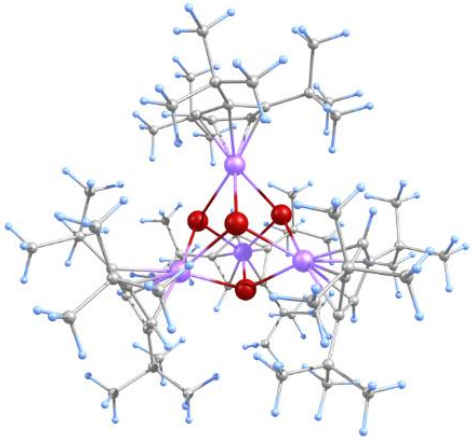
Table S8: Cartesian coordinates of the optimized geometry of [{Cp''Zr}$_2$Sb$_6$] in the RI-B3LYP-D3/def2-TZVP level of theory. Total energy = -2551.97736891102 hartree.



Sb	-2.0614117	-0.1917940	-1.6966749
Sb	-0.5399553	2.2269774	-1.3138853
Sb	-2.1374956	-1.1784190	1.0100256
Zr	-0.5803419	1.1798409	1.3313900
C	-2.3941009	2.0948161	2.8064733
H	-3.3842502	1.6807714	2.7223520
C	-0.2534703	2.4880714	3.4653400
H	0.6707279	2.4439081	4.0160622
C	-0.5674837	3.4544910	2.4735669
C	-0.2857735	5.4412041	0.9447577
H	-0.3228256	4.8294162	0.0429050
H	0.3413191	6.3091213	0.7337667
H	-1.2939355	5.8025964	1.1540244
C	0.2884141	4.6612389	2.1311305
C	-1.8950289	3.1908559	2.0573476
H	-2.4461806	3.7407248	1.3137233
C	-2.8135585	-0.1370835	4.7440155
H	-3.6969272	0.5035128	4.7431571
H	-2.8942855	-0.8132699	5.5968681
H	-2.8291016	-0.7419127	3.8369493
C	-1.5245279	0.6830219	4.8518264
C	-1.3838396	1.6610805	3.6987176
C	-0.3250667	-0.2699355	4.9396080
H	-0.4013977	-0.8856218	5.8383130
H	0.6190602	0.2745790	4.9871265
H	-0.2837958	-0.9362333	4.0784595
C	-1.5874051	1.5252578	6.1439726
H	-2.4196727	2.2304078	6.1078719
H	-0.6680518	2.0950983	6.2858746
H	-1.7241104	0.8759852	7.0117330
C	0.2791398	5.5806559	3.3709670
H	-0.7405982	5.8677078	3.6336473
H	0.8519146	6.4892034	3.1718608
H	0.7217590	5.0808576	4.2337235
C	1.7370494	4.2609313	1.8215230
H	2.1749038	3.6770157	2.6323980
H	2.3510336	5.1532518	1.6825400
H	1.7980168	3.6656984	0.9108995
Sb	2.0614466	0.1917865	1.6966841
Sb	0.5399949	-2.2269949	1.3138747
Sb	2.1375329	1.1784045	-1.0100226
Zr	0.5803743	-1.1798514	-1.3313985
C	2.3941118	-2.0948196	-2.8065063
H	3.3842623	-1.6807742	-2.7224042
C	0.2534731	-2.4880802	-3.4653382
H	-0.6707352	-2.4439168	-4.0160430
C	0.5675027	-3.4544972	-2.4735693
C	0.2857764	-5.4411795	-0.9447166
H	0.3228191	-4.8293807	-0.0428713
H	-0.3413178	-6.3090939	-0.7337196
H	1.2939397	-5.8025749	-1.1539703
C	-0.2884037	-4.6612304	-2.1311037
C	1.8950543	-3.1908595	-2.0573715
H	2.4462193	-3.7407275	-1.3137563
C	2.8135032	0.1371323	-4.7440156
H	3.6968994	-0.5034260	-4.7431105
H	2.8942315	0.8133002	-5.5968832
H	2.8289875	0.7419844	-3.8369634
C	1.5245097	-0.6830304	-4.8518492
C	1.3838365	-1.6610869	-3.6987351
C	0.3250131	0.2698777	-4.9396708
H	0.4013469	0.8855614	-5.8383776
H	-0.6190908	-0.2746735	-4.9872158
H	0.2836914	0.9361785	-4.0785266
C	1.5874493	-1.5252759	-6.1439851
H	2.4197482	-2.2303877	-6.1078586
H	0.6681246	-2.0951602	-6.2858996
H	1.7241436	-0.8760062	-7.0117494
C	-0.2791483	-5.5806691	-3.3709254
H	0.7405846	-5.8677442	-3.6336005
H	-0.8519409	-6.4892022	-3.1718050
H	-0.7217568	-5.0808751	-4.2336896
C	-1.7370328	-4.2608962	-1.8214985

H	-2.1748879	-3.6770061	-2.6323915
H	-2.3510232	-5.1532059	-1.6824773
H	-1.7979862	-3.6656284	-0.9108964

Table S9: Cartesian coordinates of the optimized geometry of [(Cp'''Ni)$_4$(μ_3-Sb)$_4$] (**2**) at the OPBE/TZVP level of theory, in the singlet spin state. Total energy: −9658.618384438727 hartree.



Sb	28.36612954452273	3.52737868439322	4.39895546683893
Sb	29.60967960299618	5.67302030865250	2.67298611473635
Sb	29.22993760496862	6.18240068148977	5.64900757841982
Sb	31.31567970738090	4.20314140295101	4.73470037815079
Ni	27.33617289745166	5.82202853080223	3.93331753809767
Ni	29.59506296476673	3.82237814021595	6.63061692978525
Ni	30.22844539539516	3.15539795160830	2.65678318804984
Ni	31.33113589161234	6.75971813491879	4.26409248657103
C	26.14534537630967	7.56548237687400	3.69202547858531
H	26.50419361497232	8.58250656088914	3.62563534672378
C	25.73986773177832	6.93743368395961	4.90205095453079
C	33.10473942393570	7.48698850955894	3.33829820566288
H	33.64021265997133	7.02315122139271	2.52290785848798
C	29.62942846321652	1.99438580445387	7.70548510524655
H	29.79553009955861	1.01068845593313	7.29090216761134
C	30.01206329239591	4.01503608832073	8.76911988916281
C	28.61051334994193	3.83794860923414	8.50352935922937
H	27.84872119079947	4.54609013272568	8.79154935307013
C	28.34725221805855	2.56981833570910	7.91902077422543
C	31.78151614826723	2.31646590449716	1.33489919863671
C	25.31667296853394	5.63613772501318	4.51466559458936
H	24.93815742544558	4.89211861103852	5.19890466923721
C	31.37046726166368	1.40687469098584	2.36905612563533
H	32.03664671207009	0.98194607667014	3.10598803822005
C	27.81938812620605	-0.12661011663479	2.77143322488801
H	27.44128667579086	0.71420650934307	3.35975478198424
H	27.38418621370393	-1.04691610847136	3.18043271702430
H	27.44128671209347	-0.01825621504143	1.74918700266618
C	32.11432265636783	8.51442021070168	3.16423453117276
C	30.67280769958636	2.81481658028555	8.25386841416063
C	25.87053787291621	6.73324617469164	2.55342464595019
C	30.58302924562350	2.59579676351447	0.54831175454367
C	29.52207389826961	1.83695462006016	1.15235791303265
H	28.51404555898958	1.79713635383820	0.76589268669447
C	31.70854404791178	8.91698419139401	4.50821695677875
C	25.33669609700785	5.48150387046709	3.08622411655108
C	30.00282982194783	1.04387806534297	2.22854471649904
C	32.48776367161141	8.11504434441125	5.41213201794522
H	32.44279368787007	8.19902715199627	6.48761420517307
C	33.41136670450484	7.29241243605357	4.71085894253015
C	25.39657363422102	7.63254963455652	6.21598195415567
C	32.04279757376723	2.13047864826456	8.47017774427519
C	27.01562714825473	1.82643385698138	7.95588925798593
C	25.81983959491241	2.77034138503074	7.80887487490711
H	25.77616123007215	3.50582432741286	8.61903962643835
H	24.88355451842926	2.19903797900930	7.83866197735686
H	25.85853516372267	3.31133325289666	6.86140579282001
C	29.81612245589570	-0.47502565232108	4.24151413020221
H	29.60352771856422	0.37633146324324	4.89141187111510
H	30.89290855421835	-0.67099984333712	4.28647542600400
H	29.30501616069489	-1.35733911227645	4.64614796396059
C	26.31196311816602	8.82047003569028	6.52049725422934
H	27.35108543327907	8.50489577403372	6.64512300751164
H	25.99348624986710	9.30701698531272	7.45120401484051
H	26.27952568775712	9.58039257616250	5.73294469935321
C	25.85157147957140	7.42794054616463	1.17251439624357
C	26.91330536347177	0.72598907593898	6.89746386863549
H	26.97820229250506	1.13514971423251	5.88512858333112

H	25.95013179158465	0.20799229697224	6.98643027528689
H	27.69625197479294	-0.03103267657832	7.00942323662033
C	29.34844047061641	-0.20241476720543	2.80865959151821
C	32.41700173628346	1.24063226145346	7.27064373418910
H	31.70834663717810	0.42676419856932	7.09919326997899
H	33.39343400357555	0.77601663304397	7.45687502859743
H	32.49509314290357	1.82421289896372	6.34867551670533
C	25.41914588940401	6.66891191158135	7.40404050592863
H	24.66409032502449	5.88287834582478	7.30576361784664
H	25.20243657901139	7.21064779094362	8.33317555939805
H	26.39506155341817	6.19079551912105	7.50830301483893
C	31.60957924791575	6.01857921256815	9.13148232976156
H	32.52553104619644	5.44800640240533	9.00201026181954
H	31.82934222730676	6.84653828331945	9.81734151920604
H	31.34000424693101	6.44553752373715	8.16218611658544
C	25.91757327894583	6.53386094465784	-0.06847173786911
H	26.81455731743089	5.91167392375710	-0.06873236877781
H	25.95977714684182	7.16925777003196	-0.96206441654692
H	25.04491526539121	5.88910155445428	-0.18599253716612
C	27.03093358547529	8.40458967772648	1.03968129700777
H	27.02130889511710	9.19491669283322	1.79459737283861
H	26.99027907712546	8.89836233311914	0.06104178896763
H	27.98455498622278	7.87445874702336	1.10978303562500
C	29.79041873096186	-1.38734650236785	1.92049965738775
H	29.35846313420362	-2.32479217806006	2.29528253351274
H	30.88102642989932	-1.49574972749517	1.91384029805419
H	29.46105710646194	-1.25560337044720	0.88375160912652
C	23.95397102730087	8.16605718516960	6.05605250354815
H	23.88487056281867	8.89426486870749	5.23938605389626
H	23.62651203839915	8.66290465092142	6.97917135568368
H	23.25043914425403	7.35357141164036	5.84250833968341
C	29.45090752509058	10.17580655520129	4.55137455806547
H	29.38989869578133	10.35904409354867	3.48091640481034
H	28.91654623751316	10.98899742057741	5.05809008299925
H	28.92304960528457	9.24243571699129	4.75673789696413
C	30.89124020596097	10.10017624130100	5.06852900102847
C	31.90241627673412	1.20394750963417	9.69961273653296
H	31.65358922166924	1.76017440612878	10.60800567201102
H	32.84617771532271	0.67255073439129	9.88136230978234
H	31.12088252476600	0.45215645958570	9.54575564631622
C	32.01947761255918	9.15023771425478	1.75828197751496
C	33.25050504319940	3.04141222998905	8.69945608476130
H	33.41068809608440	3.71529773058894	7.85566446980012
H	34.15080517818759	2.42164461619811	8.79700555289754
H	33.17375175417737	3.62988909380022	9.61486562374906
C	26.93483882138970	1.16217185893536	9.34966272864166
H	27.75401010223030	0.45025109200327	9.50303695420878
H	25.98858549694187	0.61448006178624	9.45524158116230
H	26.98510392816154	1.90955129488063	10.15018981953765
C	30.45481359221046	5.17822395407695	9.68403323575752
C	24.62172906221970	4.27115970378252	2.44735048565612
C	30.31263410807616	3.17732732712058	-0.85673295370087
C	33.25398947887899	10.06790460297406	1.59460986974201
H	33.26846839192014	10.87706927830177	2.32967086003725
H	33.25627687802815	10.52129597334120	0.59473598350081
H	34.18520513651178	9.50169533899468	1.70611127121417
C	25.46877469945591	3.50061680543960	1.42721121158558
H	25.77656359884996	4.10593109206572	0.57755290930713
H	24.89881149962646	2.64556280418458	1.04118563993270
H	26.37363500462919	3.11496306127890	1.90442238726548
C	33.64277338226320	4.08065606942804	1.06271213153058
H	33.21752012676599	4.58546240361704	0.19818793927225
H	34.73269693171617	4.20187047990244	1.01227089403791
H	33.28114983715419	4.59072626709390	1.95791546050192
C	24.55129090162645	8.26193125451156	1.10229889691164
H	23.65672270755143	7.63871145631086	1.19119887981003
H	24.49523289291377	8.79561016508370	0.14409314268121

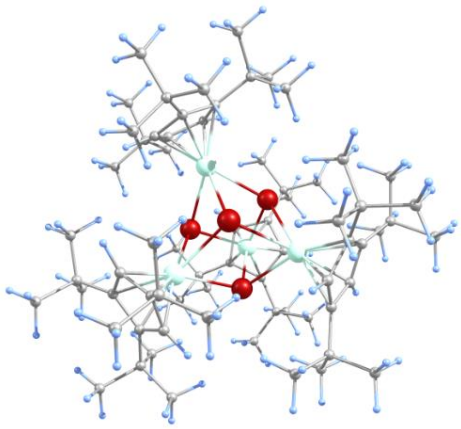
H	24.51596183126885	9.00836414426854	1.90364632210020
C	31.22095719100141	4.31635146847350	-1.32692630402158
H	31.20412493242568	5.16129896247315	-0.63425898187897
H	30.86230493898809	4.68063712476414	-2.29766589010318
H	32.25547177099664	4.00499303219285	-1.47617714351953
C	30.42564385710431	2.01585357642243	-1.87001927530795
H	31.42987702282489	1.58426059124535	-1.89632993911757
H	30.18992940816786	2.37334151669577	-2.88128438721903
H	29.72463426040521	1.20908993463418	-1.62900514885141
C	33.28530325109760	2.59166784272737	1.12422818844325
C	30.76996248869125	9.97486064958621	1.44147963938610
H	29.85641255911171	9.39239399492311	1.57053502982508
H	30.80845336056662	10.29183075590937	0.39213384328692
H	30.69754183656332	10.88343876653138	2.03941059244120
C	32.10782176340535	8.07913416535452	0.65903964307011
H	33.06094620371748	7.54500637199606	0.65444412563705
H	32.01186401000221	8.55925755732422	-0.32318562455344
H	31.30351280996812	7.34381982361562	0.75130739254039
C	34.11165535710225	1.99583852613525	2.27913592402010
H	33.81868094024876	2.40101524668541	3.25222436214152
H	35.16908756505726	2.24138325907811	2.12671683654870
H	34.03813538675771	0.90338146038737	2.32370676293018
C	28.87860055976726	3.72233112261586	-0.95116118869503
H	28.11449274327198	2.95059409966435	-0.82716239679199
H	28.72252610282333	4.16684533668446	-1.94162496557567
H	28.70621989435737	4.49665821867953	-0.19958727328708
C	29.29655135937977	6.16620370512000	9.91815546887224
H	28.91899270895155	6.58739697546188	8.98058276066765
H	29.66208964648282	7.00073027593587	10.52805452515251
H	28.45836624929838	5.71538111063799	10.45996897762303
C	35.16904057141318	5.44625253606564	4.56707279317287
H	34.43787765439601	4.64416567137646	4.70516083757834
H	36.12539985209292	5.10753854037785	4.98497693134422
H	35.31692629200090	5.59034037819281	3.49298379996153
C	23.29939712002193	4.73221346838279	1.80060955668089
H	22.67244396716684	5.26220073125280	2.52751437674968
H	22.73530263347881	3.85943484354310	1.44700306352764
H	23.45056723865519	5.39147987547092	0.94466675342798
C	30.82471484560223	4.62611480554328	11.07635643013228
H	29.99841111886707	4.04199707599941	11.49913066717678
H	31.03288251970306	5.45604019675274	11.76411926797061
H	31.71165443741795	3.98898748812882	11.05775611293967
C	34.72087835042277	6.73462753455050	5.26253103632631
C	30.78656786563200	10.01112313015992	6.60247558569035
H	30.32682539330529	9.07453942207385	6.93119528535126
H	30.15562828354367	10.83055357929543	6.96654498040385
H	31.75884166466803	10.11208022515346	7.09706404646598
C	31.62353923669989	11.42689351485169	4.77774866654015
H	32.66107120262446	11.38892583247933	5.12844194979695
H	31.12303855910819	12.24930788998182	5.30529610224359
H	31.63446174840827	11.68425051443895	3.71701652347985
C	24.21711191835839	3.24042141890525	3.51830459195681
H	25.08037327741639	2.85391416586301	4.06727612741935
H	23.73350949406334	2.38757033273715	3.02668602013725
H	23.49643491133843	3.64180776333713	4.24034566722785
C	33.78250382738043	1.87511347762564	-0.14792237412168
H	33.53312935913112	0.80783717694579	-0.12162530325069
H	34.87527085307503	1.96058942567577	-0.21876801700547
H	33.36447631526099	2.29526251585374	-1.06435148639928
C	34.65299692547628	6.48865705236581	6.76995735096337
H	34.46794498805260	7.41109637586542	7.33029194260418
H	35.60620569354717	6.08059566173444	7.12770350219756
H	33.86577719408712	5.77684181924746	7.01856442298377
C	35.79156738700265	7.81998042525317	5.00829830391109
H	35.92194223254741	8.01516299148294	3.93819442669168
H	36.76025426293096	7.49915679308725	5.41388534874686
H	35.52146431105360	8.76592694878993	5.49221425366577

Tables10: Selected Meyer bond orders for [(Cp'''Ni)$_4$(μ_3-Sb)$_4$] (**2**) in the singlet spin state, calculated at the OPBE/TZVP level of theory.

B(0-Sb, 1-Sb) :	0.31	B(0-Sb, 2-Sb) :	0.25	B(0-Sb, 3-Sb) :	0.26
B(0-Sb, 4-Ni) :	0.71	B(0-Sb, 5-Ni) :	0.69	B(0-Sb, 6-Ni) :	0.69
B(0-Sb, 7-Ni) :	0.10	B(1-Sb, 2-Sb) :	0.31	B(1-Sb, 3-Sb) :	0.31
B(1-Sb, 4-Ni) :	0.62	B(1-Sb, 5-Ni) :	0.11	B(1-Sb, 6-Ni) :	0.65
B(1-Sb, 7-Ni) :	0.67	B(2-Sb, 3-Sb) :	0.35	B(2-Sb, 4-Ni) :	0.67
B(2-Sb, 5-Ni) :	0.65	B(2-Sb, 7-Ni) :	0.68	B(3-Sb, 5-Ni) :	0.59
B(3-Sb, 6-Ni) :	0.72	B(3-Sb, 7-Ni) :	0.65		

Table S11: Cartesian coordinates of the optimized geometry of [(Cp'''Co)$_4$(μ_3-Sb)$_4$] (**3a**) at the OPBE/SVP level of theory, in the unrestricted singlet spin state. Total energy: −9156.10473923027 hartree.

Sb	-0.92743399225559	1.11513047067921	-1.14014022001331
Sb	1.00276063420058	-1.09802823459449	-1.25173465844681
Sb	-0.98124075315992	-1.05919968240592	1.18417328095972
Sb	0.95783705420896	1.11390016918754	1.23698145574804
Co	-1.68250050350963	-1.44640190706671	-1.32059719968311
Co	1.68277738247495	-1.37871831106909	1.21638098614527
Co	-1.57207535851745	1.54783397353725	1.31026912683108
Co	1.65353100817180	1.44400220166090	-1.19820458975416
C	-2.74548248263480	3.25584196106953	0.89346701878036
C	-3.53270656065321	2.13024078023505	1.29759248798996
C	-1.82678296343743	3.46271240247823	1.96097078696737
H	-1.07562856646799	4.24752980973105	1.97052041434460
C	-2.09575796784503	2.57830689145515	3.07090437974506
C	-3.20466203270497	1.71456856280552	2.63833557125824
C	-3.11275832145668	4.30217197726327	-0.16082553186184
C	-4.21188348076717	0.79129301050166	3.36257788846807
C	-4.88414716943766	-0.15968851963701	2.35346613973255
H	-5.54754516731395	0.36706045086450	1.64889532213028
H	-5.51308821539160	-0.88828960023687	2.89116700223996
H	-4.13875415432218	-0.71362773955085	1.76605036416001
C	-5.33685252816715	1.67970907832270	3.94625324523849
H	-4.98123930994697	2.36590038593517	4.72731711972542
H	-6.12812424913193	1.05062423068608	4.39153579038906
H	-5.80375432093473	2.29314821959663	3.15809239636429
C	-3.62748941775590	-0.08964417568556	4.47334568280445
H	-2.79626533676846	-0.70619201261659	4.09897491529216
H	-4.40328240291215	-0.77409636358431	4.85577097837560
H	-3.27034213264283	0.48977941735369	5.33488056692111
C	-1.42248917834167	2.86615797006693	4.43730186006257
C	-2.48322807809489	3.36336440826621	5.44185761278441
H	-3.07053680963633	4.19886152646374	5.02568754000545
H	-1.99313672095259	3.72558535905319	6.36164377467054
H	-3.18107164458596	2.57066203109086	5.73968263028339
C	-0.66752864602068	1.67033219509075	5.02324699249630
H	-1.30391215700512	0.79307218314230	5.16778006561527
H	-0.23386763376152	1.93177144736832	6.00422524582093
H	0.15274570907594	1.37567332120660	4.35427123096220
C	-0.38701177630145	4.00279618071635	4.31257820103452
H	0.41299554274763	3.75647423298710	3.59806136972623
H	0.09281376271533	4.16763606175358	5.29214425559200
H	-0.84055316445409	4.96147596945967	4.01382437235930
C	-1.89615847916882	5.12194120796288	-0.60800030184964
H	-1.46049554409346	5.70438585990157	0.21768810483902
H	-2.18299047721207	5.83915137760370	-1.39521984601818
H	-1.10969030577363	4.46958458205075	-1.01093714261360
C	-4.11793825740337	5.24974980346677	0.53800510317226
H	-5.02716951408043	4.71187982454299	0.85319853500480
H	-4.42674994245282	6.05932591740506	-0.14692411295396
H	-3.67799578397823	5.71368409038236	1.43579168250508



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H	-4.07861098759274	4.51494727098372	-2.09740184474983
H	-4.72348685898836	3.16926598488882	-1.14020238066005
C	2.78297595305340	-3.20214594920152	0.84933909372946
C	3.61821735588040	-2.12583191114088	1.27544893280113
C	1.81821639322413	-3.35110833631545	1.88615491397804
H	1.03052095607645	-4.09872994791793	1.87639522501702
C	2.09995183859466	-2.48412683325423	3.00054038102523
C	3.26501326157525	-1.67710912851077	2.59651534626107
C	3.13133666608257	-4.27402359689074	-0.18642596661876
C	4.29128033475556	-0.79009196067561	3.34094169379667
C	4.99412889975247	0.15444915573681	2.34608974471469
H	5.65024389488161	-0.38035356654154	1.64080057897547
H	5.63596278246605	0.86370522613139	2.89464300842379
H	4.26316701661741	0.72953134271337	1.76011421972918
C	5.38690316630615	-1.71275974951507	3.92703246396900
H	5.00373731322688	-2.39876845709416	4.69549106112592
H	6.18786968494422	-1.10939526483955	4.39027073603364
H	5.84859435727474	-2.32835045253215	3.13777907349838
C	3.72575977964307	0.09599523796964	4.45774226080572
H	2.91615650152439	0.74481381699465	4.08954145762085
H	4.52125533121896	0.75004021415617	4.85282992634550
H	3.34642588435634	-0.48244941037988	5.31049515458033
C	1.40556781403957	-2.75716037398783	4.35844048940936
C	2.43851904192043	-3.31531808080081	5.36062586003664
H	2.99346218184687	-4.16630615639361	4.93186172847638
H	1.92850130100388	-3.67326555075818	6.27134602411531
H	3.16722923150717	-2.55789373629136	5.67642747441011
C	0.70018268361655	-1.53692451017442	4.95570994924280
H	1.36809158785413	-0.68354533573839	5.10013903239505
H	0.26255588819555	-1.78656200198426	5.93802061091561
H	-0.11472697290987	-1.21037439906042	4.29505647433917
C	0.32012951055444	-3.84368867954760	4.21339338482129
H	-0.45773187108442	-3.55234635888581	3.49139135303017
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H	0.73144229217474	-4.81935164433692	3.90962593626599
C	1.89345761260582	-5.05234157112275	-0.64970742396701
H	1.43245080487302	-5.62179562586314	0.17112261651981
H	2.16748234905922	-5.77825349538926	-1.43346614971201
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H	4.36484135627224	-6.08632668757700	-0.12594544598850
H	3.61074354283265	-5.68424941091608	1.44063103197127
C	3.86751823174528	-3.72270302211235	-1.41367623271500
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H	4.80229633128084	-3.20981130510011	-1.14145467517356
C	-2.80328280348704	-3.25997616746123	-0.91043396979679
C	-3.62553081627122	-2.17452018041854	-1.33030456675318
C	-1.86158259134891	-3.43986856421694	-1.96582262757130
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C	-2.14295230506438	-2.57926603447155	-3.07889920522337
C	-3.27934881336886	-1.73577861360460	-2.65852342442480
C	-3.14777556394926	-4.31621901395027	0.14184474030788
C	-4.28728424681906	-0.81889065954322	-3.39013476405297
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H	-4.47133956275573	0.75000160535258	-4.88123883947720
H	-3.32449599965805	-0.50518580582288	-5.34990161437522
C	-1.45608232035653	-2.85654080327325	-4.44008138721795
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H	-3.08497171609682	-4.20366986885737	-5.04570912050218
H	-2.00359145398832	-3.71318400726989	-6.37289092594416
H	-3.20846702450934	-2.57425433390676	-5.75368598410163
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H	-0.26320908175571	-1.90646810120171	-5.99565420644242

H	0.10969526317293	-1.35784561326871	-4.34096390227744
C	-0.41104373910801	-3.98340376395263	-4.30768012656788
H	0.38194168232592	-3.72598492091684	-3.58938156452728
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H	-0.85823276768915	-4.94456611571319	-4.00723959393952
C	-1.91105825715161	-5.10017975423515	0.59902233362186
H	-1.45810104892789	-5.67551200173224	-0.22238436301861
H	-2.18307916134885	-5.82095510920256	1.38823836024942
H	-1.14345717874821	-4.42585902503770	1.00217318158430
C	-4.11865472743163	-5.29604391375273	-0.56127592969697
H	-5.04651956777754	-4.78999112331528	-0.87473767616993
H	-4.39809197951426	-6.11844947692627	0.12103782736756
H	-3.66296440303410	-5.74138720700595	-1.46076619950977
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C	3.24276956122520	1.67804262833926	-2.58075728677723
C	3.13285647782102	4.29161884680158	0.19878476620419
C	4.27057146270305	0.78888188823874	-3.31962490652896
C	4.97103407307712	-0.15376173194540	-2.32179564039212
H	5.62511085037532	0.38243735568873	-1.61571164876706
H	5.61448758301539	-0.86298132142506	-2.86827348016963
H	4.24008295445531	-0.72910367148551	-1.73653413483768
C	5.36850020537618	1.71158373248537	-3.90173303885904
H	4.98925592586165	2.39569221796113	-4.67376264414023
H	6.17225696746633	1.10749700482987	-4.35900886132119
H	5.82598497653413	2.32897346091154	-3.11135214196853
C	3.70812613678844	-0.09793322177749	-4.43751309731918
H	2.89690134987515	-0.74592024242176	-4.07152206030665
H	4.50468190217542	-0.75292995579987	-4.82872106250870
H	3.33234816590510	0.47949940173955	-5.29254265359635
C	1.39637207012575	2.76059095571947	-4.34710363634764
C	2.43261656524069	3.31020364958230	-5.35079375359761
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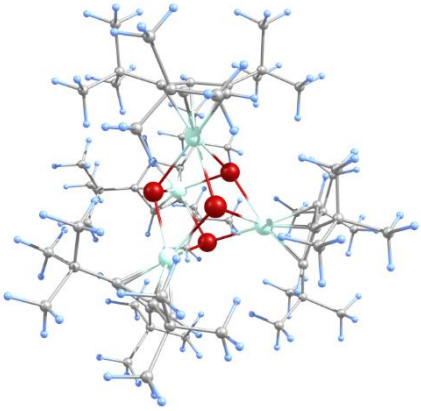
H	1.92473138299723	3.66601562408773	-6.26345883340921
H	3.15857686398708	2.54846751542942	-5.66199715389592
C	0.68584632411428	1.54090970092947	-4.93890898832434
H	1.35058435077067	0.68466915594427	-5.08040493958680
H	0.24900536483470	1.78875938438720	-5.92195540703971
H	-0.13024033597088	1.21879685250260	-4.27727451846587
C	0.31702010750661	3.85404914410508	-4.20861700467800
H	-0.46390487190217	3.57209199445112	-3.48631432704631
H	-0.17947986656300	4.00086719653426	-5.18270857045895
H	0.73297968239185	4.82971428544970	-3.91116590077069
C	1.90462017600705	5.09514820918502	0.64422038766867
H	1.46150761721503	5.66806215124229	-0.18413225056940
H	2.18300263524539	5.82047670943593	1.42699132936281
H	1.12657508749534	4.43473878597909	1.05084410694429
C	4.11403108434899	5.24847281570553	-0.52060332790932
H	5.03401193041050	4.72622353780574	-0.83077109920228
H	4.40749345120780	6.07674227583468	0.14857186208540
H	3.66017034205066	5.68709722447347	-1.42430683523819
C	3.84040221603449	3.72846177969937	1.43768471639102
H	3.19573283842243	3.03186550958637	1.99502068840200
H	4.11359366536948	4.54911948170530	2.12294552681017
H	4.77031435543566	3.19950152697486	1.18053469023800
H	-4.33739522534300	1.70035876785161	0.70409621157552
H	-4.45565562854017	-1.77526180446159	-0.74992082043653
H	4.46651782517549	-1.74792155936349	0.70755887690279
H	4.42266550426918	1.73013612922093	-0.67478229921409

Table S12: Cartesian coordinates of the optimized geometry of [(Cp'''Co)$_4$(μ_3-Sb)$_4$] (**3a**) at the OPBE/SVP level of theory, in the triplet spin state. Total energy: −9156.10520769705 hartree.

Sb	-0.91428130448516	1.07853662861176	-1.15029788612519
Sb	1.01962621423413	-1.11097927407631	-1.27334469142508
Sb	-0.91408410308650	-1.07932724158541	1.14997380145124
Sb	1.01541543472010	1.11325644922133	1.27486923356345
Co	-1.65604294543192	-1.45877331131480	-1.29841708261901
Co	1.65464354250331	-1.43634666574489	1.18366186523384
Co	-1.66330263369410	1.46021441712267	1.29177053622707
Co	1.65202476096509	1.44057082435357	-1.18516607810352
C	-2.78067624589300	3.24125968214741	0.89505440669445
C	-3.60798283448098	2.15861663410308	1.31606984175493
C	-1.84033715945533	3.42032832047745	1.95390335789913
H	-1.06408314121079	4.18004057034648	1.94824440273773
C	-2.12939301335461	2.56255569588859	3.07064676542574
C	-3.26446718087868	1.72456325252400	2.64622721087632
C	-3.12238588180212	4.29434702005712	-0.16099804268537
C	-4.27163516619109	0.80545864385153	3.37515109654554
C	-4.95233914401073	-0.14090290085187	2.36633493905470
H	-5.62079705497268	0.38888074500808	1.66882209644079
H	-5.57758355575326	-0.87246099074000	2.90462762304413
H	-4.20937537536164	-0.69122424897723	1.77181619201338
C	-5.38878279766014	1.69447221786663	3.97203298200357
H	-5.02285775435735	2.37556265459677	4.75293839105109
H	-6.17852528752644	1.06659919737602	4.42179518346458
H	-5.86013646569349	2.31350701354047	3.19095550271625
C	-3.68114722549928	-0.08262489391418	4.47707423430959
H	-2.85480604573609	-0.70043994446497	4.09351769532982
H	-4.45660125335583	-0.76571359092147	4.86284612282048
H	-3.31482975044052	0.49206218685819	5.33794787936022
C	-1.45139774641714	2.84654138338491	4.43512366523559
C	-2.50481866877337	3.35402274614889	5.44214278121585
H	-3.08636057206328	4.19314514299513	5.02512056034372
H	-2.00945088347934	3.71405420748902	6.36008932724615
H	-3.20874519762864	2.56796681505731	5.74368878913204
C	-0.70136126365739	1.64725368227654	5.02186300223852
H	-1.34018009236851	0.77160156756780	5.16656965591403
H	-0.26661644002010	1.90708471994285	6.00296099889573
H	0.11870258945603	1.35229426440586	4.35312011004554
C	-0.40720063598670	3.97444129428303	4.30331093955551
H	0.38865247964068	3.71472186781086	3.58900367333545
H	0.07466678060003	4.14131189713094	5.28164772414481
H	-0.85390258946519	4.93425020547682	3.99784276344970
C	-1.88825140158594	5.09069367905514	-0.60251970783657
H	-1.45025385869785	5.66923879109809	0.22465847861770
H	-2.15776732316258	5.80935821960373	-1.39444011332696
H	-1.10898218399817	4.42438728745651	-0.99671617313264
C	-4.11091314342120	5.26430334997631	0.53112851966353
H	-5.03756132961687	4.74931809842463	0.83326508658644
H	-4.38976922261474	6.08514157267006	-0.15320935604872
H	-3.66947342411329	5.71237910469255	1.43633475296604
C	-3.81407664432246	3.71259924402506	-1.40020269452959
H	-3.16130510295542	3.00792546359540	-1.93728041133539
H	-4.07983090305168	4.52235816388002	-2.10115563751007
H	-4.74600831310820	3.18576402029361	-1.14590498385035
C	2.78637391721680	-3.22372431506071	0.82851516642591
C	3.59002648959352	-2.11798610508605	1.23680063639383
C	1.81989586993099	-3.36151335362315	1.86339557378908
H	1.03819903861210	-4.11607445896372	1.86235425150697
C	2.10108054794787	-2.48363217083915	2.98116705643121
C	3.24336464484173	-1.66903526033976	2.56809759475952
C	3.14648411911546	-4.30168413866018	-0.19594962055192
C	4.27100960336579	-0.77577605741504	3.30229878333104
C	4.96350420072882	0.17072715268841	2.30230501069032
H	5.61881872531190	-0.36258712579291	1.59512921957671
H	5.60458308694787	0.88343302695411	2.84691134107657
H	4.22802177607212	0.74206089041639	1.71846601481482
C	5.37523375917179	-1.69552138094380	3.87737024140277
H	5.00197656210481	-2.38071139154432	4.65137205601228
H	6.17970587101347	-1.08900252084094	4.33010255040493
H	5.83021673149625	-2.31142708952961	3.08440902703465
C	3.71119353332555	0.10666441550586	4.42474663290723
H	2.89669276272067	0.75350953179192	4.06407390593425
H	4.50762934982737	0.76270858707854	4.81443653915097
H	3.34039681543111	-0.47420571501857	5.27953814715086



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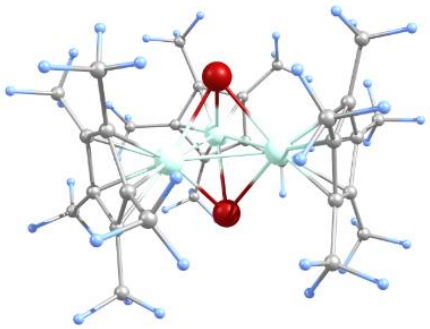
C	2.45031813706000	-3.30668283722571	5.34130968104825
H	3.00847728214430	-4.15657462142240	4.91448203212414
H	1.94592867561475	-3.66312641603474	6.25564314575645
H	3.17560410459453	-2.54321906469130	5.64988762287198
C	0.69618163558096	-1.54362433078829	4.93701885483133
H	1.35859598658676	-0.68598955770858	5.08062832200256
H	0.26062745463808	-1.79579906442361	5.91950405567924
H	-0.12114491804695	-1.22127468431624	4.27696319637793
C	0.33444980743722	-3.85668773693597	4.20226700839957
H	-0.45008396732961	-3.57629462909401	3.48328204784283
H	-0.15792617861630	-4.00819476472304	5.17770465400770
H	0.75343636719283	-4.82988066316489	3.90089190909109
C	1.91437758537851	-5.08781154993103	-0.66159636970069
H	1.45008171643431	-5.65317284970460	0.16033450454551
H	2.19530670010950	-5.81823821229512	-1.43865817667175
H	1.15340390732275	-4.41654232630526	-1.08230272459616
C	4.09836069586004	-5.27124324284065	0.54593487233716
H	5.02016420365994	-4.76227003632745	0.87254963946847
H	4.39217969763857	-6.10544811144068	-0.11567189996646
H	3.62124208470913	-5.70121435942013	1.44185304988469
C	3.88784724078388	-3.75406605554860	-1.42182175802436
H	3.26448160744198	-3.05189368837640	-1.99571932814989
H	4.16397100276718	-4.58199932082251	-2.09708391007948
H	4.82011973010174	-3.23833211365084	-1.14607190509955
C	-2.77608657043939	-3.23958567004522	-0.89393048620618
C	-3.60154709497791	-2.15525878452614	-1.31485077975596
C	-1.83684762961915	-3.42099268393870	-1.95313867798544
H	-1.06194437865612	-4.18208532179447	-1.94777729728619
C	-2.12551739494715	-2.56376094872654	-3.07040830370016
C	-3.25935027081311	-1.72384238122047	-2.64611091978885
C	-3.11982818433545	-4.29182812085362	0.16230709738007
C	-4.26722878214756	-0.80557034617998	-3.37540782707149
C	-4.94812663521877	0.14124694962457	-2.36724053323039
H	-5.61600102293838	-0.38820360242600	-1.66892868530881
H	-5.57392253472501	0.87195775406639	-2.90603032119421
H	-4.20524408533959	0.69247991883472	-1.77351114267571
C	-5.38407670326807	-1.69580745248639	-3.97107997644789
H	-5.01781077556589	-2.37724433959885	-4.75151426416525
H	-6.17440689385685	-1.06893032415959	-4.42118593177307
H	-5.85472173905586	-2.31450961291347	-3.18932305236509
C	-3.67800619201817	0.08194565732366	-4.47847862126447
H	-2.85261289659061	0.70165257063518	-4.09589375077353
H	-4.45463394285121	0.76333221146063	-4.86492236366644
H	-3.31096294824937	-0.49315520878857	-5.33874423631415
C	-1.44766352386275	2.84865814688916	-4.43482183287305
C	-2.50070295396353	-3.35710880991049	-5.44165275889367
H	-3.08200481673064	-4.19608187208703	-5.02397099661176
H	-2.00510333877719	-3.71774766624652	-6.35923430261748
H	-3.20495440931194	-2.57163091927962	-5.74389781979100
C	-0.69781011733217	-1.64926972165253	-5.02168089249737
H	-1.33675251802388	-0.77379439756027	-5.16687501296054
H	-0.26246642334655	-1.90917049268684	-6.00250121800956
H	0.12168668362142	-1.35398314158197	-4.35236179728114
C	-0.40311141839405	-3.97611380724308	-4.30221859862101
H	0.39344943239036	-3.71544133809808	-3.58906954154346
H	0.07798218970587	-4.14434828143376	-5.28071822028354
H	-0.84939164838305	-4.93560423810639	-3.99508126499437
C	-1.88670678712097	-5.08946718448283	0.60470633314355
H	-1.44859444092484	-5.66833903428675	-0.22215891738720
H	-2.15718702612230	-5.80776310752580	1.39662998951896
H	-1.10729128256954	-4.42360502647608	0.99933845959687
C	-4.10879501247742	-5.26068190903269	-0.53069205334704
H	-5.03453122509414	-4.74457559228378	-0.83370456197088
H	-4.38921241430130	-6.08111996355180	0.15349790939226
H	-3.66699337301873	-5.70931043127324	-1.43543118189626
C	-3.81189822107385	-3.70955475201711	1.40094813364017
H	-3.15906276850010	-3.00501004792204	1.93813998614212
H	-4.07811279699987	-4.51914437501015	2.10192359721871
H	-4.74361173042615	-3.18256066310718	1.14628900955439
C	2.78631781903001	3.22432622597283	-0.82946025585414
C	3.58889508787151	2.11740534187953	-1.23591145187143
C	1.82171476452154	3.36408615226985	-1.86596956752985
H	1.04118090886475	4.11986744194263	-1.86561177663839
C	2.10242049950182	2.48486750204691	-2.98280186726656
C	3.24311078195068	1.66859096676475	-2.56782618309403
C	3.14560926306206	4.30226191762272	0.19543206753730

C	4.27039100359687	0.77462977032679	-3.30132656214770
C	4.96300257646554	-0.17096602348160	-2.30060765621613
H	5.61711879212497	0.36307428505765	-1.59288134260627
H	5.60509504876988	-0.88323309824278	-2.84458918159867
H	4.22765487973105	-0.74308495744379	-1.71735060532332
C	5.37455336632228	1.69401776796565	-3.87701055294891
H	5.00117871508120	2.37850452100004	-4.65155017071843
H	6.17901380010073	1.08718646449738	-4.32937457019227
H	5.82958316663862	2.31057272150837	-3.08457721287221
C	3.71028056028041	-0.10864980064407	-4.42293315836632
H	2.89490590827320	-0.75397884392719	-4.06158714618419
H	4.50614369297595	-0.76607339015924	-4.81145506028013
H	3.34053526294578	0.47158930818307	-5.27860304720845
C	1.41090820166822	2.75951726575604	-4.34236556131993
C	2.45108266657563	3.30557127792420	-5.34422744858942
H	3.00979734749520	4.15582058881108	-4.91885354248441
H	1.94607555626295	3.66107204588361	-6.25860401349601
H	3.17581178764469	2.54151352569204	-5.65264868043758
C	0.69690432151969	1.54339330352496	-4.93744541232601
H	1.35945890231793	0.68590935137666	-5.08123362609440
H	0.26055602766398	1.79484106988554	-5.91976902115417
H	-0.11975534264267	1.22131939919196	-4.27641101754503
C	0.33586451348449	3.85718616438998	-4.20454658329251
H	-0.44863817701827	3.57722181714233	-3.48535871775553
H	-0.15644029267513	4.00818682461989	-5.18009736194707
H	0.75494927088146	4.83052381862969	-3.90377052824221
C	1.91336541108149	5.08827197835918	0.66068658533379
H	1.44947145914901	5.65393794698065	-0.16127780031389
H	2.19410794260302	5.81856128809259	1.43794779882932
H	1.15203375980904	4.41708739100878	1.08088865897300
C	4.09809525805688	5.27206918581933	-0.54532645340943
H	5.01994813886893	4.76307667806838	-0.87179470303697
H	4.39180527851087	6.10577174594150	0.11695728560817
H	3.62158146589050	5.70275165580891	-1.44122528293775
C	3.88619512539971	3.75389839956556	1.42153197306268
H	3.26249178165521	3.05141410142766	1.99468027404432
H	4.16217955461724	4.58132355966647	2.09746285178507
H	4.81843717213728	3.23813473667985	1.14569944105984
H	-4.43754622660121	1.75811684267442	0.73610139738839
H	-4.42985031885907	-1.75278719992030	-0.73447474545113
H	4.42482693281284	-1.72365708400999	0.65974264335479
H	4.42204672210992	1.72164411151575	-0.65751159433261

Table S13: Selected Meyer bond orders for [(Cp'''Co)$_4$(μ_3-Sb)$_4$] (**3a**) in the triplet spin state, calculated at the OPBE/TZVP level of theory.

B(0-Sb, 1-Sb) :	0.53	B(0-Sb, 2-Sb) :	0.27	B(0-Sb, 3-Sb) :	0.30
B(0-Sb, 4-Co) :	0.52	B(0-Sb, 6-Co) :	0.69	B(0-Sb, 7-Co) :	0.55
B(0-Sb,147-C) :	-0.13	B(1-Sb, 2-Sb) :	0.30	B(1-Sb, 4-Co) :	0.50
B(1-Sb, 5-Co) :	0.79	B(1-Sb, 7-Co) :	0.60	B(2-Sb, 3-Sb) :	0.53
B(2-Sb, 4-Co) :	0.69	B(2-Sb, 5-Co) :	0.55	B(2-Sb, 6-Co) :	0.51
B(2-Sb, 57-C) :	-0.13	B(3-Sb, 5-Co) :	0.60	B(3-Sb, 6-Co) :	0.50
B(3-Sb, 7-Co) :	0.79	B(4-Co, 6-Co) :	0.16	B(4-Co, 7-Co) :	0.12
B(4-Co, 98-C) :	0.39	B(4-Co, 99-C) :	0.60	B(4-Co,100-C) :	0.57
B(4-Co,102-C) :	0.41	B(4-Co,103-C) :	0.38	B(5-Co, 6-Co) :	0.12
B(5-Co, 7-Co) :	0.19	B(5-Co, 53-C) :	0.39	B(5-Co, 54-C) :	0.61

Table S14: Cartesian coordinates of the optimized geometry of [(Cp'''Co)$_3$(μ_3-Sb)$_2$] (**3m**) at the OPBE/TZVP level of theory, in the singlet spin state.



Sb	0.11389417875039	-0.02119927888256	1.78649239039132
Sb	-0.00539365778615	-0.04363123771272	-1.92328605399182
Co	0.88808682281100	-1.37640866287519	-0.08852098585645
Co	-1.52450215035696	-0.07650206583724	-0.01649880348559
Co	0.80655898586835	1.35753306369451	-0.09959415414357
C	-3.24382205788528	0.12057191689996	-1.15691007531088
C	2.65808702757706	-2.21749288149677	0.52323201130729
C	2.66751870732670	2.27739161455834	-0.16274569301666
C	1.55665186776325	-2.94807111002193	1.08745941684458
C	0.75962113235899	-3.44500300652500	0.00272985022651
C	0.71831218930339	3.27879049959302	0.60277933368779
C	-3.16407315703314	0.35391592738748	1.16065031882289
C	1.95083572151999	2.66743759717047	1.01951903227132
C	2.53885321165157	-2.26761412448404	-0.91300952218714
C	-3.15355094880531	-1.19218293688179	-0.57987250949705
C	-3.36917033765138	0.93995017993471	2.52097983738698
H	-2.96335115824036	1.95196166276067	2.60554847575281
H	-2.90207851684174	0.33562419974607	3.30377305510658
C	1.88522035459550	2.64284450999597	-1.31039495447435
C	-3.25179026842743	1.07054303328328	-0.08138189296164
C	-0.30175061605792	3.99142491853675	-1.69885274256992
H	-1.25901528430442	4.14123130018538	-1.19822493146516
H	-0.49513478175413	3.47013341751407	-2.64109458194857
C	-3.10588743538384	-1.04947616988487	0.85359105857826
C	0.67865145298199	3.26538953631856	-0.83831721516921
C	-3.33924609428804	-2.46649022427371	-1.33458673845169
H	-3.00806953100244	-3.33302923390041	-0.76137620681998
H	-2.80190419290621	-2.46780510229284	-2.28636640940296
C	3.84123600421772	-1.73212877499408	1.29349553185286
H	3.56077645881056	-1.31049698678733	2.26328218446960
H	4.40657978417529	-0.97378449362150	0.74906755001988
C	1.36235937960745	-3.02971318257808	-1.23351865739631
C	4.09481921148395	1.85013287175253	-0.20217633908149
H	4.31269669541678	1.18882324112690	-1.04363905727710
H	4.40640005589092	1.35239432900990	0.71840875730491
C	-3.22772598696244	-2.14979636025535	1.85638017431983
H	-2.63552177453610	-1.96067261694036	2.75639547655076
H	-2.91599273479925	-3.11360301256109	1.45031238451106
C	-0.21833307119553	4.01380164463443	1.50379015673392
H	-0.34090557210444	3.51538908761174	2.46962518886909
H	-1.20867208549903	4.13305552137925	1.06125003586729
C	-3.58718488099171	2.51648054646247	-0.21965265216595
H	-3.25678447602656	2.93142117000336	-1.17393304618454
H	-3.16361929830653	3.12323035767612	0.58291414019040
C	1.41103549019726	-3.34169567815560	2.52304790829883
H	1.93414245875690	-4.29338041173087	2.70948955628432
H	1.83645395326929	-2.59762649835432	3.20224221373250
C	3.57784605165303	-1.83900344743998	-1.89712543573597
H	4.20119761324314	-1.02730018003566	-1.51543269638702
H	3.14277068146521	-1.50704477184351	-2.84433912013908
C	2.36534590371561	2.62613283665229	-2.72675889220211
H	1.54122741095304	2.57073265894678	-3.44377899876752
H	3.03073460482519	1.78223783298205	-2.93047572563000
C	-3.55147484855405	0.42464165446877	-2.58889389815223
H	-3.13597047882689	-0.32376160343743	-3.26994235604488
H	-3.16101115231163	1.39741547356708	-2.90121015838753
C	-0.32682413025867	-4.45765701608652	0.13381510407433
H	-1.02563102495606	-4.43274898833699	-0.70494027733401
H	-0.89549046009987	-4.34263568151848	1.05904926996044
C	2.50651526941115	2.67740091696944	2.40824844971074
H	3.18096963088443	1.83584063827207	2.59275824066908
H	1.72145932440349	2.63500366383376	3.16888240061044
C	0.97950514515160	-3.51859457422886	-2.59434029261957
H	1.29293900703347	-2.82896128234471	-3.38307244292266
H	-0.10085250285261	-3.65890434607573	-2.69579576102211
H	0.36480857771401	-3.48307656173399	2.81005069467419
H	0.11478642352913	-5.46720721307779	0.15303467649206
H	4.52916016974276	-2.57004330086099	1.48975491795174
H	4.25149098978496	-2.68071799661491	-2.12365590568308
H	1.45787163743959	-4.48997444234632	-2.79692748523497
H	2.93160722042060	3.54628178187338	-2.94427830736136
H	4.73773805791017	2.73706259995230	-0.31799589398332
H	3.08390603951965	3.60047009284921	2.57835562442279

H	0.16864549173223	5.02510160371290	1.70416431296881
H	0.09014949080666	4.98883693712016	-1.95166659096283
H	-4.64171892996071	0.44374481378454	-2.74514997141318
H	-4.68074899079799	2.64342611956270	-0.17550516260844
H	-4.44506853399954	1.00082634649778	2.74839651994335
H	-4.27773956669307	-2.25741401069217	2.16930250657834
H	-4.40685789521602	-2.61614074055941	-1.55865258598794

Table S15: Selected Meyer bond orders for [(Cp'''Co)$_3$(μ_3-Sb)$_2$] (**3m**) in the singlet spin state, calculated at the OPBE/TZVP level of theory.

B(0-Sb, 2-Co)	0.94	B(0-Sb, 3-Co)	0.96	B(0-Sb, 4-Co)	0.96
B(1-Sb, 2-Co)	0.97	B(1-Sb, 3-Co)	0.92	B(1-Sb, 4-Co)	0.95
B(2-Co, 3-Co)	0.47	B(2-Co, 4-Co)	0.48	B(3-Co, 4-Co)	0.47

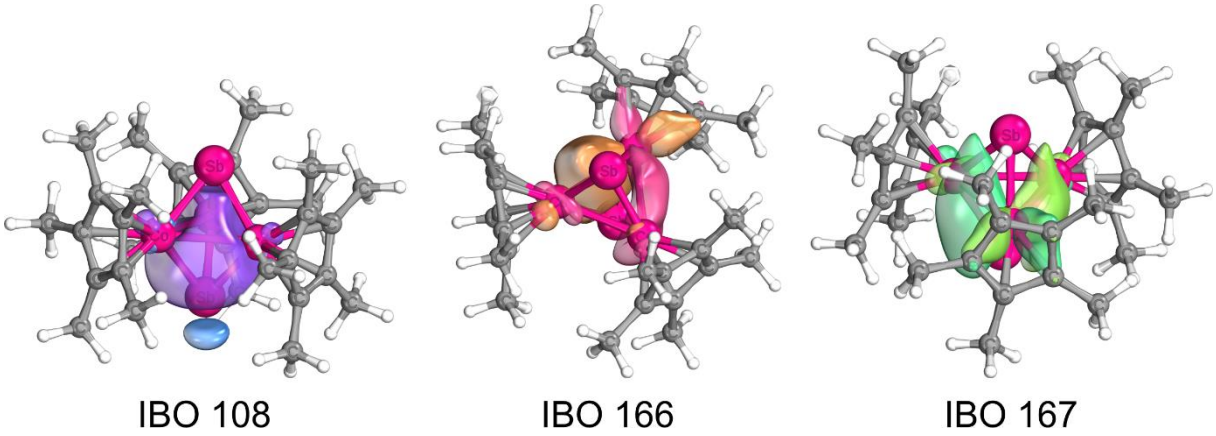
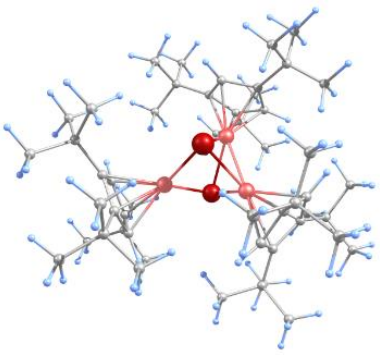


Figure S16: Selected Intrinsic Bonding Orbitals of [(Cp'''Co)$_3$(μ_3-Sb)$_2$] (**3m**) in the singlet spin state, calculated at the OPBE/TZVP level of theory. IBO 108: SB2 1.174 Co4 0.284 Co3 0.210 Sb1 0.147 Co5 0.137 (other: 0.047); IBO166 Co3 1.001 Sb2 0.380 Co5 0.331 Sb1 0.114 Co4 0.094 C10 0.021 (other: 0.059); IBO 167: Co4 1.031 Co5 0.316 Sb2 0.301 Sb1 0.141 Co3 0.119 (other: 0.091).

Table S16: Cartesian coordinates of the optimized geometry of [(Cp'''Fe)$_3$(μ_3-Sb)$_2$] at the OPBE/TZVP level of theory, in the doublet spin state.

Sb	3.13565562751790	19.92303483979375	5.42214204916052
Sb	2.72445041538463	16.23533020234116	4.57459754717904
Fe	3.38878228974659	17.69147760844119	6.52695623668602
Fe	3.85991216561666	18.26980563757314	3.63048326141166
Fe	1.35005801350535	18.18054532209338	5.31113500035496
C	5.02213725625285	18.21282204333016	8.00812357721525
C	-0.39724897585977	18.52687515155236	6.47951065400245
H	-0.38423854995653	18.74323546533278	7.53808641923326
C	-0.43309449068513	19.54045777407334	5.45622778781457
C	3.09313964838218	18.87560466430457	9.85906798512115
C	3.76375546790331	18.05859095139635	8.73287731479488
C	4.24601232908666	16.00028162903688	7.67768576901582
C	-0.52380611880783	17.22417746085858	5.92371203447455
C	5.48363321991858	17.49964750056737	2.34090197299322
C	3.30650674443877	16.72922640500196	8.45984894507343
H	2.40627537565475	16.30878690070417	8.87781619776794
C	5.24255833876460	16.95797722935563	7.34891460370681
H	6.11810683128083	16.74181226742506	6.75576622690728
C	-0.49671128488117	17.42549755785723	4.51658876713294
H	-0.57681978531840	16.63052527322671	3.79130285726382
C	3.63225728368216	16.94109307140597	0.35634822260588
C	6.51179540985272	16.35253015040133	2.44259836173431
C	6.22071138202027	19.18504789280823	8.10011190247343
C	5.83793163572760	18.77479889031159	2.90340780723600
H	6.67950311689444	18.92983244177289	3.56365143183661

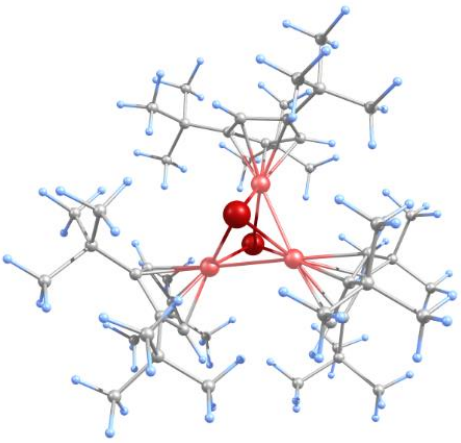


C	-0.79111427468854	20.98436078816541	5.88150828356096
C	4.31447001445403	17.75017347605890	1.48818298819362
C	2.88683855390213	15.67944242729369	0.81225284707377
H	3.51629927275859	14.98511168748264	1.36732548946207
H	2.49355808297303	15.14496678619010	-0.06268713305640
H	2.04239170848870	15.93727612951324	1.45659780360680
C	4.04005595759580	19.14924950444687	1.61361963481440
H	3.23390128017499	19.65470201879470	1.10376133358730
C	-0.13072558824262	21.35477282499870	7.21641855966894
H	-0.43956603016658	20.71114494487123	8.04439570817978
H	-0.41906271251387	22.37679002076997	7.49027949969955
H	0.95801400613564	21.32726862332099	7.12835432374883
C	4.99363330257766	19.81270918696159	2.42935646553006
C	3.07033946895194	13.73723123041215	7.61682018782063
H	2.53324477008559	13.94861493480277	6.68740883424911
H	2.42099182349535	13.99882477714299	8.45806518872743
H	3.24382781430232	12.65490439896714	7.66506565867402
C	4.40796785695304	14.48083164973111	7.66342356069534
C	-0.40901845724464	22.11538252606113	4.92059957346870
H	0.66799817351034	22.12746976329643	4.72773961240634
H	-0.66998907521806	23.07523603368273	5.38353850100173
H	-0.93709412532719	22.07967248075519	3.96813659863365
C	-0.49271497311100	18.82110035763255	4.19134074012103
C	-1.07180534214951	15.97274541694386	6.60431852029080
C	2.69184705898725	20.29932950100996	9.46679730386388
H	3.51909367292616	20.89630368868384	9.08963318330716
H	2.27167698271642	20.82287262894430	10.33606056592164
H	1.92886308112727	20.26264239215867	8.69087849284292
C	-2.31869172567665	21.01560632699772	6.11780775846203
H	-2.89133470209949	20.77864253981742	5.21796689061871
H	-2.62394896183460	22.01501735083186	6.45366837727910
H	-2.60797761106941	20.30005011870103	6.89549131039051
C	-0.76626609214550	19.25020842111012	2.73384962031270
C	7.61201574233857	16.59337242214407	1.38493108193379
H	7.22908444831314	16.56628532085047	0.36246188818832
H	8.38911150711183	15.82177849659706	1.47078125568827
H	8.09388054219612	17.56691891629865	1.53227408889443
C	5.29576395297526	21.30845101369126	2.40389143407377
C	5.90801377172440	20.65345837922736	8.40281424577434
H	5.21355245413078	21.07610843973422	7.66919912977241
H	6.83696560471044	21.23378155264024	8.35016108345700
H	5.50037634909011	20.81231051866948	9.40274356412897
C	4.02630350919563	18.90693806146830	11.08805431012088
H	4.35730772191746	17.89860664048185	11.36164234592243
H	3.48575432120124	19.32532295272442	11.94666242368666
H	4.91237390808183	19.52460502902398	10.93457038485633
C	4.02702121180309	22.16488428123302	2.32772827001568
H	3.42418739181268	21.93840265594583	1.44182865256288
H	4.29634737805416	23.22716290838049	2.27344175752982
H	3.40290218275029	22.01891077738735	3.21413611022660
C	7.16964157453275	18.64333117380371	9.19455764469854
H	6.69833132294466	18.60638397236198	10.17955792527081
H	8.05558166863868	19.28679961279658	9.27068039024173
H	7.51155291991510	17.63096534404871	8.95269190934175
C	-0.79054404928761	18.01634122640625	1.81397820126145
H	0.14142178559805	17.44932500426831	1.86291548005294
H	-0.92794380740011	18.34327482860807	0.77687070378143
H	-1.62158833965014	17.34275839751202	2.05070760280726
C	5.95915192681657	14.93301040012370	2.27925753322320
H	5.14312532968868	14.74068944569608	2.98152679939595
H	6.75554060873761	14.20802858611035	2.48814305120341
H	5.60027971720791	14.72149024127802	1.27131154510981
C	-2.60870371909548	16.14114972548156	6.60902000058080
H	-2.91401265784241	17.02248838479112	7.18452004015942
H	-3.08489275346168	15.26212162800207	7.06299318383723
H	-3.00452436922393	16.25006735895257	5.59272229985310
C	2.60073565517452	17.81078718277440	-0.38490216872733
H	1.81270530431311	18.18162462049369	0.27237045950961
H	2.11810107926175	17.20400210000795	-1.16005739467683
H	3.06593048288715	18.66631480841858	-0.88746606615912
C	5.28456682511805	13.98552579758871	6.51181138883948
H	5.39988398857631	12.89608016812830	6.57207195682285
H	6.28839872245574	14.41933444114586	6.53870433748694
H	4.83266931386537	14.21949689307443	5.54371739313647
C	0.28173325670599	20.20972138417428	2.16270243993691
H	0.29106901285364	21.17587114333021	2.66192645045091
H	0.08797747202208	20.38875731475929	1.09739572672901

H	1.27823477957732	19.77902311406263	2.27271019906056
C	4.67026698425791	16.56369586600785	-0.72161116232561
H	5.22295968475351	17.44573752077814	-1.06396651659865
H	4.15140343186875	16.13958500984710	-1.59086951291487
H	5.39326428790344	15.81882009368153	-0.38663223890636
C	7.02276816086930	19.18969420228994	6.78934252709937
H	7.48132497948241	18.22261712973320	6.56844946945443
H	7.84161994483712	19.91460267452419	6.87005704893499
H	6.39078440087256	19.47556651569937	5.94706266323879
C	7.20984147154986	16.38190974245949	3.81171965788301
H	7.82171091710404	17.27668991356584	3.95680983238629
H	7.88329912529385	15.52091404979208	3.89813994172879
H	6.47475565898562	16.32638905812367	4.61602457582257
C	-0.60762051043613	15.82120294340948	8.05244558987510
H	0.47357074400069	15.69039466028554	8.10078482460263
H	-1.08056160460719	14.94176705362560	8.50654128969289
H	-0.88020922943129	16.68531351983002	8.66652718417837
C	-2.17429185843420	19.86904579435795	2.60922541495212
H	-2.93718075223064	19.20661221737972	3.03476311257230
H	-2.41457181815981	20.01261086927731	1.54818528068945
H	-2.26107541613221	20.84274083506659	3.09183923240867
C	1.80074466915061	18.19175271392994	10.34095079435673
H	1.08398056612378	18.05629184361087	9.52807755876007
H	1.32799571069376	18.82721539053763	11.09951904618654
H	1.98880388811556	17.21836758727613	10.80767560796722
C	5.11385235960952	14.12443411954946	8.99271867060791
H	4.51898602052423	14.43758914661014	9.85808834032529
H	6.09425956918084	14.60777216960070	9.06600266043900
H	5.26540494744872	13.03936680133140	9.06062909195552
C	6.13222418231551	21.76273089282030	3.60372015168888
H	5.59763486207758	21.60552433186651	4.54557582142415
H	6.35463473132907	22.83366785830989	3.52101837428587
H	7.09085593095071	21.23627727316016	3.65771306836400
C	-0.73685501795580	14.69168587770103	5.83193226835478
H	-1.17042830723367	14.69222629111556	4.82690280029660
H	-1.14633005847419	13.82015634409252	6.35801136627787
H	0.34312845043891	14.55324811764622	5.73252718015323
C	6.12458564726133	21.54866741780808	1.12070025941777
H	7.06070915616128	20.97971790708160	1.13621544477210
H	6.37545915876250	22.61294069386107	1.02654272668837
H	5.56784332608372	21.25252560013529	0.22444027648810

Table S17: Cartesian coordinates of the optimized geometry of [(Cp'''Fe)$_3$(μ_3-Sb)$_2$] at the OPBE/TZVP level of theory, in the quartet spin state.

Sb	2.87869613152581	19.98999495689126	5.21031972888739
Sb	2.58737248340026	16.26293367637830	4.40539044733478
Fe	3.53882181771265	17.74626491803244	6.25646497291353
Fe	3.88225608059737	18.25022020904473	3.78526316468168
Fe	1.24635909033264	18.16537553578363	5.19110652084977
C	5.17128516389206	18.26917571464328	7.92566260492100
C	-0.39431287213503	18.41869419570741	6.41117313319832
H	-0.35891478014636	18.59394817415814	7.47700298932380
C	-0.46146968226722	19.46769728905288	5.42532627725952
C	3.20775616184742	19.06021313379300	9.68541973102982
C	3.88276157130804	18.20008863194857	8.59367136562274
C	4.26745592169636	16.11779553684032	7.54338077973533
C	-0.53151949517234	17.13404977227749	5.81517073600654
C	5.42907707099023	17.44525808064930	2.49483495110725
C	3.34243385015928	16.91232591029263	8.28293279819194
H	2.40226862888599	16.55078249386253	8.66567001962405
C	5.34029852411965	17.01242458710135	7.26175903277765
H	6.24248839056530	16.73047309649340	6.74169101087253
C	-0.52872542455346	17.38166050201106	4.41585958853302
H	-0.61001821775984	16.61140021193727	3.66350991063567
C	3.59562031778064	16.96393179680921	0.48094112000997
C	6.45012883446347	16.29040905891968	2.55018730171098
C	6.41003828350417	19.18289760576106	8.04672156212608
C	5.77708492914900	18.69113976208398	3.12641035436885
H	6.64154571063710	18.82255783294304	3.76032785450471
C	-0.85857377359182	20.88457122809519	5.91051556237837
C	4.25934844825698	17.71598319570854	1.66738977985261

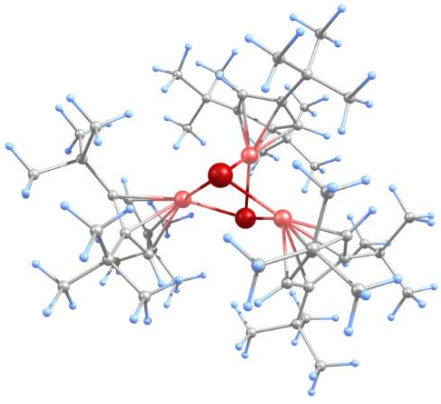


C	2.83906998466204	15.67813784325545	0.83781845785253
H	3.44742521700451	14.95421536408125	1.37890469065920
H	2.48477554091611	15.19201387974924	-0.08081760871318
H	1.96271521009473	15.89677398978784	1.45443397172684
C	3.95351401884335	19.10200364146546	1.87462227770439
H	3.14425276761927	19.62181710259971	1.38652129037876
C	-0.20129523172008	21.22694857665996	7.25424227133724
H	-0.46604601671157	20.53345616413232	8.05669371979424
H	-0.53360329767529	22.22136716098359	7.57599394351592
H	0.88604579672553	21.25610680066437	7.15602131008690
C	4.93075757745928	19.75008071537937	2.68415971916863
C	3.01943766105583	13.88932592378486	7.63734529151879
H	2.44279062502834	14.08890895946125	6.73054862273351
H	2.42009690311432	14.18872222913362	8.50288985827867
H	3.16560306922897	12.80413582456450	7.70748554122581
C	4.37817502082762	14.59169188781010	7.60065228270185
C	-0.52878567118458	22.06712791120890	4.99300732055559
H	0.54662636937870	22.13549374749617	4.80106680031434
H	-0.83093953512456	22.99608706501659	5.49259670448454
H	-1.05544806295281	22.04425469804458	4.03964686355857
C	-0.52875211290078	18.78888020872121	4.13141169812083
C	-1.05156236188583	15.86594527209336	6.48466069601755
C	2.93073788755002	20.51436474567200	9.28904772337313
H	3.83398618265362	21.10306269217894	9.14763731936838
H	2.33729896458521	21.00717754278526	10.07020509552570
H	2.36200531407636	20.54830030918902	8.36086692970412
C	-2.38363230658105	20.85374696583354	6.16387143512855
H	-2.95822064236721	20.62700577224440	5.26307815491322
H	-2.71898384645490	21.82995081683788	6.53712777461653
H	-2.63797930914110	20.10287461346767	6.92032516965596
C	-0.85381245425073	19.26568922127947	2.69904897851049
C	7.54656866254302	16.56631262254521	1.49667364874827
H	7.16415938240610	16.58060732948538	0.47443674678179
H	8.31825800992727	15.78662994663081	1.55368104524437
H	8.03648132107312	17.52957402684502	1.68155970364835
C	5.28422842791905	21.23712777988749	2.62375701305044
C	6.16110783103623	20.66704626657348	8.33509317876856
H	5.47864118155141	21.11676041269651	7.60809380262125
H	7.11375395364403	21.20626340695482	8.27036213198975
H	5.77497981385821	20.84885387625856	9.33963991260183
C	4.06745452829258	19.02920451602393	10.96729492761564
H	4.29626389446497	18.00095732567162	11.26958041967824
H	3.51375380328079	19.50412433840094	11.78721416581041
H	5.00953887132624	19.56969293145836	10.86065790015680
C	4.06852224150068	22.13213276868452	2.36260470955870
H	3.55315172637722	21.87389812979722	1.43107254385780
H	4.39167138438952	23.17678202572815	2.27376450593687
H	3.34461988535547	22.07950457293573	3.18215872398912
C	7.29962644074342	18.60650973658327	9.17292866123075
H	6.79516390581506	18.59402052092750	10.14230655087524
H	8.20740923603244	19.21494473911337	9.27414262856767
H	7.60838036923883	17.58037745127228	8.94628932871478
C	-0.87573997547100	18.06745894173659	1.73370582704379
H	0.06237013884279	17.50906619790764	1.75327131359540
H	-1.02651167385607	18.43067441401876	0.71034158219384
H	-1.69741048225976	17.37702539902170	1.95335526712216
C	5.88233879425578	14.88331547381153	2.33884566820984
H	5.05066517215020	14.68646758093535	3.02112068713429
H	6.66382865151078	14.14131227719731	2.54305812541298
H	5.53834908836570	14.70337574565166	1.31964584393139
C	-2.58987150095120	16.02163453242594	6.52385448790207
H	-2.88976945843416	16.90002114985576	7.10639167247847
H	-3.04704444981591	15.13844177164838	6.98906209101060
H	-3.01091010609244	16.12597806184064	5.51722493325698
C	2.58600930461785	17.87437713418239	-0.24062319795626
H	1.78118240423064	18.21039258973227	0.41328900609030
H	2.12453682191342	17.31078948567863	-1.06012366429832
H	3.06475191057202	18.75470626965523	-0.68359826893093
C	5.19674425055524	14.00688557321032	6.44887330872941
H	5.27380375570988	12.91805735047104	6.55988018730234
H	6.21609210771557	14.40256368279385	6.42584260699051
H	4.72377034468789	14.21179080551869	5.48460901650809
C	0.15658579803305	20.26919978533844	2.13784964852071
H	0.19823109251062	21.19572921785364	2.70633720896974
H	-0.09689810343221	20.52381111031593	1.10068454078744
H	1.15384977141972	19.82969421260022	2.16084743595470
C	4.65951503860793	16.64370241568681	-0.59104829183627

H	5.23572482053255	17.53649534401764	-0.85808043120234
H	4.15747648206049	16.28964307276231	-1.50037042990832
H	5.35840954150637	15.86358456838227	-0.28799461310107
C	7.24694431969812	19.13916346470991	6.75958176657112
H	7.65802262437964	18.14832918101837	6.55431712119703
H	8.10018953754895	19.82032172493593	6.86001933543001
H	6.65256119746767	19.45249165299045	5.90140323128923
C	7.16012832056290	16.26708185798532	3.91131210953960
H	7.79027018896074	17.14585016184462	4.07272666601031
H	7.81657357551314	15.39072661750349	3.96717838132160
H	6.42831562102156	16.20821387330308	4.71551128110769
C	-0.55836594994701	15.70597865615458	7.92345339719250
H	0.52794974498653	15.62626249744463	7.95674409531163
H	-0.98288439518305	14.79642703530967	8.36616424789240
H	-0.86372974071050	16.54385553155212	8.55917279586946
C	-2.27969878819752	19.85280539832431	2.63590505052237
H	-3.01158488686405	19.16263463420421	3.07151735088318
H	-2.55995447961814	20.01368697250870	1.58725706565784
H	-2.37381292587541	20.81335639246621	3.14321426957099
C	1.84794458633512	18.45763387362221	10.08284955200071
H	1.17795460469607	18.37563965316857	9.22517293659191
H	1.37170437505338	19.11262844456808	10.82172906949437
H	1.94642248686587	17.46923366325728	10.54540080005134
C	5.11633347852499	14.27319753862850	8.92197870766532
H	4.56575810334442	14.65431288387801	9.78947764942403
H	6.11695490078232	14.71821155960634	8.93626578347930
H	5.22712331035912	13.18754506879809	9.04202193612797
C	6.01173341653946	21.73756409270050	3.87478429450486
H	5.38927705094757	21.62975514343491	4.76902344315827
H	6.25723388619246	22.80098486546471	3.76512301522364
H	6.95219656891087	21.20364075736235	4.04326800096714
C	-0.72857747243996	14.59754792828004	5.68688738314511
H	-1.18294890155329	14.61388841983029	4.69108013716509
H	-1.12700916168859	13.71721285419598	6.20687449012912
H	0.34838209205775	14.45812845009445	5.56027806494350
C	6.24509174022958	21.38086307360170	1.42069800222219
H	7.15701358071458	20.79108294183471	1.56373850957559
H	6.53612751556126	22.43122311712432	1.29262089145842
H	5.77262903748854	21.04686637675612	0.48986775366832

Table S18 Cartesian coordinates of the optimized geometry of [(Cp'''Fe)$_3$(μ_3-Sb)$_2$] at the OPBE/TZVP level of theory, in the sextet spin state.

Sb	3.17793896082564	19.81348372346898	5.45169885967660
Sb	2.86105207481670	16.30957771847973	4.70470440461899
Fe	3.26887138258852	17.66309817621872	6.82903578983144
Fe	3.50001963171297	18.38354501006198	3.37478383026012
Fe	1.38229986445284	18.20806659884054	5.07916603332967
C	5.00031155760115	18.26090504621275	8.23715467124480
C	-0.25869758124130	18.43691051611707	6.30558226475279
H	-0.22828650202411	18.56599446590629	7.37896822576305
C	-0.29294835323765	19.52251380562591	5.35860479173859
C	3.13083341194597	18.86757657709163	10.18248946729678
C	3.80233491200608	18.05655796724960	9.05131298405709
C	4.29013604191838	16.01979151029293	7.96101990805797
C	-0.39051254835313	17.17724420161739	5.65505109164135
C	5.27864280942364	17.45633901938483	2.23410901137311
C	3.39211059665078	16.70931824215814	8.82299891214657
H	2.53984985850189	16.24999551982147	9.30228027074174
C	5.22997530058745	17.01261334302837	7.56820057968853
H	6.07344232024294	16.82916595302132	6.91957669192364
C	-0.38268533739577	17.48382567963059	4.26571752897951
H	-0.44921531715485	16.74317224632452	3.48236438615690
C	3.52345787315700	16.87781238170949	0.18067916368254
C	6.28944610669219	16.30238929440240	2.41233519326666
C	6.16588787437084	19.27736828338086	8.25365208564290
C	5.58359160923778	18.71785217513078	2.84729413362466
H	6.36192479861761	18.86115070764209	3.58239011321273
C	-0.61194891029838	20.93861216274076	5.89253404304329
C	4.20711260657415	17.72627842153802	1.27824933612993
C	2.71848109957842	15.68709047125689	0.72529798191405
H	3.32822630758222	14.98022884980012	1.28652518923603

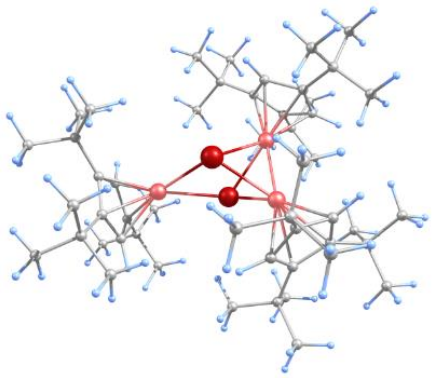


H	2.25691455842017	15.13913818599881	-0.10661293488238
H	1.91918565073001	16.02387098622192	1.39178258532245
C	3.94445780617138	19.12686930185663	1.36038045272575
H	3.21464388867966	19.63896407410272	0.75123491834599
C	0.06834831587596	21.19357815246223	7.24276884873294
H	-0.26017827129516	20.50178917532204	8.02226676335044
H	-0.18293768714248	22.20271119133261	7.59160172613191
H	1.15582386480411	21.13343182607862	7.14887933412279
C	4.81235627986327	19.77645357789911	2.28500648820771
C	3.16166637529506	13.73698290242057	7.86047996840130
H	2.63334785092231	13.93854933917036	6.92369436787920
H	2.49580893539880	13.98972829751703	8.69181029380454
H	3.35092243448854	12.65737914553403	7.91203140935162
C	4.48591700840550	14.50459720354280	7.92665533501345
C	-0.21073456359497	22.12277517498127	5.00677764959200
H	0.85898416299676	22.10183573726798	4.77680423282458
H	-0.41114894951994	23.05611819963712	5.54764739040001
H	-0.76976913122753	22.17736987705298	4.07370094853292
C	-0.36740791125667	18.90061826370313	4.03634629649817
C	-0.89817258041748	15.88055106448978	6.27546708541768
C	2.66843695381775	20.27299391098425	9.78480453507186
H	3.46505223182185	20.89586525923191	9.38283130962240
H	2.25600523717819	20.78918903850311	10.66170616279610
H	1.88168724778194	20.21278602677486	9.03345514688726
C	-2.13493353069650	20.98975960773015	6.15309634309709
H	-2.72405517866555	20.81623328352591	5.25054365196992
H	-2.41437496999002	21.97310042842302	6.55286223279479
H	-2.42726220436308	20.23445875536564	6.89129618602380
C	-0.70639995235587	19.43752725364483	2.62700697844336
C	7.42020786779201	16.50972133721115	1.37969780172861
H	7.06961303126366	16.43808697638297	0.34757606822219
H	8.20015580023238	15.74960293290353	1.52118094267286
H	7.88833181795461	17.49340740154797	1.50249363013455
C	5.16003580065564	21.26453115831407	2.27045456126105
C	5.81521562064122	20.73876717983896	8.54946401122270
H	5.06843700964214	21.12753793919542	7.84972094614337
H	6.71848146295804	21.35146176015509	8.44133732195522
H	5.45760550328695	20.89483208879678	9.56915956946171
C	4.09293423132100	18.95392911299355	11.38518878830397
H	4.46051129996938	17.96177211595965	11.67138834483058
H	3.56621327958869	19.37743926079293	12.24992931695998
H	4.95650256489996	19.59197346688571	11.19052592985722
C	3.91771960111809	22.15867927273515	2.18864762153043
H	3.31666911224163	21.95118943436701	1.29712635556869
H	4.21746882029856	23.21307505798251	2.13832648928906
H	3.27971402144255	22.03160714376090	3.06750750140475
C	7.18189804392928	18.79152020357765	9.31335588300391
H	6.75956627919271	18.77567250377437	10.32120394091810
H	8.05669389891123	19.45495501751581	9.32797515313014
H	7.53228881620384	17.77891456934339	9.08463989000062
C	-0.79111138748525	18.27507268381852	1.62304770464753
H	0.13340278549858	17.69423112789260	1.58654581665961
H	-0.96798956781902	18.67828583255216	0.61925981286267
H	-1.62016683247812	17.59545978491169	1.84776539315834
C	5.73730433778565	14.87908888118880	2.27965993716361
H	4.91662240612600	14.70805580299951	2.98322263735201
H	6.53118155875114	14.15866759019629	2.51265628467155
H	5.38380738224614	14.64177679999441	1.27599379974838
C	-2.44014511011605	15.99139229007633	6.27315022762122
H	-2.78072209214244	16.85632466752700	6.85353973980211
H	-2.88705625866874	15.09190040605225	6.71641719793071
H	-2.83356006825650	16.09454562079709	5.25523561761578
C	2.53888393184551	7.73684379794487	-0.63373427444565
H	1.75170209159132	18.17394205111272	-0.01623815460227
H	2.04983309531171	17.10228153967529	-1.38211222084574
H	3.04513998049248	18.54398576158727	-1.17514526131910
C	5.37725828977171	14.04661107020480	6.77052493280573
H	5.51874830757545	12.95960474731461	6.81830958544794
H	6.37103726621720	14.50372109021126	6.80858500707474
H	4.92460347772292	14.28104033328845	5.80333078492168
C	0.32015685610934	20.42573791329111	2.06982728746218
H	0.40477028583148	21.33404579271198	2.66162015309359
H	0.04809938880008	20.71804648674969	1.04714052821103
H	1.30747173388666	19.95962337681579	2.04888982896062
C	4.55811756526729	16.38107842437608	-0.84819163213121
H	5.14073806496582	17.21620508263787	-1.25251646229614
H	4.03707616193120	15.90223215539836	-1.68701034573537

H	5.25653638574301	15.64744064922721	-0.44370096510202
C	6.90660976777048	19.27720173592851	6.90477103809349
H	7.43171426401562	18.33698618469658	6.71158904457845
H	7.66853328404544	20.06623366857387	6.90800349972326
H	6.21951304589315	19.46982679931431	6.07767703255363
C	6.94629147293032	16.37567383592375	3.80073821478710
H	7.57756482369913	17.26032521898266	3.92355677295621
H	7.59260115939049	15.50233697076554	3.94623851210641
H	6.18679534105914	16.37862143440535	4.58516020777723
C	-0.43301419968958	15.70630498617006	7.72194018622989
H	0.65702287778333	15.69684232468006	7.78168770732353
H	-0.80956422802753	14.75975401275890	8.12935242593731
H	-0.80580733030665	16.50572577513375	8.37150040368069
C	-2.11103611017134	20.07579069290542	2.61676193762870
H	-2.85680355175184	19.39896779534195	3.04958687950774
H	-2.41034034090756	20.28047332061055	1.58113174222371
H	-2.15688870855676	21.02286326604269	3.15540179168963
C	1.87293975118066	18.14712975301755	10.70661820857475
H	1.13117496783560	17.97569882657537	9.92008019101610
H	1.40119133697317	18.77612875904259	11.47121109372695
H	2.10603405109829	17.18698029878867	11.18012273318715
C	5.19455691913144	14.13963295904039	9.25169484365825
H	4.58277626294974	14.40792234900988	10.12036189480462
H	6.15549695049260	14.65767145602528	9.34448811899773
H	5.38648019848333	13.05968555657198	9.29303081749804
C	5.99755991075271	21.68592085535044	3.48164456542126
H	5.44826324452460	21.54958215653068	4.41866953623986
H	6.26048608563156	22.74782061766703	3.40152612407806
H	6.93536172099804	21.12393307041852	3.54586457251291
C	-0.51248977795823	14.63997641934292	5.46297446648284
H	-0.88956683368795	14.68577926451009	4.43615948795359
H	-0.94173701882467	13.74192449718230	5.92493090472938
H	0.57302265577133	14.50833991158030	5.41524414191229
C	6.01115683022662	21.49504362866079	1.00063401734252
H	6.92384397785525	20.88884871320896	1.01549902246355
H	6.30570746278461	22.54973681448452	0.92834014372851
H	5.45460949504947	21.23849506722861	0.09213204102656

Table S19: Cartesian coordinates of the optimized geometry of [(Cp'''Fe)$_3$(μ_3-Sb)$_2$] at the OPBE/TZVP level of theory, in the octet spin state.

Sb	3.18667129656319	19.46364873818217	5.10939552558090
Sb	2.84157289730264	16.74526895876496	4.53222126982828
Fe	3.09214478795879	17.65597032399416	6.93207038185227
Fe	4.29638727278587	18.23530955600211	2.99588533912021
Fe	1.07930480919611	18.16956536756333	5.69970987857179
C	4.84091001069946	18.13758674158765	8.24779301888166
C	-0.74571998260567	18.61717157304644	6.74199302860563
H	-0.81189420962070	18.89567462694147	7.78473245722814
C	-0.70363616816703	19.56124919897485	5.65814595918509
C	2.99987064124095	18.72943010756834	10.22346453750104
C	3.64798604820206	17.92355441402026	9.07371714910817
C	4.13284200729029	15.90598859114437	7.95037848007299
C	-0.83432030455161	17.28053410902726	6.25698480825174
C	5.89149469672492	17.57811590103556	1.81850216043211
C	3.23423203500867	16.56995508502501	8.82620088207062
H	2.40286328887613	16.09183607460532	9.32279376533717
C	5.06568488773066	16.89811685136626	7.56247601049451
H	5.87842864607076	16.72961263032855	6.87095926064370
C	-0.73663909771277	17.39924520605636	4.84451484734142
H	-0.76445031175542	16.56525443790653	4.15980095011456
C	3.96127826100421	16.98298460763004	-0.09772367109660
C	6.88685924018639	16.41084045257939	1.99673897779523
C	5.97574638003187	19.18733303256352	8.22378137880903
C	6.24360024188108	18.86129846331732	2.37329793686874
H	7.07503053015797	19.02718728836470	3.04551668438324
C	-0.92788754753888	21.05366231726123	5.98692049345846
C	4.71377708392841	17.82738456345087	0.95914817755476
C	3.20158449031445	15.77859170994113	0.47924444221517
H	3.84246255488089	15.08500834013526	1.02235939272585
H	2.71713843869229	15.21839693544711	-0.33163761791799
H	2.42203167509323	16.11154063237468	1.17168402294579

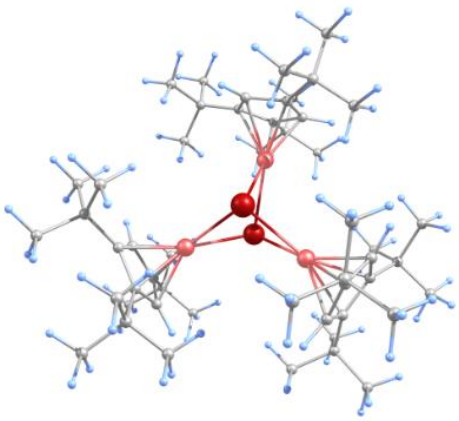


C	4.44421504148412	19.23465729586763	1.07036128474561
H	3.62819156416310	19.73964976296476	0.57267202108171
C	-0.24274406945875	21.43683283503967	7.30963056555151
H	-0.63822237290917	20.89293442405485	8.17212819952642
H	-0.40968594126226	22.50275317212083	7.50682305086497
H	0.83619428587697	21.27093518185458	7.25533779147236
C	5.38808994891660	19.88702001212074	1.89902211919333
C	2.92016949761133	13.70991518344749	7.52131933527572
H	2.47062372151833	14.04061871768132	6.58073450517037
H	2.20765674849431	13.91134999469810	8.32731649799611
H	3.05542868545491	12.62221670429633	7.46742290017564
C	4.26745709672840	14.40032279631527	7.75574228525209
C	-0.42442174588963	22.07702317344415	4.96396368063893
H	0.65384364219867	21.98314162998488	4.79971001478431
H	-0.60760027045363	23.08623880128838	5.35325000703737
H	-0.93278315606125	22.01826643134277	4.00113248842700
C	-0.68931633247921	18.77471660460257	4.43406440137169
C	-1.35735274498940	16.05993876253483	7.00278840406012
C	2.37089325521003	20.04926008031218	9.76163076054686
H	3.07246286216139	20.69888902160977	9.23916908258606
H	1.98014412078650	20.60406089956208	10.62515481925096
H	1.54227990303880	19.84453993609872	9.08180294965484
C	-2.44841547261095	21.25092470761722	6.18313300876653
H	-3.01853815057073	21.02610447139869	5.27741404123167
H	-2.66018272487162	22.29166595588200	6.46078396999216
H	-2.82878126424530	20.60621748503667	6.98316217901188
C	-0.85290843022703	19.11249231377433	2.93447888939293
C	8.00038293245290	16.55743387257724	0.93842852545338
H	7.61566309260148	16.47783782166861	-0.08206785818909
H	8.76186007312196	15.77710943278846	1.07108989399094
H	8.49898333733537	17.52958832178183	1.02706659785379
C	5.59282528492082	21.38990234240982	2.02959268057919
C	5.55056094915450	20.64944015303502	8.40026547472041
H	4.81336214277461	20.94421082339128	7.64613771174379
H	6.42618850791824	21.29871082771713	8.27694787021123
H	5.13983469808357	20.86732268051785	9.38770455858817
C	4.02062299396897	18.99348425734476	11.34742199416954
H	4.49954334077882	18.06358262568980	11.67530165723005
H	3.50464673957775	19.42503678866934	12.21461644059810
H	4.80147456163778	19.69673622106431	11.05757512723543
C	4.26608478988240	22.15917901868691	1.98644304105632
H	3.71984533516037	21.99050388340644	1.05148175449693
H	4.45376644873229	23.23777773182899	2.06022266279491
H	3.61374681753565	21.87044187789685	2.81627668140260
C	6.99370175957773	18.81533199534073	9.32643563452752
H	6.57119768164543	18.87202981820356	10.33135707561428
H	7.85568918500524	19.49455474695736	9.28684551420194
H	7.36579316448827	17.79471818821769	9.18116106338024
C	-0.86742799190101	17.82539065046875	2.08737334106314
H	0.05020793839472	17.24269268523680	2.21049654487856
H	-0.94319862044032	18.09898990429944	1.02845580536727
H	-1.72580533868832	17.18386502084750	2.31756306410572
C	6.29129230045756	15.00134839187402	1.90855420693600
H	5.47908519021533	14.86513875918373	2.63034910539532
H	7.06867209930821	14.26308117815709	2.14214722348071
H	5.91335345101001	14.75588884130027	0.91532350421533
C	-2.89779990516701	16.17149190464763	7.00282054392996
H	-3.23221262770470	17.08274631844766	7.51213558577655
H	-3.34438177705965	15.31370744971450	7.52280985474757
H	-3.29887110996299	16.19312459154794	5.98271305558807
C	2.90424787720369	17.84205445069620	-0.81644596397509
H	2.14984984424912	18.23442120356055	-0.12727594002825
H	2.38044969133663	17.22102459290184	-1.55290853985534
H	3.35147570898577	18.68266446958220	-1.35891770641701
C	5.20861570267436	14.05198724057001	6.59843594748683
H	5.27492056880875	12.96303812205969	6.48298667765926
H	6.22605555371752	14.42074741013994	6.77101709884782
H	4.84931285252755	14.46665445243578	5.65114994956447
C	0.26079185802823	19.98762414454614	2.34601172634519
H	0.37728642410554	20.93851236265324	2.86020993085298
H	0.04416382998565	20.20265427349450	1.29150770149829
H	1.22118481579599	19.46691111441531	2.39562139634189
C	4.93268504400995	16.51672898361299	-1.19971721923443
H	5.48405053916628	17.36570151815355	-1.61954853787921
H	4.36880656500107	16.04805724058383	-2.01648709522549
H	5.66219728825350	15.78343104328932	-0.85012978528572
C	6.75167015485980	19.12301917079872	6.89582317124587

H	7.31669702104529	18.19275215516972	6.78188556101493
H	7.48487888474043	19.93836701365393	6.86692326726851
H	6.08851567776801	19.23159017728785	6.03342395885409
C	7.55961557567840	16.49338325458341	3.38093803242647
H	8.18160210395266	17.38544699043565	3.50206865888561
H	8.22021644932855	15.62843236468492	3.51804450415034
H	6.81446697866357	16.48201841854738	4.18291289808694
C	-0.87516322136220	16.01656779861646	8.45266454346446
H	0.21553161177826	15.98278005370219	8.49386698238303
H	-1.27403056344151	15.12924801959211	8.96007421446064
H	-1.21195537642604	16.88949410983864	9.02211617794849
C	-2.22701526678413	19.77484833392153	2.70159808928111
H	-3.03372045837071	19.17325989669730	3.13704652520663
H	-2.41661927516779	19.85735785468346	1.62392022828429
H	-2.29286713091335	20.78066563241180	3.11817833891580
C	1.86607672513431	17.92570580898404	10.88497177619176
H	1.06878524087412	17.68394974885165	10.17902443199309
H	1.42331849759435	18.53169358765816	11.68472037459546
H	2.22598632093511	16.99836224678315	11.34420863008364
C	4.88255347555392	13.85065576212967	9.06328256416825
H	4.22316294895515	14.03045662472347	9.92007526652161
H	5.84741051075636	14.32467069991001	9.27840951836561
H	5.04653876272976	12.76826018786397	8.98227866833499
C	6.34043658696455	21.76113231006382	3.31578244477867
H	5.78828859400731	21.44218047822821	4.20505196953033
H	6.47366079379927	22.84854475528752	3.37211087165931
H	7.33814730417670	21.31113995161133	3.35357545542888
C	-0.97055553048166	14.75244295373936	6.30130866125426
H	-1.39861765312691	14.68536267545101	5.29561529159354
H	-1.35289528249617	13.89480659517736	6.86926778877634
H	0.11390337797038	14.64805475311198	6.21748617631793
C	6.45489620883944	21.82216008346953	0.82230769789906
H	7.42026513923935	21.30402565601403	0.81892031893179
H	6.64911142861755	22.90227751616057	0.85817290343483
H	5.95276947845506	21.60007142136345	-0.12643072060578

Table S20: Cartesian coordinates of the optimized geometry of [(Cp'''Fe)$_3$(μ_3-Sb)$_2$] at the OPBE/TZVP level of theory, in the decet spin state.

Sb	3.13168234147571	19.47983915814254	5.29954635514073
Sb	2.72141546526593	16.76960782121692	4.91282787348694
Fe	3.91205874899109	17.76300733128919	7.13220982729803
Fe	4.13564672665142	18.15675237381077	3.20442445797587
Fe	0.68909142915651	18.47915378150896	5.29645873906961
C	5.46262166448420	18.06447991509368	8.55333694265986
C	-1.11623996985466	18.62671534959455	6.33129291379186
H	-1.15108717056237	18.81637445087184	7.39617501569447
C	-1.15462617918253	19.66152489656672	5.32382816668539
C	3.38306949754803	18.80620131792906	10.24853661862376
C	4.16104512743750	17.92519564997191	9.24492698546929
C	4.67045613476481	15.86804649636857	8.20228427081994
C	-1.09186806469961	17.33171137535411	5.73384600089492
C	5.73306183443960	17.49791083752124	1.98729963294763
C	3.72021566037431	16.58632647666079	8.97471627033538
H	2.78797684847875	16.16970912443811	9.32870909615012
C	5.71138386543641	16.78956946862705	7.93771216518403
H	6.58793234327566	16.56361465731857	7.34667567271568
C	-1.09758836031952	17.57980886022640	4.32669528662093
H	-1.06902207673965	16.80418370508723	3.57522415532128
C	3.76312591176425	16.84146475724209	0.13237284929014
C	6.73514282816052	16.33845324317157	2.17486785988272
C	6.61357564405591	19.09463528564431	8.57796363990350
C	6.08439330994694	18.79100816827676	2.50939963080845
H	6.92232551959503	18.97486632950017	3.16823186193955
C	-1.39399105810692	21.11527837716862	5.78590112725305
C	4.53814355453050	17.72189005209588	1.14194788415902
C	3.00734120757082	15.66979320505324	0.77826355973908
H	3.65924265470552	14.98689307743539	1.32217094748644
H	2.48566489827090	15.08808313842322	0.00630581499177
H	2.25779402017975	16.03659727542463	1.48743828149976
C	4.25974307912698	19.12597716659704	1.22797000227682
H	3.42993944840535	19.61338832006905	0.73583649104229

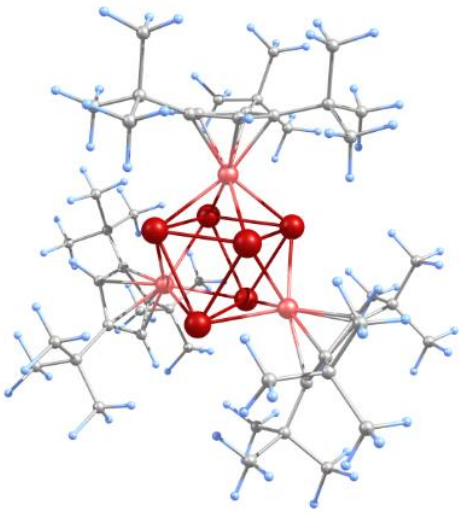


C	-0.79981392662857	21.34394662016436	7.18975431693590
H	-1.31087656571857	20.76852068424033	7.96818054887760
H	-0.90873499478071	22.40101656529149	7.46020700927642
H	0.26750235711711	21.10209937174877	7.22005957742265
C	5.20589220277886	19.80006227583930	2.03939183490026
C	3.29723290785274	13.76141421754159	7.87690447983752
H	2.73702981252569	14.19457730316942	7.04276329229366
H	2.71931311291803	13.91740485042925	8.79445130365176
H	3.36345495465227	12.67805088827650	7.71659748142104
C	4.70373280804407	14.36400841341783	7.97199027579549
C	-0.78428568834173	22.20979942893898	4.90148354304139
H	0.30283781808340	22.10082516253789	4.82575936925992
H	-0.98582423600020	23.18996822938874	5.35101447536763
H	-1.20097949442723	22.23517620258368	3.89451162481191
C	-1.18657756328688	18.96958611345001	4.03651914593286
C	-1.38129865915624	16.00409049657177	6.42341827191345
C	2.89383013976993	20.14010828792086	9.66182247588200
H	3.70314515357282	20.77722655402168	9.30657549141514
H	2.33743674732026	20.70223471623862	10.42411323083258
H	2.22052585324601	19.95992767012021	8.81870265395543
C	-2.91792560109137	21.33580769565859	5.89907934480084
H	-3.42509707261282	21.24953205883420	4.93523694657233
H	-3.12787643376800	22.33712646541625	6.29780457280949
H	-3.36828385576367	20.60297787946883	6.57825631020463
C	-1.31357318058157	19.44304921414875	2.57416160359071
C	7.82327453559245	16.45674683315760	1.08709247887321
H	7.41613277517811	16.34713999604647	0.07822381970997
H	8.58988344366957	15.68261923992612	1.22539624115100
H	8.31976772062354	17.43262356223640	1.13704519855835
C	5.40431134166939	21.30553183508908	2.14293161998488
C	6.20085357033274	20.56381612831100	8.71940373902467
H	5.50817703877985	20.86471907165878	7.92643060198129
H	7.09177665877460	21.19854949671656	8.63697491997889
H	5.74501047900802	20.79283392378828	9.68451348297783
C	4.23196691871409	19.05957303458885	11.50871669988529
H	4.58404803982331	18.11577888143487	11.94101277899257
H	3.62632819172361	19.57040078750357	12.26851461557176
H	5.10331538572959	19.68676119563295	11.31475943301515
C	4.07367381252452	22.06721705691505	2.09849334533482
H	3.52583138529527	21.88899662172281	1.16622606107226
H	4.25572565362867	23.14730867961689	2.16366176382681
H	3.42496255055962	21.78028263365140	2.93184739590210
C	7.56593153198085	18.72666411177959	9.73572054609617
H	7.07553442527169	18.79016659743249	10.71141598391888
H	8.43056165270904	19.40353236272860	9.75144019388342
H	7.94168255446016	17.70361470750808	9.62203141889120
C	-1.44654911159358	18.23648709759613	1.62672200270217
H	-0.56065149648972	17.59334437870622	1.63802618793495
H	-1.56606626522698	18.59963937154023	0.59902153968607
H	-2.32403749020527	17.62229783078923	1.86050478237104
C	6.13901403373564	14.92645938195188	2.14280713940227
H	5.34331431178910	14.81212752178275	2.88665641279080
H	6.92209265443071	14.19545988911947	2.38009320760774
H	5.73820141806607	14.65112800657013	1.16669833927565
C	-2.90734110099167	15.92554588431614	6.64216618818071
H	-3.26154741744500	16.74144579715666	7.28224879387527
H	-3.18028889047099	14.97658413699938	7.12257784231049
H	-3.44683619224695	15.98840522941089	5.69041078488196
C	2.70023122199631	17.67766067685445	-0.60382808266905
H	1.94806065390874	18.08886239103806	0.07642159899049
H	2.17360725839883	17.03371214972807	-1.31828750428783
H	3.14375488898260	18.50240281472883	-1.17301598512924
C	5.49288720169145	13.99130615193534	6.71181826089848
H	5.50943644499780	12.90137291581971	6.58634137445105
H	6.53458059758520	14.32556446546421	6.76564586092695
H	5.04166087947398	14.42756565159057	5.81548961239198
C	-0.08994323432070	20.23882081788495	2.09265504939498
H	0.07290167271960	21.15195102062632	2.66323265528807
H	-0.21328018188059	20.52010720070326	1.03862506415266
H	0.81797744778255	19.63325867684848	2.17489049984979
C	4.70945419829575	16.32267378430715	-0.96737733606863
H	5.25880635389137	17.14939879497547	-1.43196669852363
H	4.12694957102235	15.82571112663469	-1.75361236664835
H	5.44022558391308	15.59833398586675	-0.60267412794430
C	7.42801937476294	19.01337786172867	7.27160194587309
H	7.96449099316161	18.06592570831019	7.16092662177934
H	8.18798182368590	19.80453263094738	7.26701598953572

H	6.78945210510169	19.15481709694809	6.39356894665030
C	7.43998938531057	16.46210610821087	3.53982581893145
H	8.06157734410798	17.35876347278133	3.62229684784492
H	8.10714786613121	15.60335456524215	3.68403043877362
H	6.71573982740266	16.46842990140694	4.36061637829656
C	-0.67872366940631	15.91405720859478	7.78269199605861
H	0.40617482453812	15.99203590961067	7.66541177435017
H	-0.90193376130836	14.95433596776101	8.26688665347909
H	-1.00882855939877	16.70312329373385	8.46787668004485
C	-2.60051936114367	20.26451526231630	2.37188361614297
H	-3.48069739459319	19.69745384435378	2.69793344741147
H	-2.72945355278446	20.49381544790902	1.30676954281571
H	-2.59458912612606	21.21331080010840	2.90867298795181
C	2.11768172281631	18.07552354592644	10.73781565014224
H	1.42701597509242	17.84435805577338	9.92004860903335
H	1.58397459981557	18.72632999916199	11.44082225377822
H	2.35364582036201	17.14652282317530	11.26948898548311
C	5.41892845355721	13.75009561958886	9.19709928073795
H	4.88884939939315	13.98782122987057	10.12663457975845
H	6.44360687354685	14.12798415862023	9.29033441258968
H	5.46794787868619	12.65720736950277	9.10355494118153
C	6.16094536589866	21.69734031588953	3.41767098298469
H	5.62162828188163	21.37747499129646	4.31481840091132
H	6.28218690820267	22.78658034070715	3.46407876125812
H	7.16421806790804	21.25919102127400	3.44882692099430
C	-0.95551768894115	14.80944237880407	5.56093476105746
H	-1.51096916817908	14.76877314099880	4.61801514030674
H	-1.15390436371664	13.87089747598904	6.09322482135171
H	0.11281431347965	14.84548319798556	5.32565372676231
C	6.25473893278735	21.72401494131495	0.92246981619506
H	7.22254542441111	21.21061532391246	0.91912361895623
H	6.44393361189431	22.80539019962088	0.94118504367152
H	5.74598331345069	21.48569607310368	-0.01870940578092

Table S21: Cartesian coordinates of the optimized geometry of [(Cp'''Fe)$_3$($\mu_{3,}\eta^{4:4:4}$-Sb$_6$)] (**6**) at the OPBE/SVP level of theory, in doublet spin state. Total Energy: -7229.209625966045 hartree.

Sb	-1.11651036573435	8.59641546661141	3.12052605158467
Sb	-2.12397948134124	10.42905034553532	5.15971357430055
Sb	-2.14388597714058	7.56423867437319	5.64755467169907
Sb	1.60230808185452	8.81283697653564	4.34120799679653
Sb	0.59064255061731	10.64484533549113	6.37197137331574
Sb	0.58779246367050	7.76693034633383	6.85152672909420
Fe	0.06715476141924	10.82870501012802	3.79590396241360
Fe	-1.42525188892950	9.35154674968862	7.41387256498297
Fe	0.04423966769283	6.71014212490692	4.53077943399306
C	-2.28788398781005	8.45446240072709	9.02485512600344
H	-2.50461465464125	7.39267284826791	9.12588712047636
C	-3.22870093360636	9.42794483148888	8.51357855030447
C	0.75131121388798	5.53803742579202	3.02650646633816
H	1.05987380729989	5.88891224756609	2.04385777790331
C	0.08009371669107	12.85144665433826	3.60223735794939
H	-0.17603580449308	13.56941147918553	4.37977031275447
C	-0.85619986237923	12.34590873932002	2.64290710583213
C	-0.58342431651268	5.07029395381643	3.33561753364096
C	-1.08065785265435	9.07041039291191	9.48945151059397
C	-4.71918229393103	9.02863947443492	8.33629968555242
C	0.80977598981948	4.92931902388756	5.19877346118824
H	1.17849817119315	4.67680014238215	6.19298478841020
C	1.30939882368668	11.47099536967567	2.19877426349782
C	-0.09269011186746	8.51092491325559	10.51756962196734
C	1.64301084461301	5.38507350385752	4.13654999155415
C	3.17019155381215	5.27805588898244	4.09680218851988
C	2.29001671882744	10.87993792655476	1.14843311114008
C	-0.54389068887985	4.67874708128145	4.74968103071178
C	-2.52811461813560	10.71961637373841	8.57803736696864
C	-1.22208239159910	10.44239037558183	9.13938104630549
H	-0.48013342235883	11.20539038795893	9.37353721969668
C	-4.20280203967313	12.56393791931953	7.71447536687984
H	-4.08907607945912	12.26422908244516	6.66223441468744
H	-4.35187972270927	13.65683530077351	7.72823381101037
H	-5.12515694858561	12.11477610665973	8.10369032431014



C	-1.83047858046783	13.11695176881877	8.02091808076016
H	-0.89191979084656	13.02007791142056	8.58558152823031
H	-2.13774956707136	14.17393803512909	8.09336621186510
H	-1.60979460949501	12.91576233630425	6.96088139981457
C	-0.09440909036492	11.44513989900902	1.84618089095068
H	-0.49850040427524	10.90106356867757	0.99251881784236
C	1.42676665641785	12.38754067690307	3.34033092485081
C	3.83259635161177	5.79758263023921	5.38206747711241
H	3.65992363113529	6.87697275919534	5.51750781818232
H	4.92336458164788	5.63291580578904	5.34200470669616
H	3.45749993914325	5.28200997482368	6.28040693705095
C	-5.35196113037220	9.42874459343715	6.99301571918647
H	-5.29549604737269	10.50156812663014	6.78414715886864
H	-6.41979959014214	9.14893604096162	6.98348716067716
H	-4.86510888774145	8.90351343704701	6.15684491690500
C	0.01604040942393	6.98048133471165	10.45946166658415
H	-0.95790161085344	6.48703192406315	10.60820924742632
H	0.69112359745775	6.61600050267572	11.25192451972554
H	0.42476444051544	6.64149140451280	9.49532123070954
C	-2.96307224551635	12.21074725832992	8.54606868408753
C	1.30806972377928	9.12821493249258	10.38132558145128
H	1.75961112154118	8.89906187011786	9.40284632512009
H	1.97971400339502	8.72841625992348	11.16025261860537
H	1.29315087255734	10.22407908360606	10.49805418947939
C	-3.20493505552532	11.87890802661468	1.75929305497199
H	-2.81218543997258	11.31374858479556	0.89921950895879
H	-4.14449633132194	12.35551535558766	1.43135085028315
H	-3.45471518315740	11.15419846838533	2.55002097257900
C	-4.89575634412864	7.49887277359843	8.44879649286214
H	-4.30982174455794	6.95713283063053	7.68994915984026
H	-5.95568357889722	7.24153446479373	8.28315545337959
H	-4.62604777285496	7.11142886803901	9.44461615595890
C	-1.28171827105720	4.19513548085781	7.15243269290228
H	-0.24702186244202	4.16276846136615	7.52413092960543
H	-1.86952290534454	3.50771629629976	7.78296500907003
H	-1.66861874365876	5.21138323860067	7.33017603109780
C	-1.42282600351581	3.78823960997879	5.67173886182235
C	-2.99268049032161	5.37575460706223	2.38421307827300
H	-3.47084947435879	5.03918352321867	3.30840459124062
H	-3.64754598081401	5.07985750851653	1.54558401149192
H	-2.96194502247893	6.47651598117685	2.40824297711807
C	3.77762207847882	6.00504782532744	2.88735225064597
H	3.40815172839506	5.59925208645551	1.93112720779913
H	4.87526997938301	5.88881481133582	2.88612199241956
H	3.55986683947970	7.08451701275209	2.91078751689844
C	-1.66146163658002	3.26920473439043	1.95194611096824
H	-0.65657604304040	2.83607499909871	1.81306203749943
H	-2.24735833841177	3.05280506463298	1.04136247186572
H	-2.14490131123432	2.73408824277323	2.77994563781887
C	-5.52800303747616	9.63000045533794	9.50795056201626
H	-5.08554350102916	9.35159876475211	10.47927665556898
H	-6.56227537517080	9.24590212361789	9.48993462178610
H	-5.58895121016053	10.72583432357401	9.46941377900463
C	3.73361483820649	10.62326743773220	1.59938777673916
H	4.27218476371589	11.54188227370682	1.86444094359549
H	4.29629286277672	10.15531171296781	0.77326877176766
H	3.77728097902222	9.93420885483955	2.45709017763018
C	-1.92132401376384	13.92519363145880	1.09388622209357
H	-1.19206080210273	14.69617625744939	1.39295938003285
H	-2.84896333548454	14.43681233965837	0.78112132176160
H	-1.51271921712518	13.40418171646168	0.21246628946321
C	1.77628174172648	9.53345663418012	0.59694966869355
H	1.75211792350675	8.76141872966102	1.38289726558868
H	2.45292286800173	9.17540778883580	-0.19790608093751
H	0.77177590569447	9.59134700601186	0.15219045897696
C	-2.21211472127534	12.94231529970850	2.25450572420713
C	-3.23258572912735	12.61778239399601	10.01774433743743
H	-4.01839612222934	12.00076437590077	10.47767495637790
H	-3.55768311670843	13.67195821136380	10.06926648865912
H	-2.32900192605638	12.51812833081414	10.63983906643843
C	-1.06318883275910	5.39070412432950	0.85299502651649
H	-0.89879152946562	6.47771497759027	0.92083090700546
H	-1.81308463492464	5.22217094259766	0.06176871989210
H	-0.12887393267182	4.91383524234229	0.51544091138845
C	-2.93034525270455	3.75267427583459	5.38889748188647
H	-3.38630942816486	4.75306410177138	5.44927770770335
H	-3.42770870982238	3.12197038710585	6.14489958922566

H	-3.17588197681367	3.32093946076026	4.41030099739729
C	-0.87039103400428	2.34639248385616	5.53448298534465
H	-0.93182769985414	1.97900998583920	4.49928126823042
H	-1.44702105424742	1.65252068992415	6.17082326172131
H	0.18564309949927	2.28264744546623	5.84210190733353
C	-0.67307395453860	8.89925290009178	11.89983746151571
H	-0.75246732407503	9.99290671138768	12.01331038891338
H	-0.02516316282836	8.52076589844024	12.71023933459997
H	-1.68048176101140	8.47523575403753	12.04876898229820
C	2.62655070750570	13.10666907146574	4.01369182480208
C	-2.84652766065740	13.74164082249928	3.40192278750918
H	-3.02543892260921	13.10895972379466	4.28472387761971
H	-3.81979834862146	14.15337681696254	3.08672737859726
H	-2.21968598892012	14.59426843285627	3.71099354690118
C	3.68498147788122	12.17872326435152	4.63172461898156
H	3.26413908524050	11.60719132682208	5.47393150582081
H	4.52197090493363	12.77865618870648	5.02934770898209
H	4.10620421139540	11.45875746270460	3.92339203523713
C	3.48037722647189	3.76829314331535	3.95340969206971
H	3.10910254334864	3.19259157511952	4.81727542963872
H	4.57043991636082	3.60274247622302	3.88290669908155
H	3.01483038307375	3.34628507248169	3.04699986735220
C	-1.58354979140993	4.79589398015884	2.18071038494647
C	3.28050313312970	14.04357844018138	2.97304429537240
H	3.79267497742178	13.50094821361938	2.16694333955423
H	4.03573731734835	14.68424502327036	3.46126577454509
H	2.53221629650053	14.70604621402081	2.50565563779974
C	2.14412402953272	14.02190734869166	5.15965749825790
H	1.5006386708766	14.84372386803477	4.80660471797353
H	3.01837563835964	14.48227853136457	5.64914889104173
H	1.59973966780274	13.45831677301243	5.93406219230886
C	2.31987188548165	11.88155023864261	-0.03363883715243
H	1.32092828656992	12.01512057915086	-0.47884037479496
H	2.99449244262737	11.51585102028201	-0.82716132622940
H	2.67478753498845	12.87600848394738	0.27528373397817

Table S22: Selected Meyer bond orders for [(Cp'''Fe)$_3$(μ_3,$\eta^{4:4:4}$-Sb$_6$)] (**6**) at the OPBE/SVP level of theory, in doublet spin state.

B(0-Sb, 1-Sb)	0.52	B(0-Sb, 2-Sb)	0.54	B(0-Sb, 3-Sb)	0.34
B(0-Sb, 6-Fe)	0.72	B(0-Sb, 8-Fe)	0.70	B(1-Sb, 2-Sb)	0.53
B(1-Sb, 4-Sb)	0.34	B(1-Sb, 6-Fe)	0.71	B(1-Sb, 7-Fe)	0.73
B(2-Sb, 5-Sb)	0.33	B(2-Sb, 7-Fe)	0.69	B(2-Sb, 8-Fe)	0.72
B(3-Sb, 4-Sb)	0.54	B(3-Sb, 5-Sb)	0.53	B(3-Sb, 6-Fe)	0.73
B(3-Sb, 8-Fe)	0.70	B(4-Sb, 5-Sb)	0.54	B(4-Sb, 6-Fe)	0.69
B(4-Sb, 7-Fe)	0.72	B(5-Sb, 7-Fe)	0.70	B(5-Sb, 8-Fe)	0.73
B(6-Fe, 7-Fe)	0.24	B(6-Fe, 8-Fe)	0.25	B(7-Fe, 8-Fe)	0.24

Table S23: Loewdin spin population in [(Cp'''Fe)$_3$(μ_3,$\eta^{4:4:4}$-Sb$_6$)] (**6**) calculated at the OPBE/SVP level of theory, in doublet spin state.

0 Sb	-0.041
1 Sb	-0.041
2 Sb	-0.039
3 Sb	-0.043
4 Sb	-0.040
5 Sb	-0.042
6 Fe	0.454
7 Fe	0.440
8 Fe	0.510

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