Supporting Information

Application of Ferrocene-Bridged *N*-Heterocyclic Carbene Stabilized Bis-Phosphinidenes in Sn(II) Complexation

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1. Experimental Details

1.1 General Methods and Instrumentation

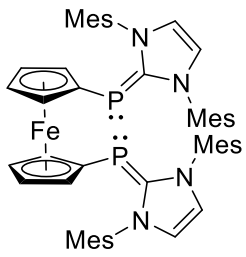
All reactions were performed in flame dried glass ware under Argon in a glovebox (model LABstar from MBraun Inertgas-Systeme GmbH) or using Schlenk technique. Standard chemicals for the synthesis reactions were purchased from the commercial distributers. All used solvents were dried over Na/benzophenone prior to use. Deuterated NMR solvents were dried over 3 Å molecular sieves (C_6D_6), potassium mirror (THF-d_8) or CaH_2 (CD_3CN). 1,1'-Bis-(dichloro-phosphine)ferrocene, IMes, ^{Me}IMes, $SnCl_2$·dioxane, $Sn(OTf)_2$, and bisNHI were synthesized according to or analogue to literature known procedures.[S1-6]

All NMR samples were prepared in an argon atmosphere using J. Young PTFE valve NMR tubes. ^{1}H, ^{13}C, ^{19}F, ^{31}P, and ^{119} Sn NMR spectra were recorded on Bruker Avance 300 MHz, 400 MHz, and 500 MHz spectrometers at ambient temperatures (300 K). The obtained ^{1}H- and ^{13}C NMR spectra were calibrated on the residual proton and natural abundance carbon signals of the deuterated NMR solvent and the chemical shifts δ reported in ppm values, relative to tetramethylsilane. The observed signal multiplicities were abbreviated as following: s = singlet, d = doublet, t = triplet and m = multiplet.

Liquid Injection Field Desorption Ionization Mass Spectrometry (LIFDI-MS) was measured directly from an inert atmosphere glovebox with a Thermo Fisher Scientific Exactive Plus Orbitrap equipped with an ion source from Linden CMS.[S7]

Quantitative elemental analyses (EA) were carried out using a EURO EA (HEKAtech) instrument equipped with a CHNS combustion analyser at the Laboratory for Microanalysis at the TUM Catalysis Research Center.

1.2 Synthesis of BisNHCP 3a (NHC = IMes)



To 1,1'-bis-(dichlorophosphine)ferrocene (1.0 g, 2.58 mmol, 1.0 eq) and IMes (1.73 g, 5.67 mmol, 2.2 eq) was added hexane (150 mL) and the suspension stirred at r.t. overnight. The precipitate was separated via Whatman filtration and washed with hexane (20 mL). The yellow solids were dried under vacuum and suspended in THF (120 mL). After cooling to -80 °C, a NaNaph solution (30 mL, 3.44 M in THF, 10.32 mmol, 4.0 eq) was

added dropwise over 10 min. After 30 min the suspension was warmed to r.t. and stirred overnight. The solvent was removed in vacuo and the resulting solids extracted with toluene (100 mL). The solids were dried and washed with hot hexane (60 + 40 mL). After drying under vacuum, the product was isolated as yellow powder (560 mg, 0.66 mmol, 25%). Crystals suitable for SC-XRD analysis were grown from a saturated Et_2O solution at -35 °C.

^{1}H NMR (400 MHz, C_6D_6, 300K): δ[ppm] = 6.49 (s, 8H, $C_{Mes}H$), 5.70 (s, 4H, NCH), 3.76 (s, 4H, $C_{Cp}H$), 3.61 (s, 4H, $C_{Cp}H$), 2.16 (s, 24H, *o*-$C_{Mes}CH_3$), 1.95 (s, 12H, *p*-$C_{Mes}CH_3$).

^{13}C NMR (101 Hz, C_6D_6, 300K): δ[ppm] = 170.51 (d, $^1J_{C,P}$ = 105.8 Hz, $C_{carbene}P$), 138.10 (*p*-$C_{Mes}CH_3$), 136.04 (NC_{Mes}), 134.45 (*o*-$C_{Mes}CH_3$), 129.32 ($C_{Mes}H$), 117.88 (N*C*H), 77.44 (s, $C_{Cp}H$), 77.37 (s, $C_{Cp}H$), 72.39 (d, $^1J_{C,P}$ = 36.4 Hz, $C_{Cp}P$), 71.55 (s, $C_{Cp}H$), 71.49 (s, $C_{Cp}H$), 20.94 (*p*-$C_{Mes}CH_3$), 18.44 (*o*-$C_{Mes}CH_3$).

^{31}P NMR (162 Hz, C_6D_6, 300K): δ[ppm] = -56.98

Elemental Analysis: $C_{52}H_{56}FeN_4P_2$

Calculated [%]: C (73.06), H (6.60), N (6.55)

Observed [%]: C (72.69), H (6.52), N (6.37)

LIFDI-MS: Calculated for $C_{52}H_{56}FeN_4P_2$: 854.33296

Observed: 854.33157

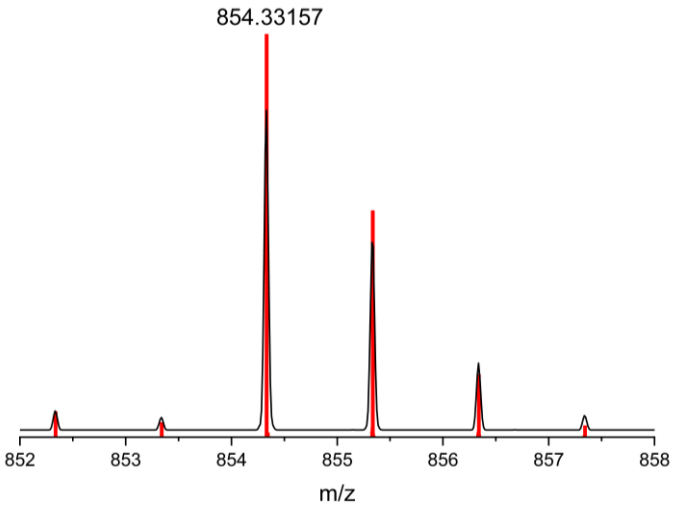


Figure S1 Measured (black) and calculated (red) LIFDI-MS for **3a**.

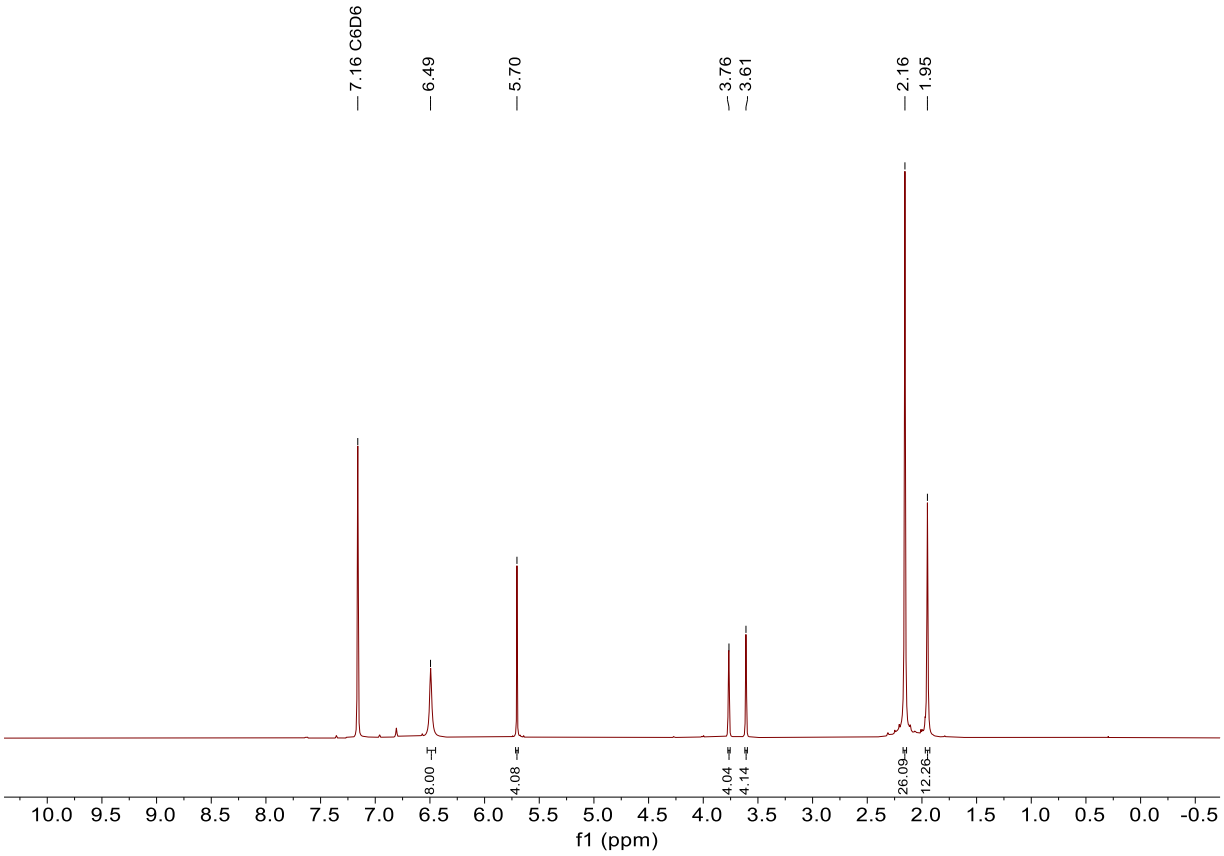


Figure S2 ^{1}H NMR of bisNHCP **3a** in C_6D_6.

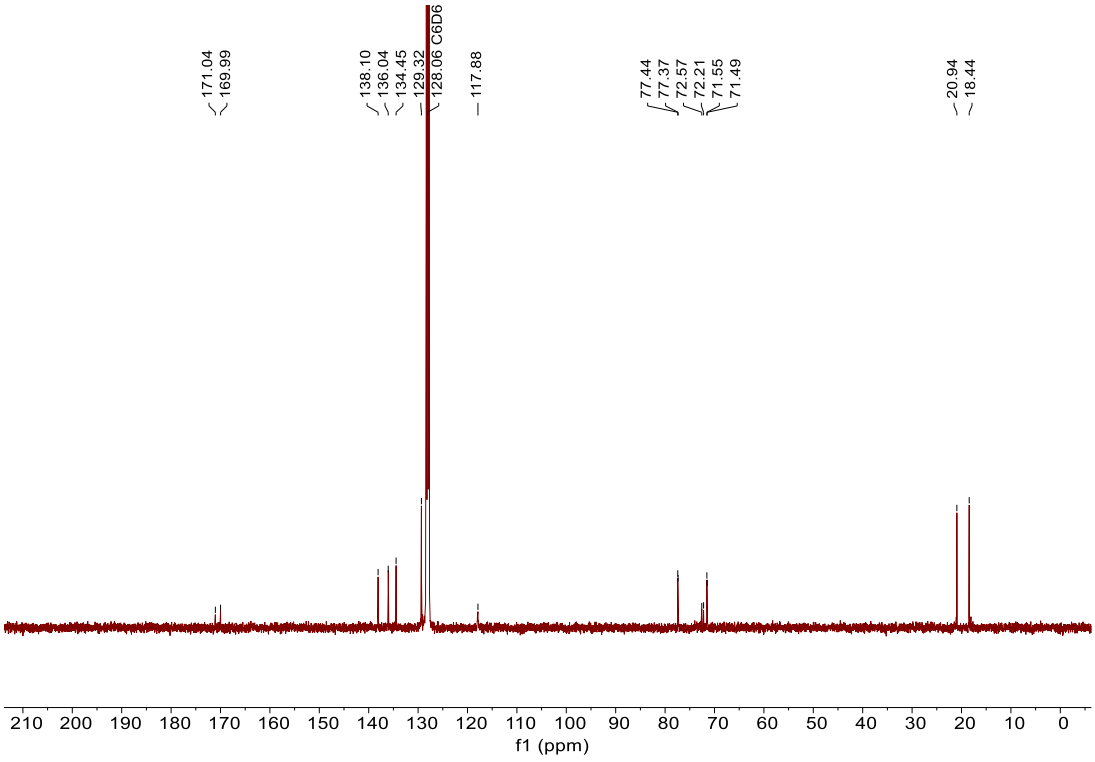


Figure S3 ^{13}C NMR of bisNHCP **3a** in C_6D_6.

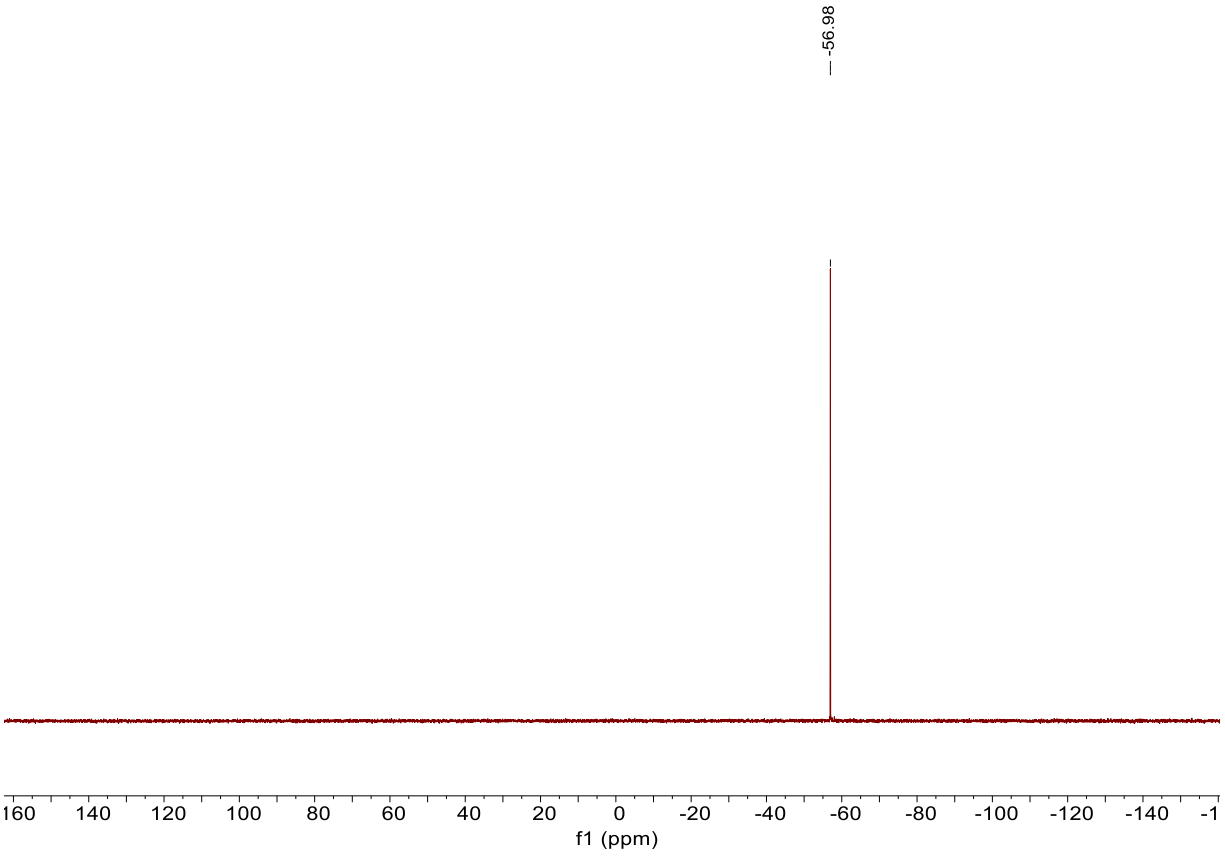
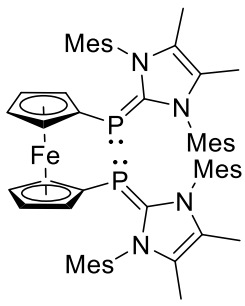


Figure S4 ^{31}P NMR of bisNHCP **3a** in C_6D_6.

1.3 Synthesis of BisNHCP 3b (NHC = ^{Me}IMes)



To 1,1'-bis-(dichlorophosphine)ferrocene (1.0 g, 2.58 mmol, 1.0 eq) and ^{Me}IMes (1.89 g, 5.67 mmol, 2.2 eq) were added hexane (150 mL) and the suspension stirred at r.t. overnight. The precipitate was separated via Whatman filtration and washed with hexane (20 mL). The yellow solids were dried under vacuum and suspended in THF (120 mL). After cooling to -80 °C, a NaNaph solution (30 mL, 3.44 M in THF, 10.32 mmol, 4.0 eq) was added over 10 min. After 30 min the cooling bath was removed and the suspension stirred overnight. The solvent was removed and the resulting solids extracted with toluene (100 mL). The solvent was removed and the solids washed with warm hexane (40 + 10 mL). The product was isolated as orange powder (1.1 g, 1.21 mmol, 47%). Crystals suitable for SC-XRD analysis were grown from a saturated Et_2O solution at -35 °C.

^{1}H NMR (400 MHz, C_6D_6, 300K): δ[ppm] = 6.52 (s, 8H, $C_{Mes}H$), 3.78 (s, 4H, $C_{Cp}H$), 3.62 (s, 4H, $C_{Cp}H$), 2.17 (s, 24H, *o*-$C_{Mes}CH_3$), 1.96 (s, 12H, *p*-$C_{Mes}CH_3$), 1.34 (s, 12H, $NCCH_3$).

^{1}H NMR (400 MHz, THF-d_8, 300K): δ[ppm] = 6.70 (s, 8H, $C_{Mes}H$), 3.28 (s, 4H, $C_{Cp}H$), 3.18 (s, 4H, $C_{Cp}H$), 2.18 (s, 12H, *p*-$C_{Mes}CH_3$), 2.06 (s, 24H, *o*-$C_{Mes}CH_3$), 1.58 (s, 12H, $NCCH_3$).

^{13}C (101 MHz, C_6D_6, 300K) δ[ppm] = 169.76 (d, $^1J_{C,P}$ = 104.9 Hz, $C_{carbene}$P), 137.96 (*p*-$C_{Mes}CH_3$), 136.52 (NC_{Mes}), 132.85 (*o*-$C_{Mes}CH_3$), 129.44 ($C_{Mes}H$), 120.26 (NCCH_3), 77.50 (s, $C_{Cp}H$), 77.43 (s, $C_{Cp}H$), 72.99 (d, $^1J_{C,P}$ = 36.8 Hz, C_{Cp}P), 71.60 (s, $C_{Cp}H$), 71.54 (s, $C_{Cp}H$), 21.00 (*p*-$C_{Mes}CH_3$), 18.23 (*o*-$C_{Mes}CH_3$), 8.68 (NCCH_3).

^{31}P (162 Hz, C_6D_6, 300K) δ[ppm] = -59.76.

^{31}P (162 Hz, THF-d_8, 300K) δ[ppm] = -59.83.

Elemental Analysis: $C_{56}H_{64}FeN_4P_2$

Calculated [%]: C (73.84), H (7.08), N (6.15)

Observed [%]: C (72.69), H (7.10), N (6.03)

LIFDI-MS: Calculated for $C_{56}H_{64}FeN_4P_2$: 910.39556

Observed: 910.39035

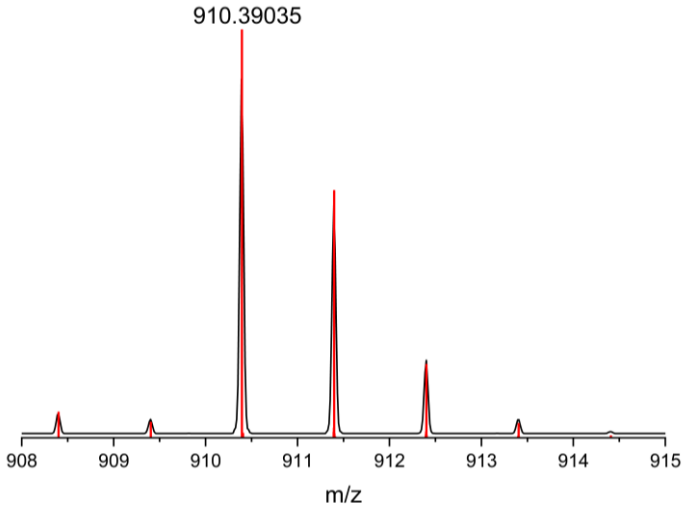


Figure S5 Measured (black) and calculated (red) LIFDI-MS for **3b**.

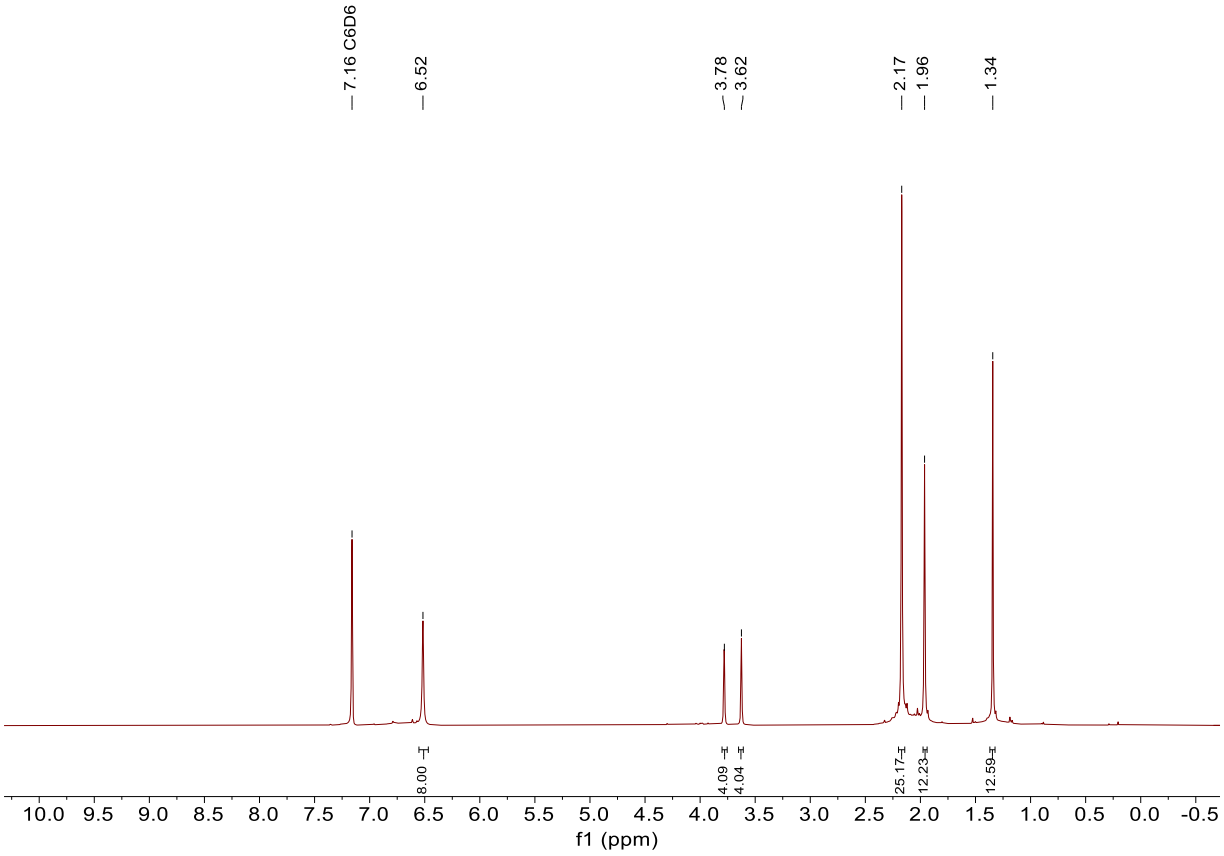


Figure S6 ^{1}H NMR of bisNHCP **3b** in C_6D_6.

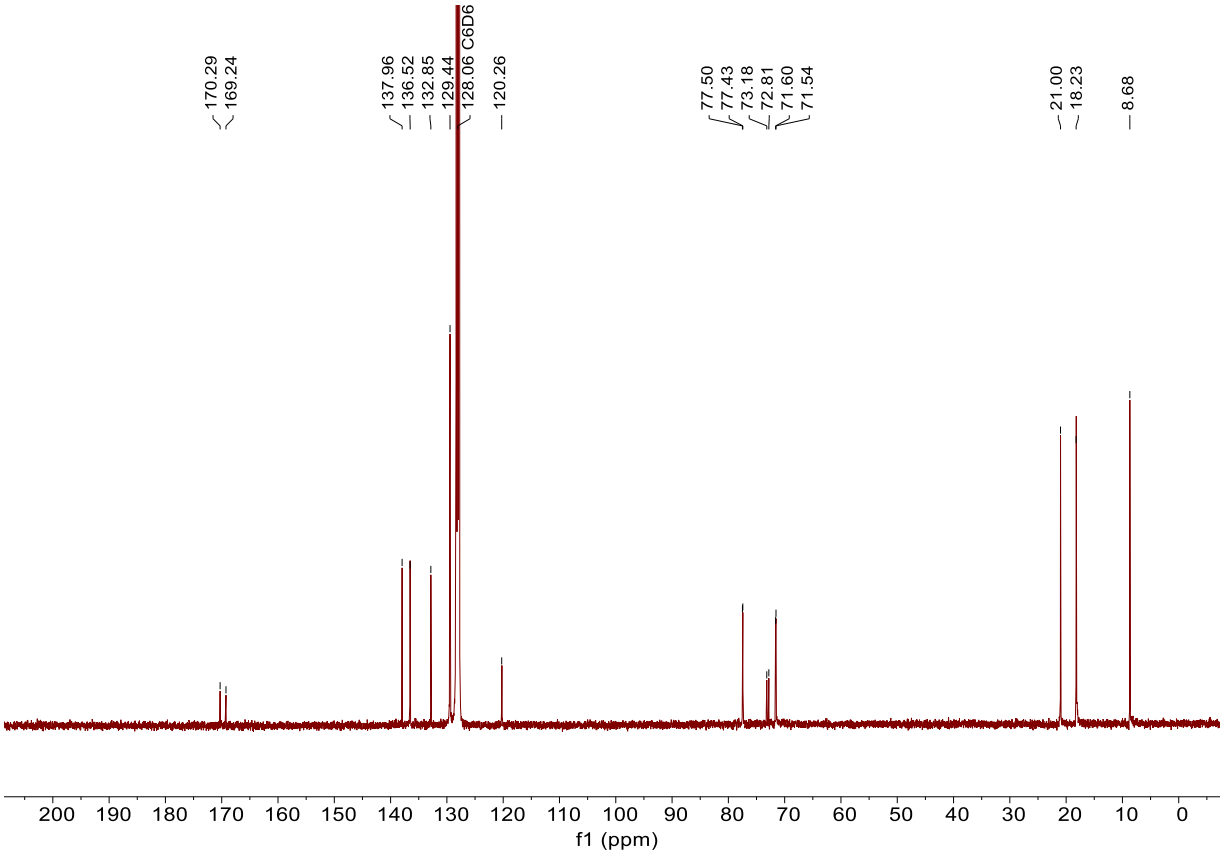


Figure S7 ^{13}C NMR of bisNHCP **3b** in C_6D_6.

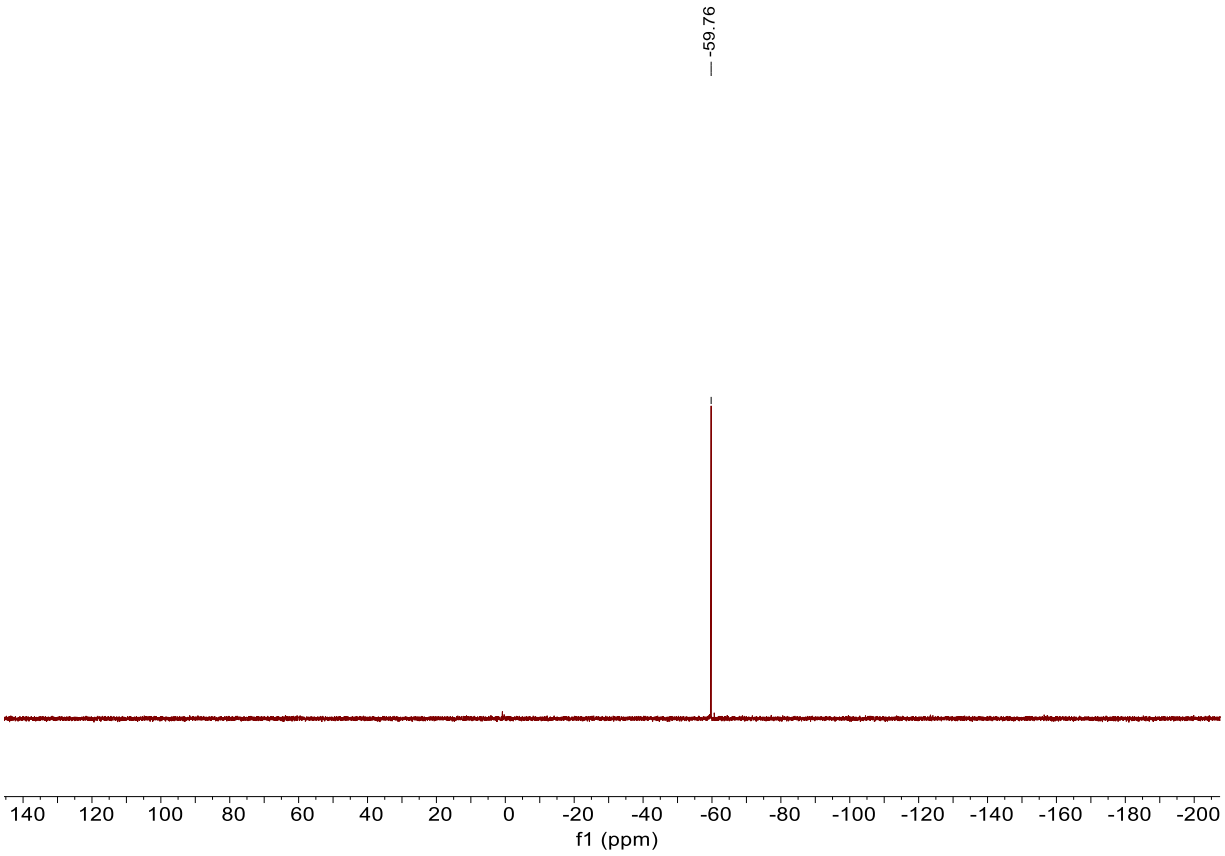
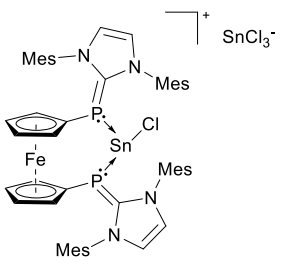


Figure S8 ^{31}P NMR of bisNHCP **3b** in C_6D_6.

1.4 Synthesis of BisNHCP $SnCl_2$ Complex 4a (NHC = IMes)



BisNHCP **3a** (30 mg, 35.1 µmol, 1.0 eq) and $SnCl_2$·dioxane (19.5 mg, 70.2 µmol, 2.0 eq) were dissolved in toluene (1 mL) and stirred overnight. The precipitate was separated from the solution and dried under vacuum to yield the product as an orange solid (23 mg, 18.6 µmol, 53%).

^{1}H NMR (400 MHz, THF-d_8, 300K): δ[ppm] = 7.49 (s, 4H, NCH), 6.94 (s, 8H, $C_{Mes}H$), 3.78 (s, 4H, $C_{Cp}H$), 3.60 (s, 4H, $C_{Cp}H$), 2.38 (s, 12H, *p*-$C_{Mes}CH_3$), 2.05 (s, 24H, *o*-$C_{Mes}CH_3$).

^{13}C (101 MHz, THF-d_8, 300K) δ[ppm] = 158.95 (d, $^1J_{C,P}$ = 34.2 Hz, $C_{Carbene}$), 141.36 (*p*-$C_{Mes}CH_3$), 136.42 (NC_{Mes}), 133.69 (*p*-$C_{Mes}CH_3$), 130.84 ($C_{Mes}H$), 126.20 (N*C*H), 80.25 (m, $C_{Cp}H$), 71.64 (m, $C_{Cp}H$), 21.50 (*p*-$C_{Mes}CH_3$), 18.02 (*o*-$C_{Mes}CH_3$).

Impurities at 138.60 ppm, 129.84 ppm, 129.07 ppm, 126.05 ppm, and 21.39 ppm are from residual toluene.

^{31}P (162 Hz, THF-d_8, 300K) δ[ppm] = -46.85 (s, satellites $^1J_{Sn,P}$ = 1151 Hz)

^{119}Sn (112 Hz, THF-d_8, 300K) δ[ppm] = 236.45 (SnCl), -21.11 ($SnCl_3$).

Elemental Analysis: $C_{52}H_{56}Cl_4FeN_4P_2Sn_2$

Calculated [%]: C (50.61), H (4.57), N (4.54)

Observed [%]: C (49.84), H (4.78), N (3.79)

LIFDI-MS:

Calculated for $C_{52}H_{53}Cl_2FeN_4P_2Sn$:	1041.1494
Observed:	1041.18906

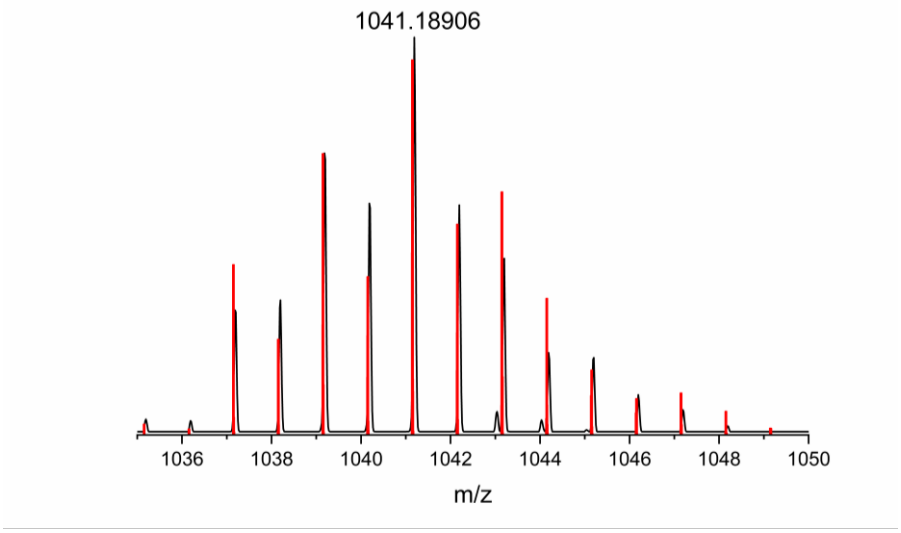


Figure S9 Measured (black) and calculated (red) LIFDI-MS for [**4a-3H]**.

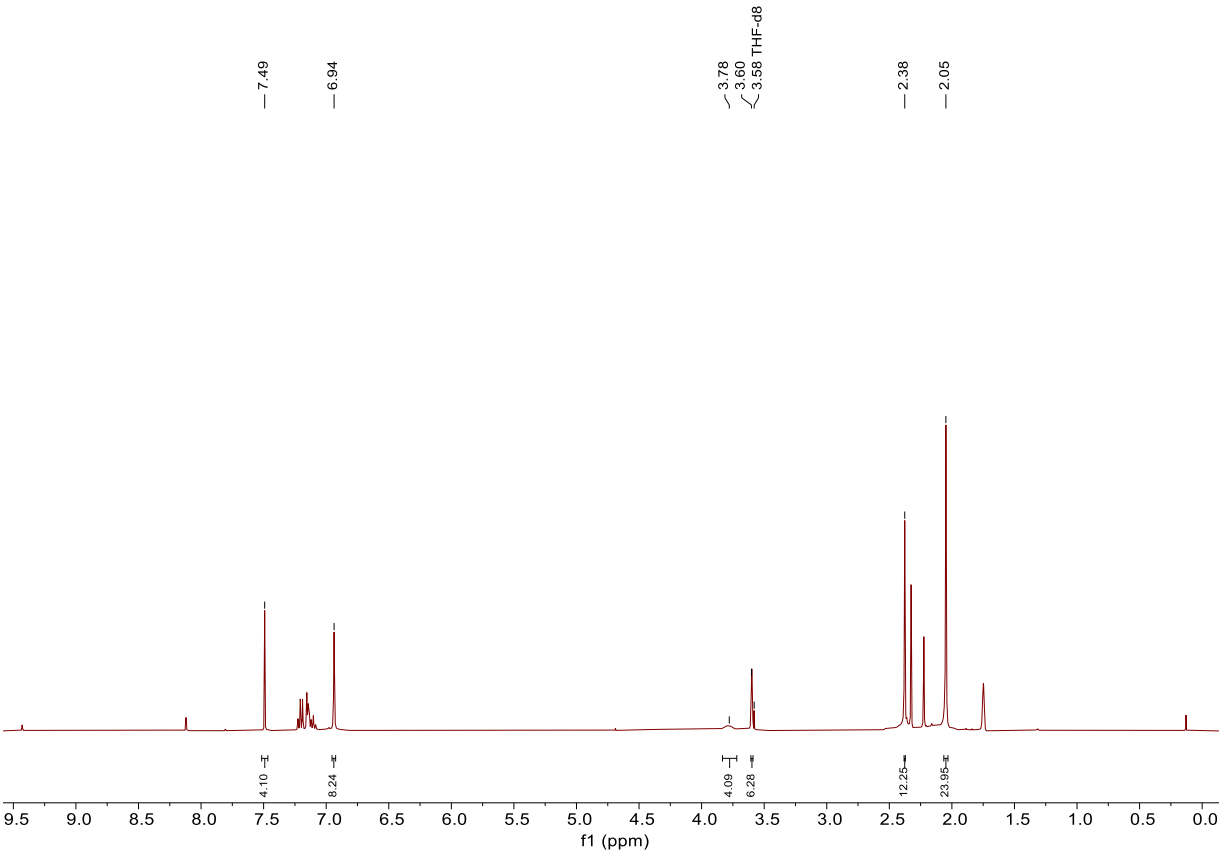


Figure S10 ^{1}H NMR of **4a** in THF-d_8.

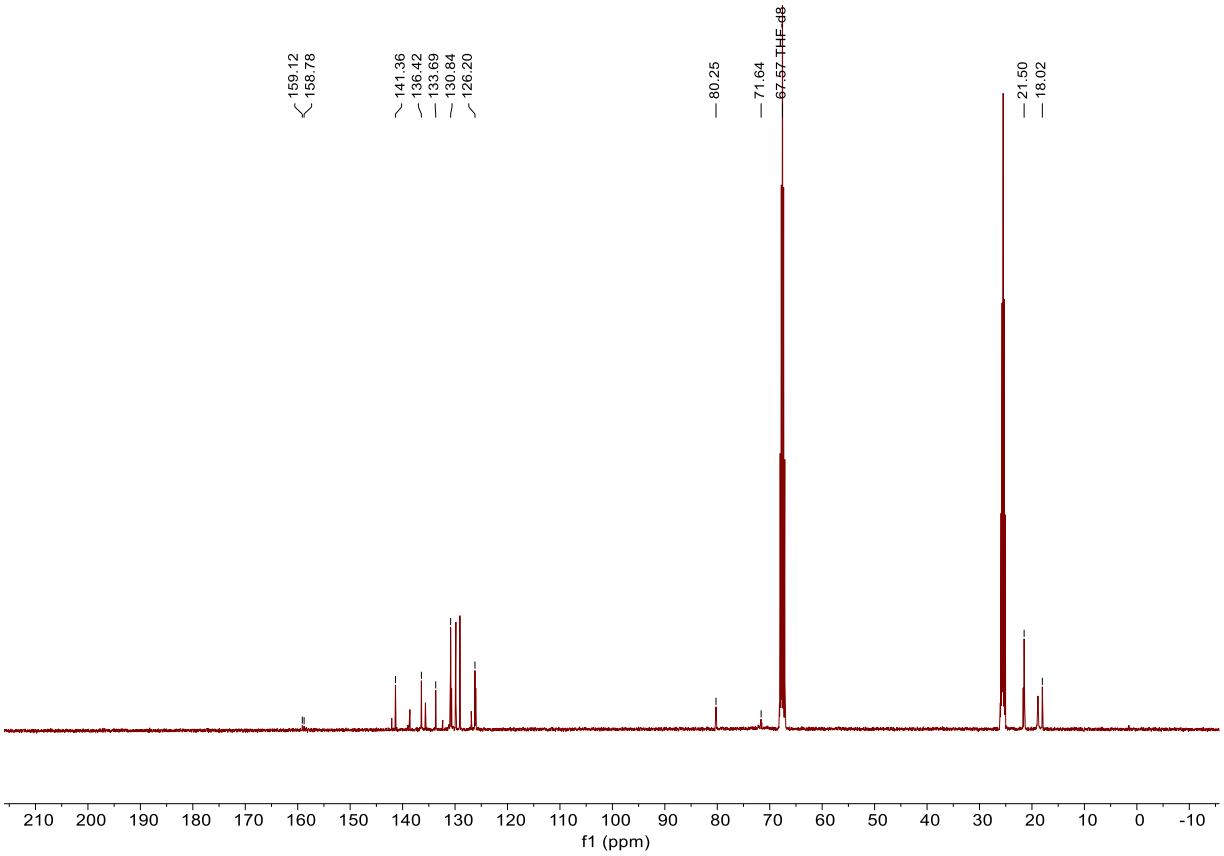


Figure S11 ^{13}C NMR of **4a** in THF-d_8.

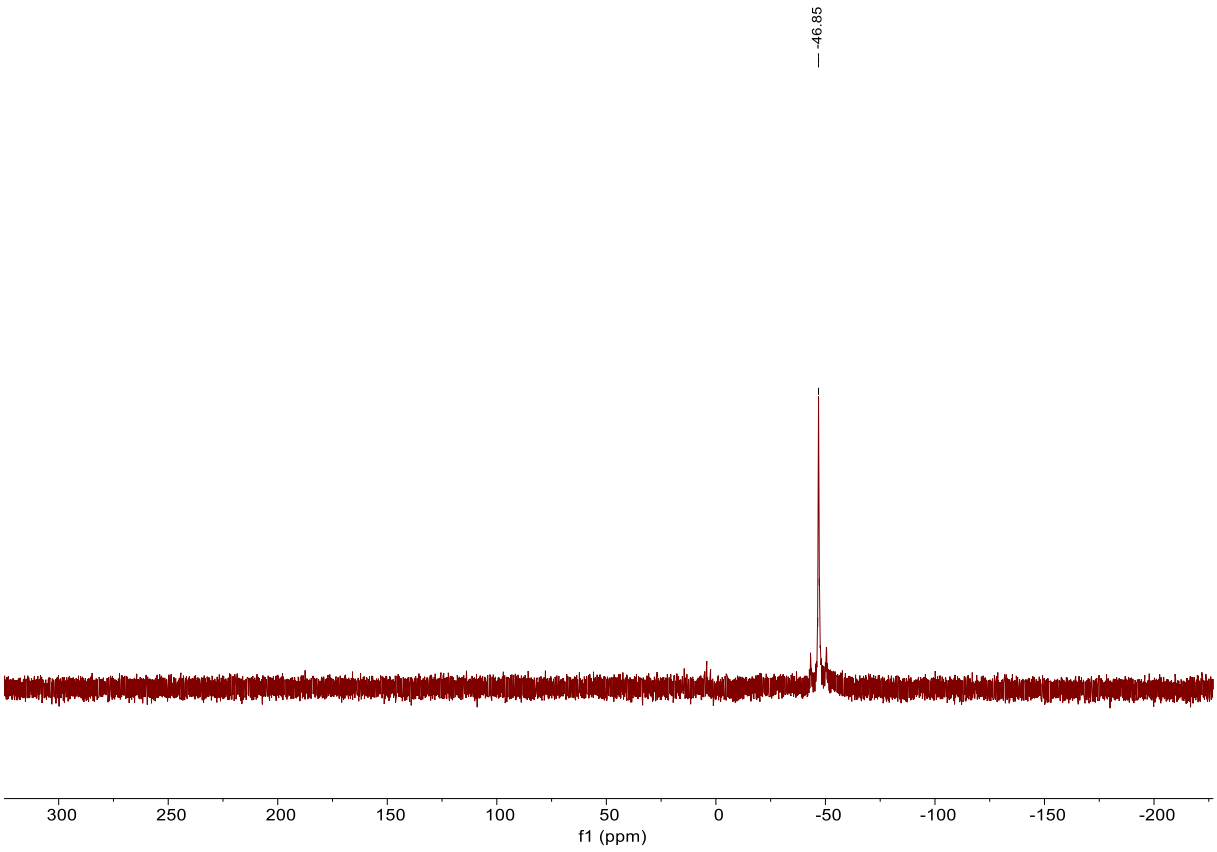


Figure S12 ^{31}P NMR of **4a** in THF-d_8.

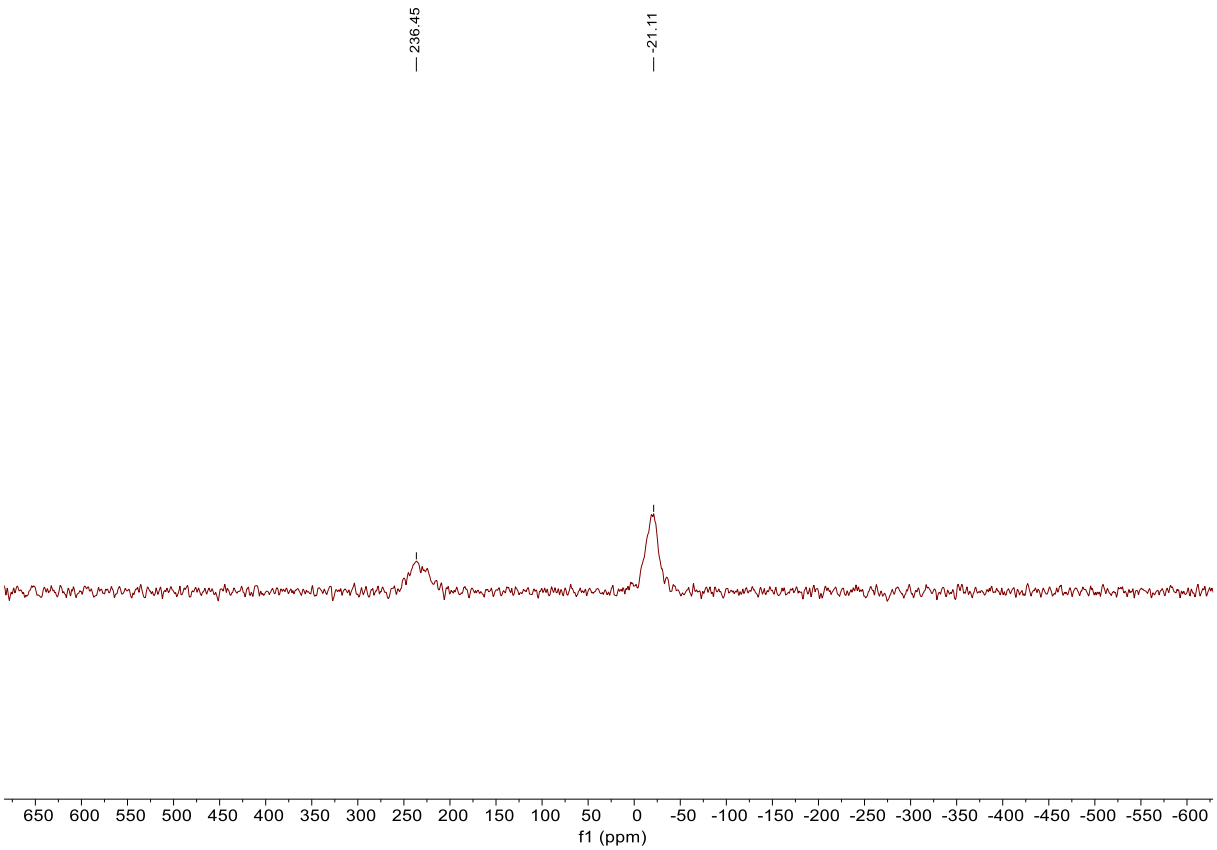
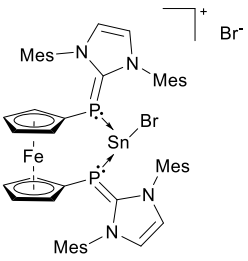


Figure S13 ^{119}Sn NMR of **4a** in THF-d_8.

1.5 Synthesis of BisNHCP $SnBr_2$ Complex 4b (NHC = IMes)



BisNHCP **3a** (20 mg, 23.4 µmol, 1.0 eq) and $SnBr_2$ (11.5 mg, 41.3 µmol, 1.7 eq) were dissolved in benzene and stirred overnight. The precipitate was separated from the solution and dried under vacuum to yield the product as an orange solid (23 mg, 20.3 µmol, 87%).

^{1}H NMR (400 MHz, THF-d_8, 300K): δ[ppm] = 7.46 (s, 4H, NCH), 6.92 (s, 8H, $C_{Mes}H$), 3.97 (s, 4H, $C_{Cp}H$), 3.78 (s, 4H, $C_{Cp}H$), 2.36 (s, 12H, *p*-$C_{Mes}CH_3$), 2.05 (s, 24H, *o*-$C_{Mes}CH_3$).
^{13}C (101 MHz, THF-d_8, 300K) δ[ppm] = 141.39 (*p*-$C_{Mes}CH_3$), 136.39 (NC_{Mes}), 133.66 (*p*-$C_{Mes}CH_3$), 130.87 ($C_{Mes}H$), 125.98 (N*C*H), 80.12 ($C_{Cp}H$), 71.29 ($C_{Cp}H$), 21.63 (*p*-$C_{Mes}CH_3$), 18.98 (*o*-$C_{Mes}CH_3$).

Shifts of carbon atoms directly bound to P were not observed in the ^{13}C NMR spectrum.

^{31}P (162 Hz, THF-d_8, 300K) δ[ppm] = -47.91 (s, satellites $^{1}J_{Sn,P}$ = 1202 Hz)

^{119}Sn (149 Hz, THF-d_8, 300K) δ[ppm] = 168.99 (bs)

LIFDI-MS: Calculated for $[C_{52}H_{56}BrFeN_4P_2Sn]^+$: 1053.1535

Observed: 1053.14239

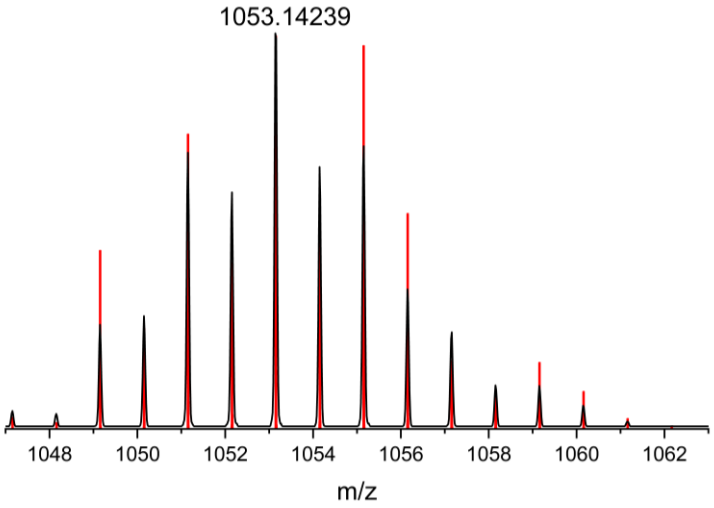


Figure S14 Measured (black) and calculated (red) LIFDI-MS for [**4b**-Br]$^+$.

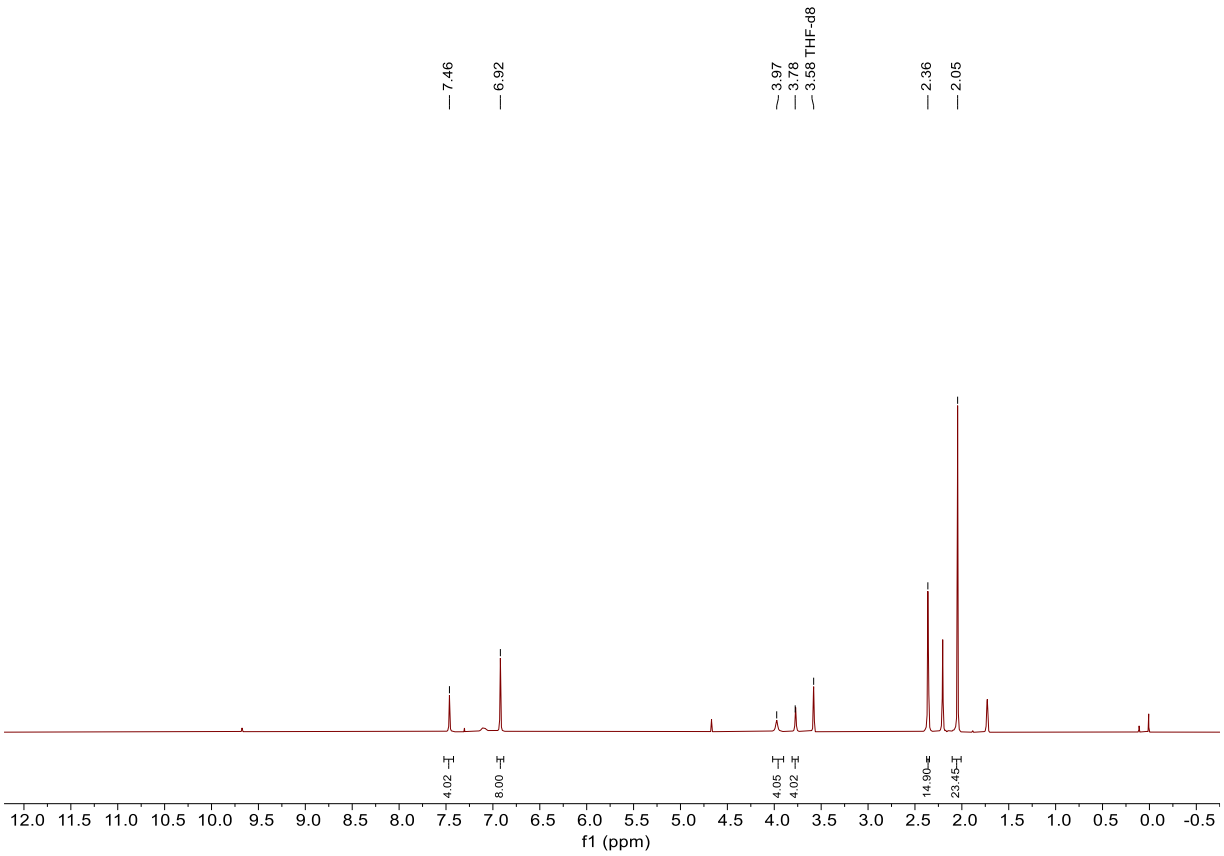


Figure S15 ^{1}H NMR of **4b** in THF-d_8.

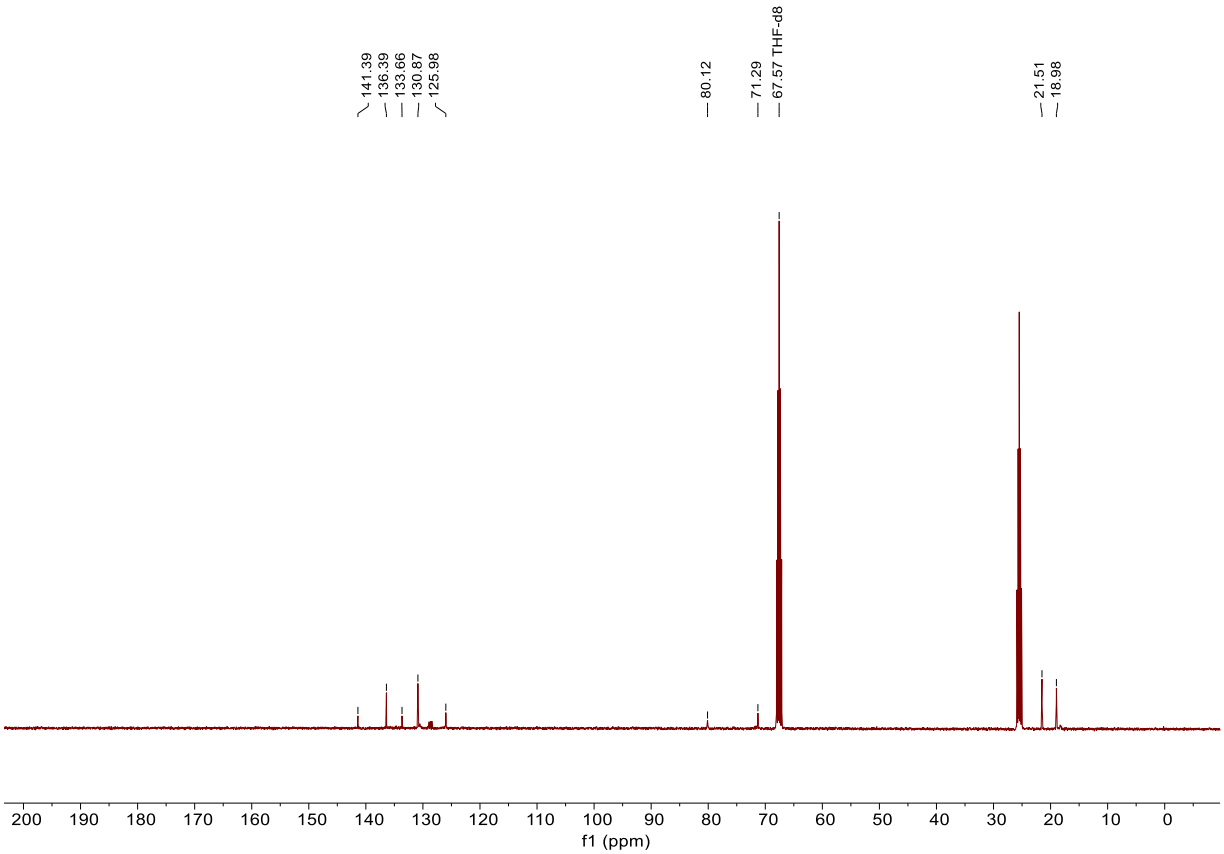


Figure S16 ^{13}C NMR of **4b** in THF-d_8.

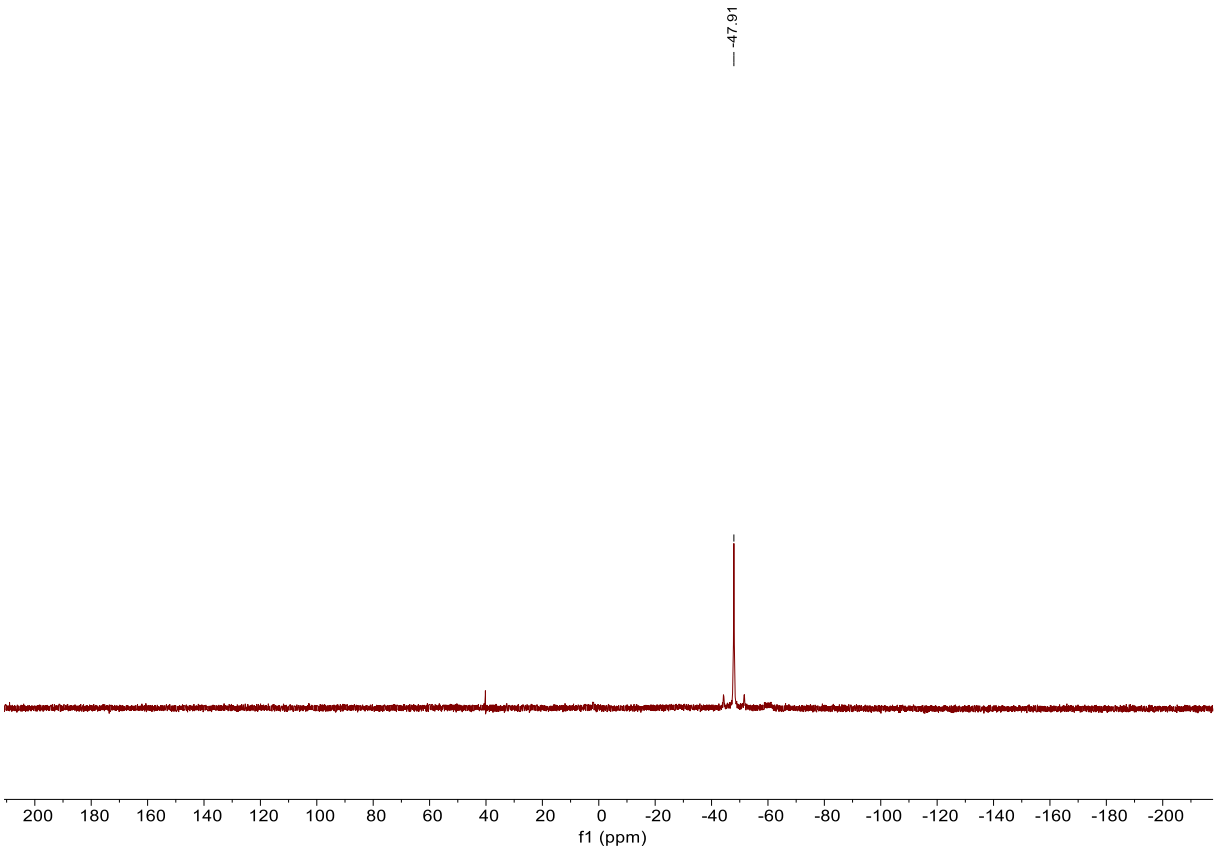


Figure S17 ^{31}P NMR of **4b** in THF-d_8.

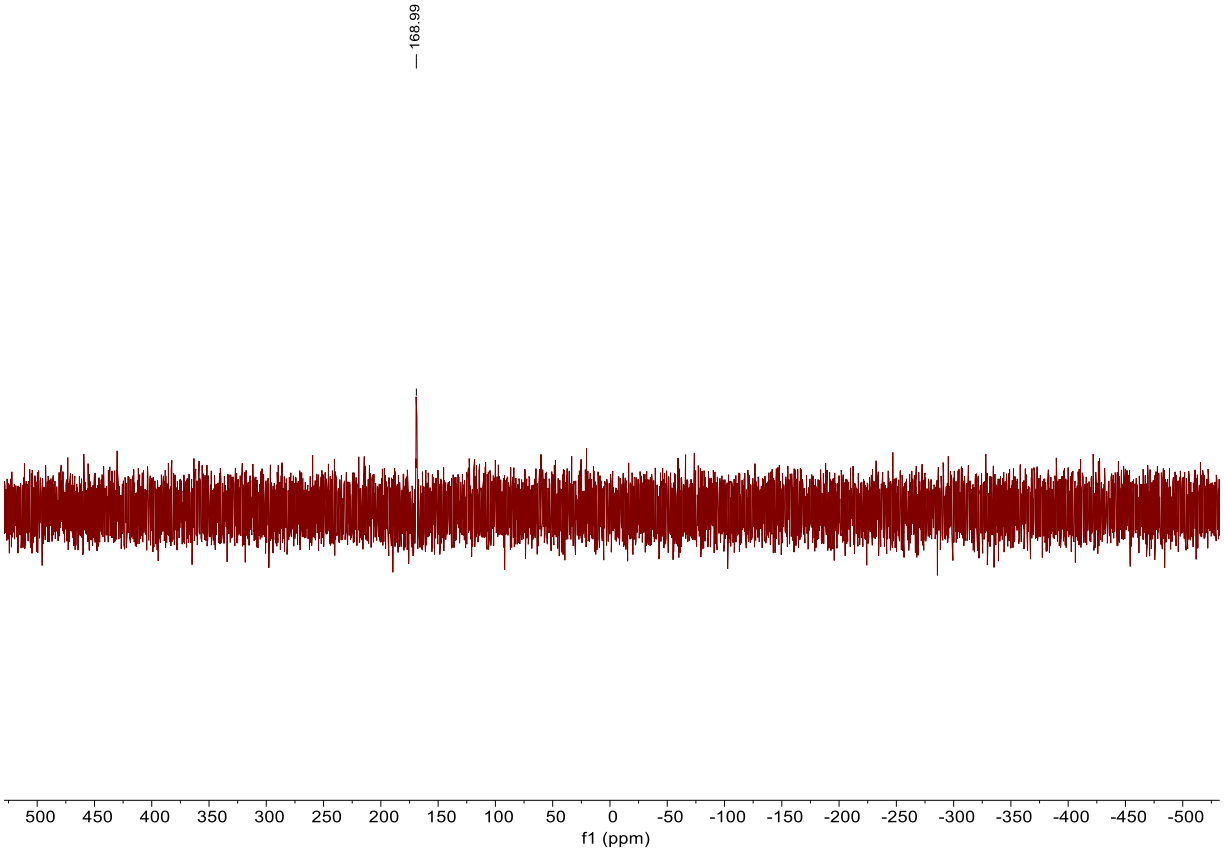
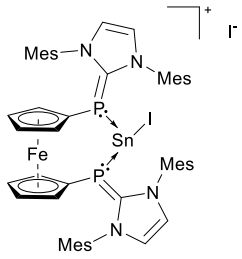


Figure S18 ^{119}Sn NMR of **4b** in THF-d_8.

1.6 Synthesis of BisNHCP SnI_2 Complex 4c (NHC = IMes)



BisNHCP **3a** (11.8 mg, 13.80 µmol, 1.0 eq) and SnI_2 (5.1 mg, 13.80 µmol, 1.0 eq) were dissolved in toluene (1 mL) and stirred overnight. The precipitate was separated from the solution and dried under vacuum to yield the product as an orange solid (15.2 mg, 12.38 µmol, 90%).

^{1}H NMR (400 MHz, THF-d_8, 300K): δ[ppm] = 7.41 (s, 4H, NCH), 6.89 (s, 8H, $C_{Mes}H$), 4.21 (s, 4H, $C_{Cp}H$), 3.71 (s, 4H, $C_{Cp}H$), 2.34 (s, 12H, *p*-$C_{Mes}CH_3$), 2.13 (s, 24H, *o*-$C_{Mes}CH_3$).

^{13}C (101 MHz, THF-d_8, 300K) δ[ppm] = 140.97 (*p*-$C_{Mes}CH_3$), 136.52 (NC_{Mes}), 133.68 (*p*-$C_{Mes}CH_3$), 130.90 ($C_{Mes}H$), 125.67 (N*C*H), 80.05 ($C_{Cp}H$), 71.08 ($C_{Cp}H$), 21.52 (*p*-$C_{Mes}CH_3$), 19.68 (*o*-$C_{Mes}CH_3$).

Shifts of carbon atoms directly bound to P were not observed in the ^{13}C NMR spectrum.

^{31}P (162 Hz, THF-d_8, 300K) δ[ppm] = -49.89 (s, satellites $^1J_{119Sn,P}$ = 1211 Hz, $^1J_{117Sn,P}$ = 1268 Hz)

^{119}Sn (149 Hz, THF-d_8, 300K) δ[ppm] = 174.43 (t, $^1J_{Sn,P}$ = 1301 Hz)

LIFDI-MS: Calculated for $[C_{52}H_{56}FeIN_4P_2Sn]^+$: 1101.13964

Observed: 1101.12756

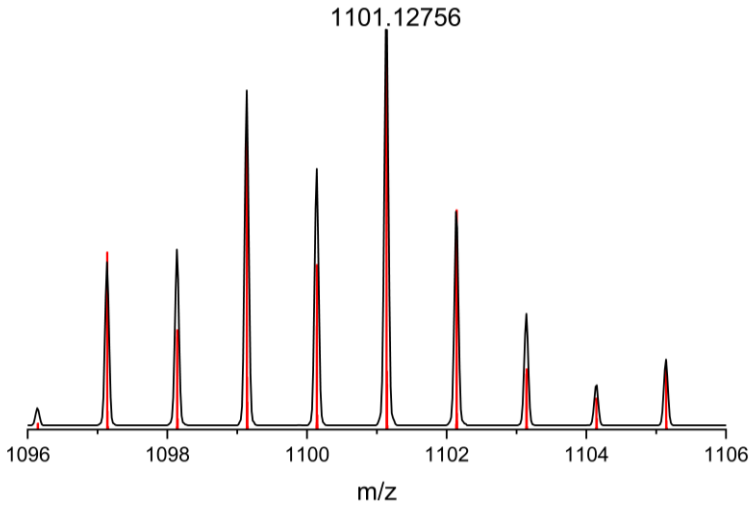


Figure S19 Measured (black) and calculated (red) LIFDI-MS for [**4c**-I]$^+$.

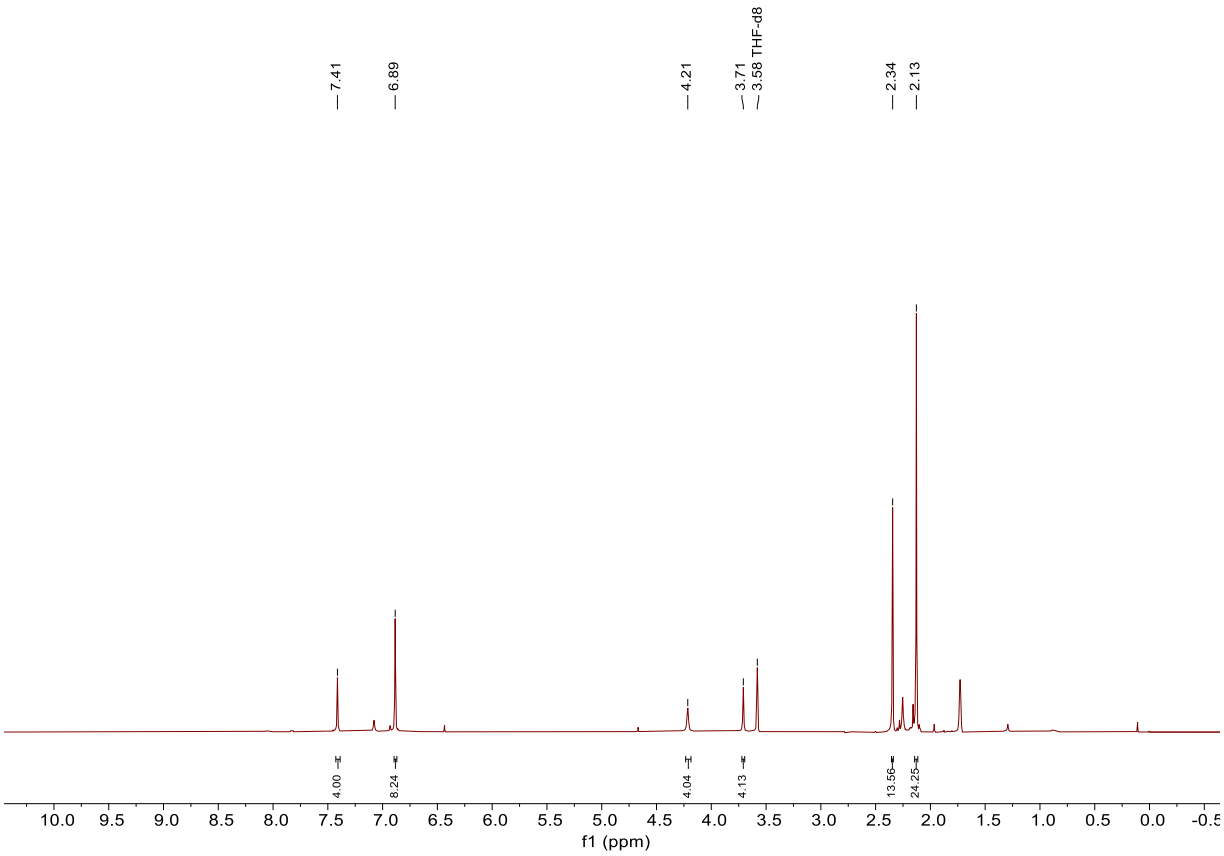


Figure S20 ^{1}H NMR of **4c** in THF-d_8.

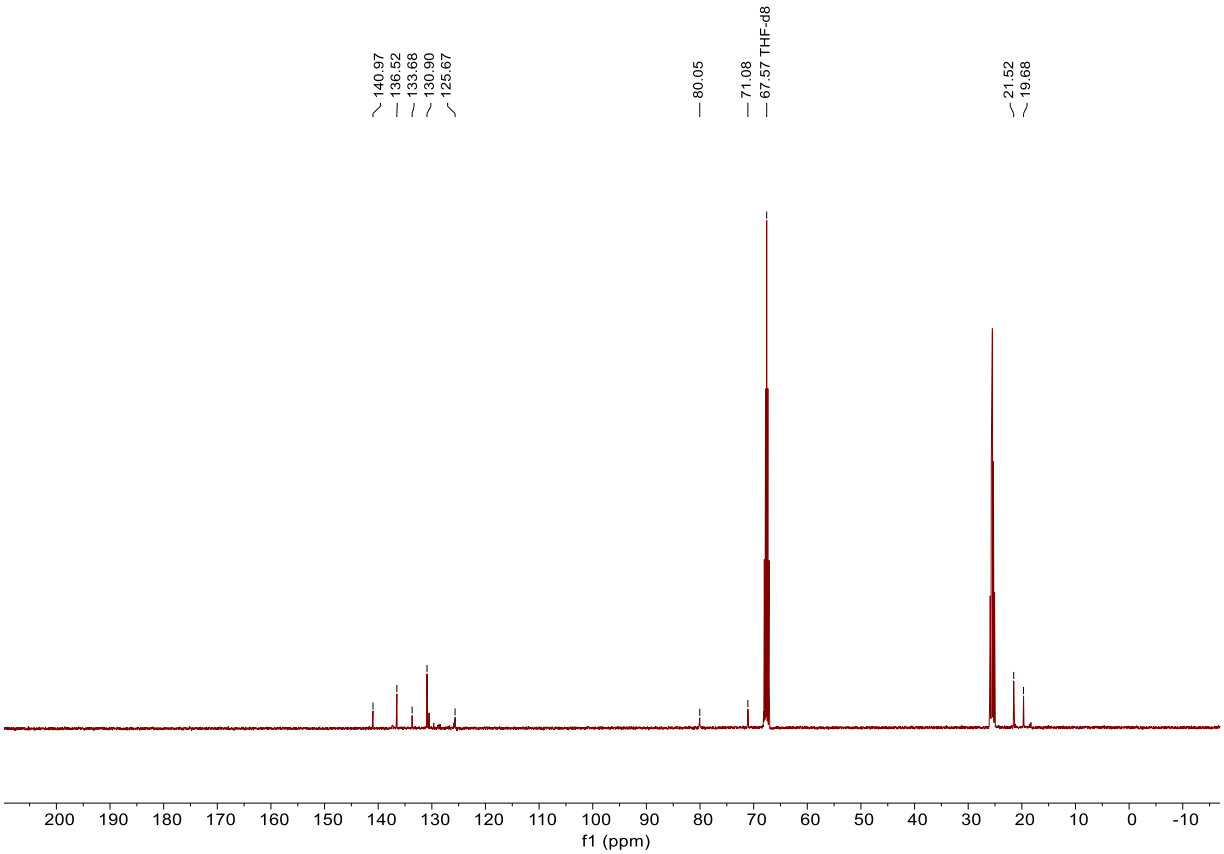


Figure S21 ^{13}C NMR of **4c** in THF-d_8.

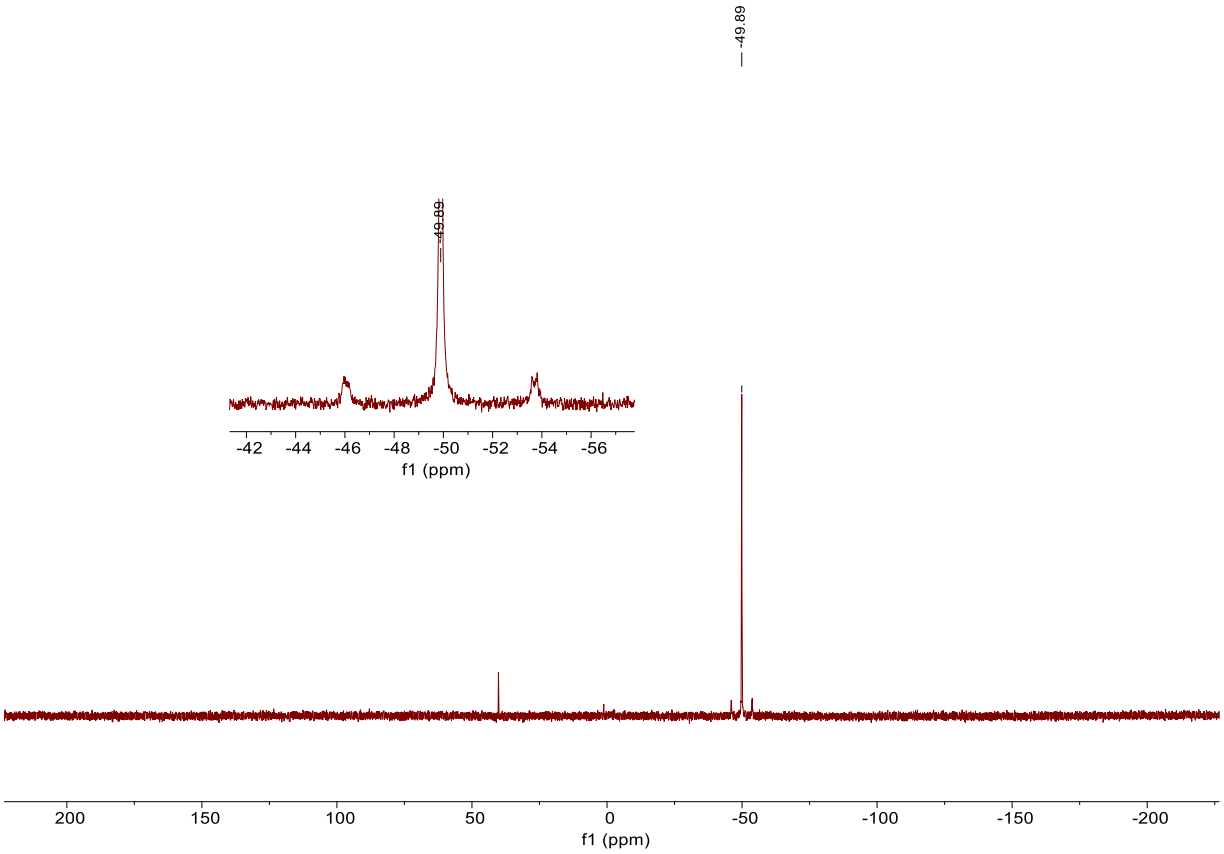


Figure S22 ^{31}P NMR of **4c** in THF-d_8.

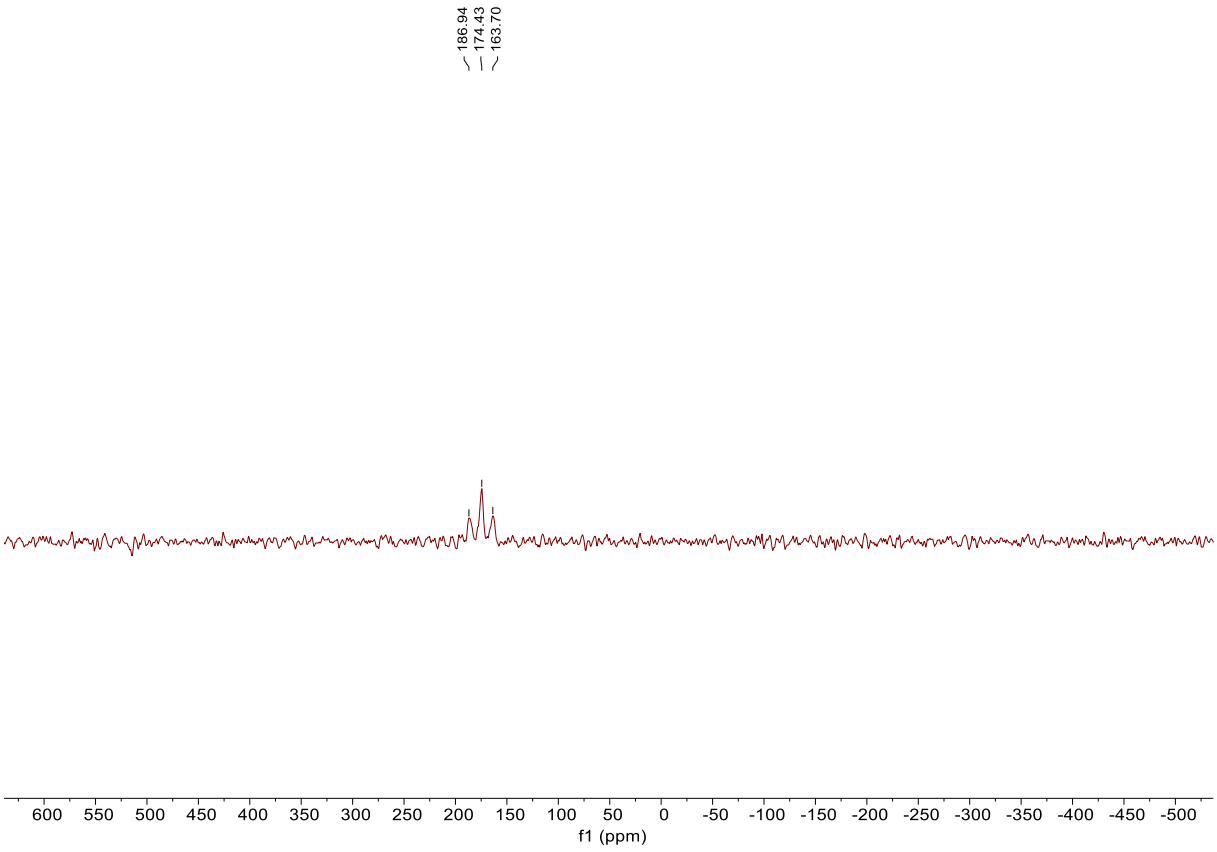
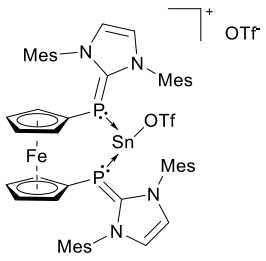


Figure S23 ^{119}Sn NMR of **4c** in THF-d_8.

1.7 Synthesis of BisNHCP $Sn(OTf)_2$ Complex 4d (NHC = IMes)



BisNHCP **3a** (20 mg, 23.4 µmol, 1.0 eq) and $Sn(OTf)_2$·dioxane (11.8 mg, 23.4 µmol, 1.0 eq) were dissolved in toluene (1 mL) and stirred overnight. The precipitate was separated from the solution and dried under vacuum to yield the product as an orange solid (23 mg, 18.1 µmol, 77%).

^{1}H NMR (400 MHz, THF-d_8, 300K): δ[ppm] = 7.53 (s, 4H, NCH), 6.95 (s, 8H, C_{Mes}H), 3.86 (s, 4H, C_{Cp}H), 3.82 (s, 4H, C_{Cp}H), 2.38 (s, 12H, *p*-$C_{Mes}CH_3$), 2.01 (s, 24H, *o*-$C_{Mes}CH_3$).
Impurities at 7.19 ppm (m), 7.11 ppm (m), and 2.31 ppm (s) are from residual toluene.
^{13}C (101 MHz, THF-d_8, 300K) δ[ppm] = 141.67 (*p*-$C_{Mes}CH_3$), 136.41 (NC_{Mes}), 135.63 (*p*-$C_{Mes}CH_3$), 131.12 (C_{Mes}H), 126.49 (N*C*H), 80.61 (m, C_{Cp}H), 71.99 (C_{Cp}H), 18.51 (*p*-$C_{Mes}CH_3$), 17.65 (*o*-$C_{Mes}CH_3$).

Impurities at 138.61 ppm, 130.53 ppm, 129.84 ppm, 129.07 ppm, and 21.48 ppm are from residual toluene. Shifts of carbon atoms directly bound to P were not observed in the ^{13}C NMR spectrum.

^{31}P (162 Hz, THF-d_8, 300K) δ[ppm] = -29.76 (s, satellites $^1J_{119Sn,P}$ = 1202 Hz, $^1J_{117Sn,P}$ = 1255 Hz)

^{19}F (376 Hz, THF-d_8, 300K) δ[ppm] = -78.72

^{119}Sn (149 Hz, THF-d_8, 300K) δ[ppm] = 432.78 (t, $^1J_{Sn,P}$= 1249 Hz)

Elemental Analysis: $C_{54}H_{56}F_6FeN_4O_6P_2S_2Sn$

Calculated [%]: C (51.00), H (4.44), N (4.41), S (5.04)

Observed [%]: C (51.87), H (4.98), N (4.10), S (4.46)

LIFDI-MS: Calculated for $[C_{53}H_{56}F3FeN_4O_3P_2SSn]^+$: 1123.18719

Observed: 1123.18977

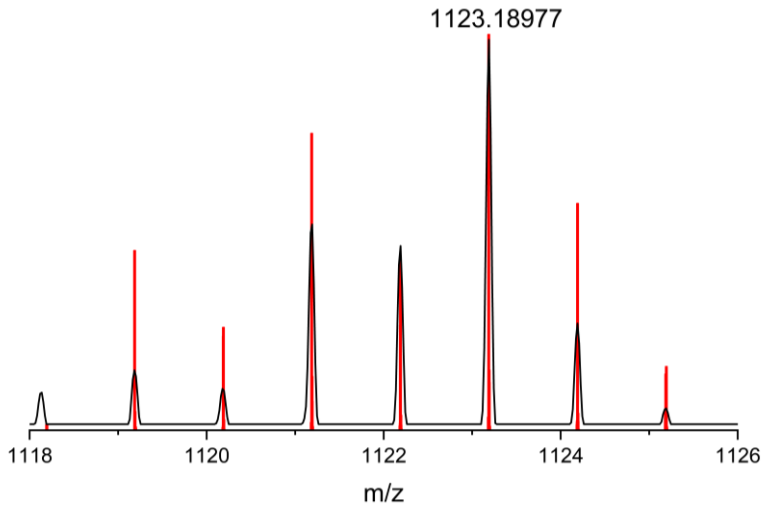


Figure S24 Measured (black) and calculated (red) LIFDI-MS for [**4d**-OTf]$^{+}$.

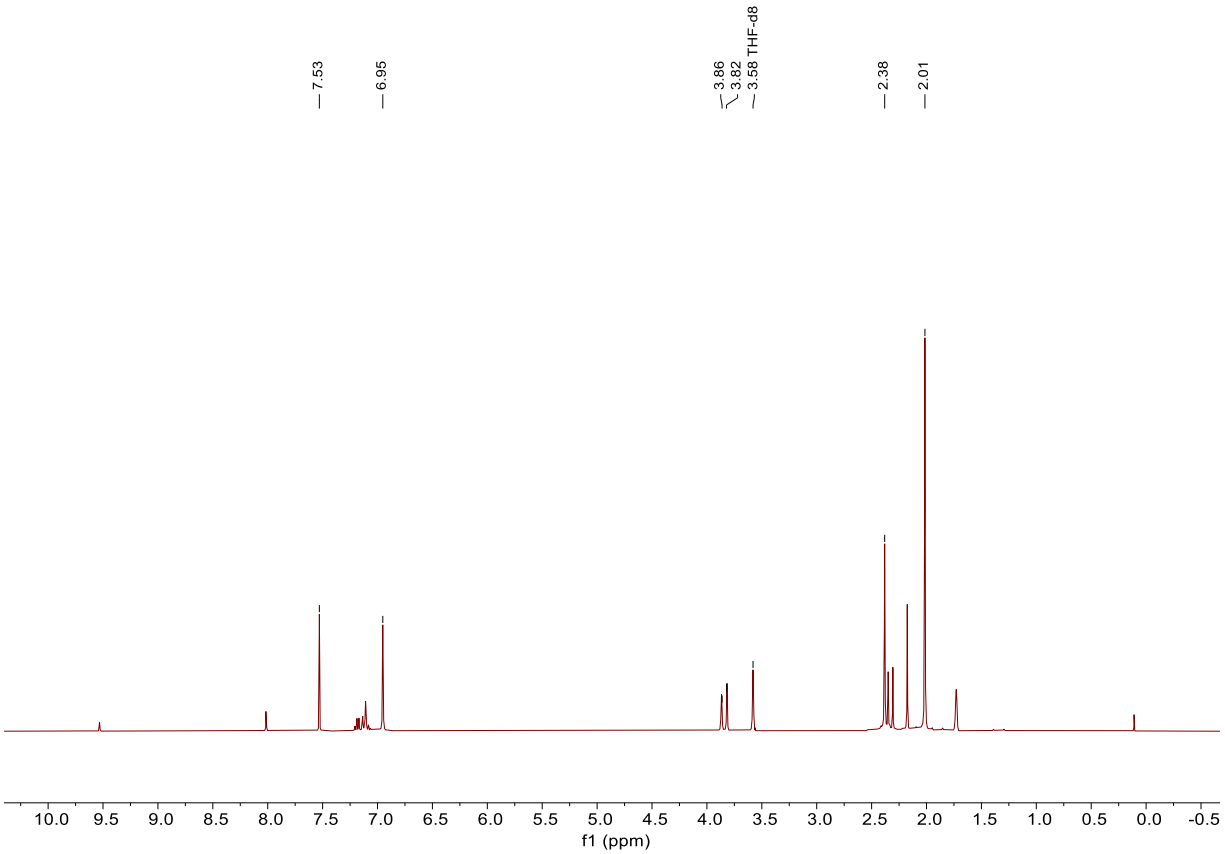


Figure S25 ^{1}H NMR of **4d** in THF-d_8.

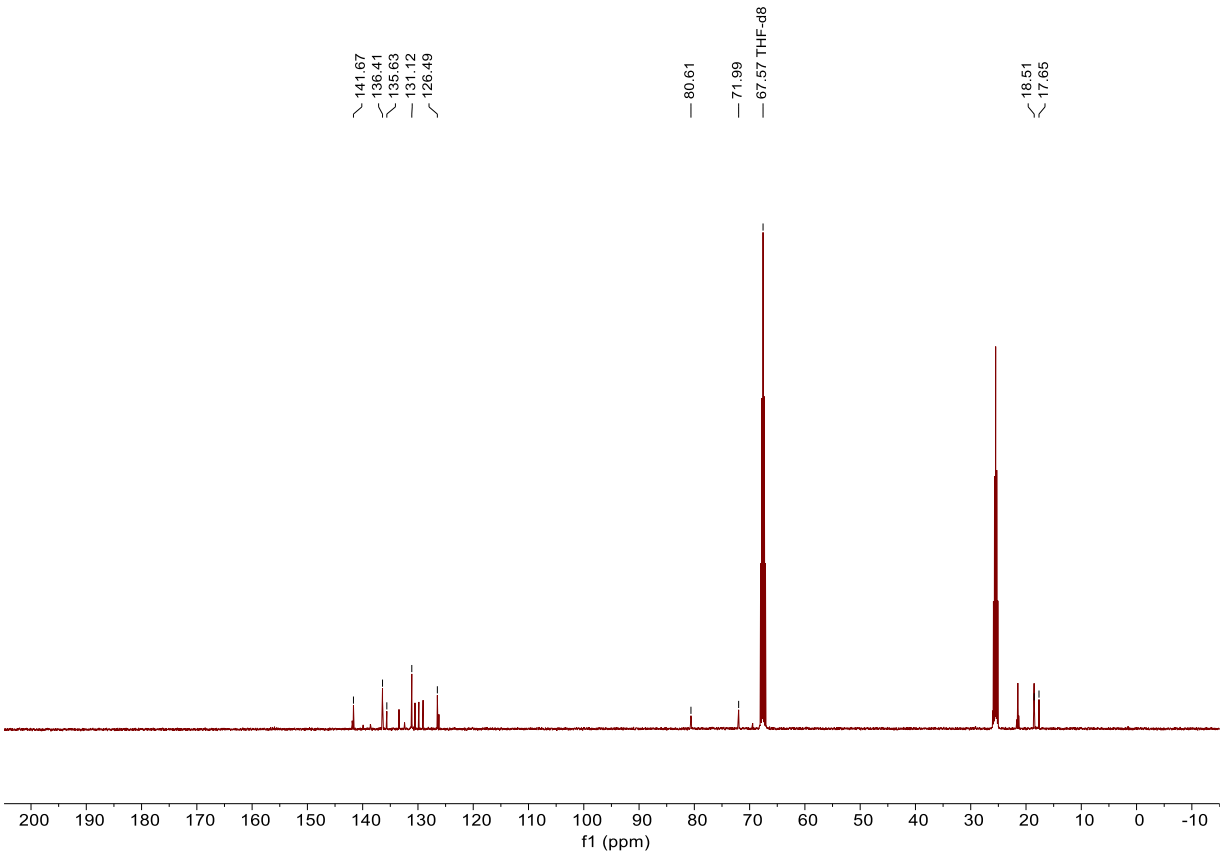


Figure S26 ^{13}C NMR of **4d** in THF-d_8.

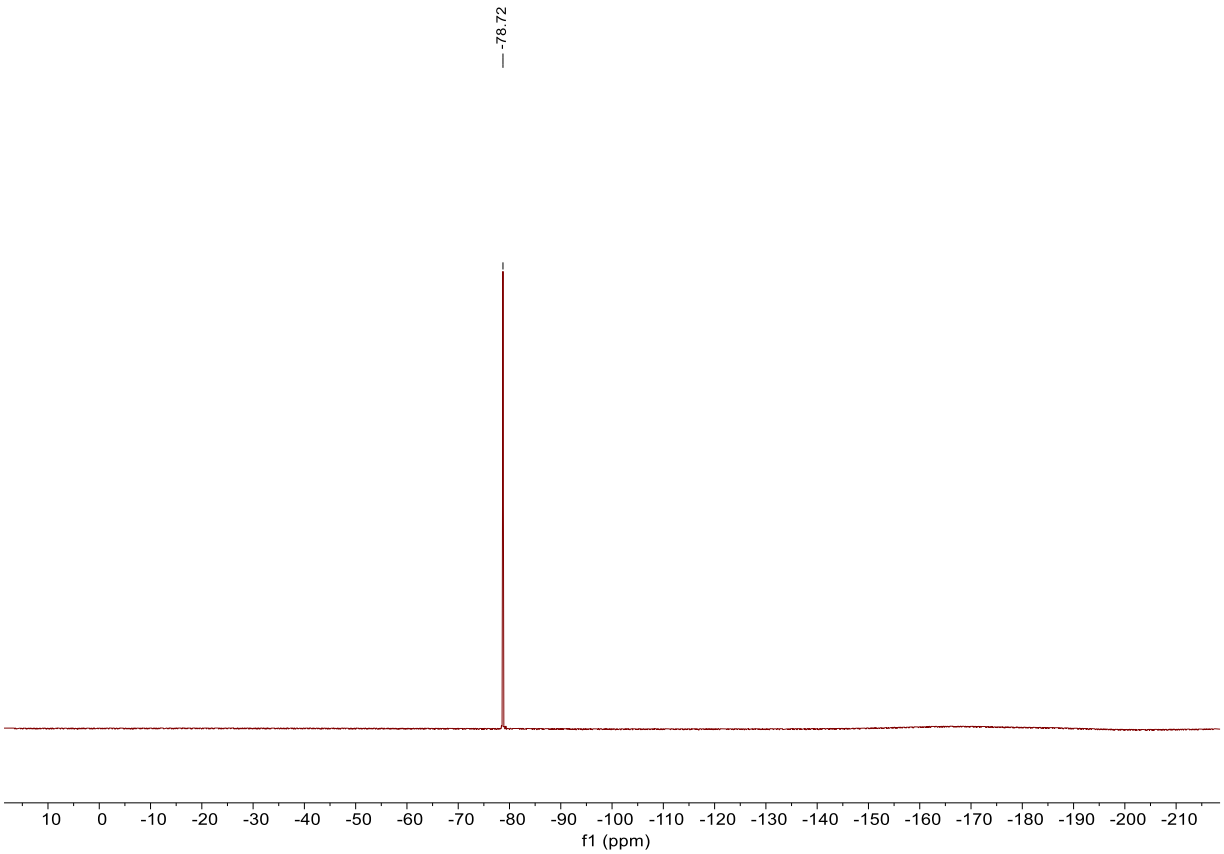


Figure S27 ^{19}F NMR of **4d** in THF-d_8.

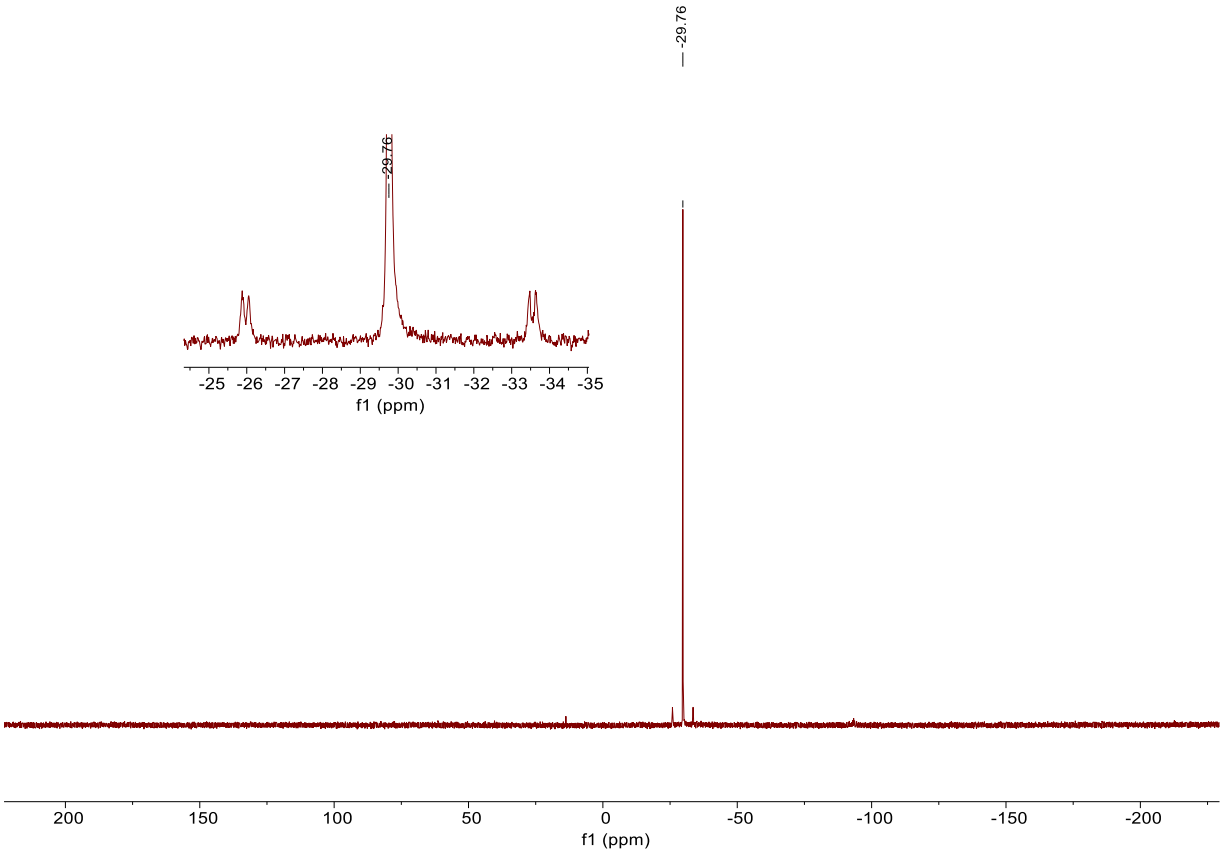


Figure S28 ^{31}P NMR of **4d** in THF-d_8.

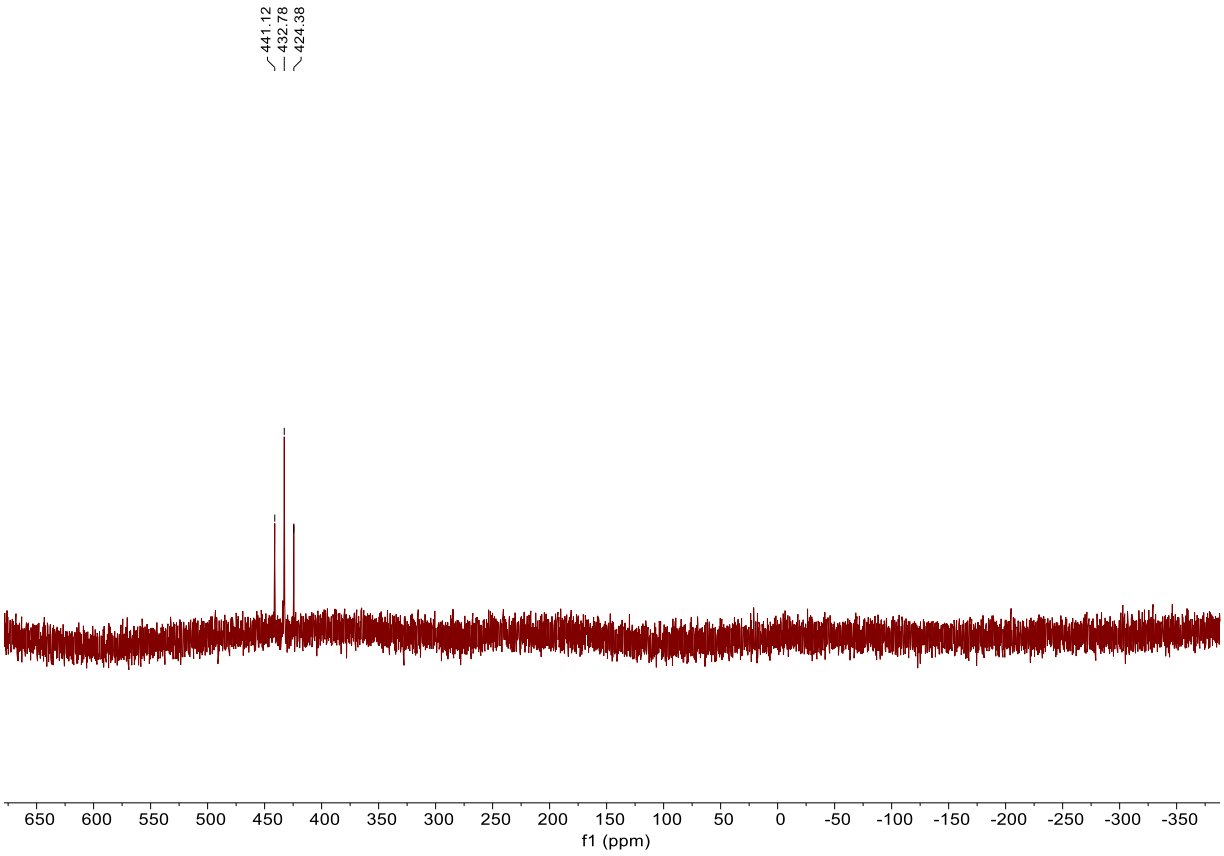
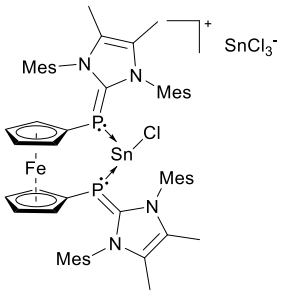


Figure S29 ^{119}Sn NMR of **4d** in THF-d_8.

1.8 Synthesis of BisNHCP $SnCl_2$ Complex 5a (NHC = ^{Me}IMes)



BisNHCP **3b** (30 mg, 32.93 µmol, 1.0 eq) and $SnCl_2$·dioxane (18.3 mg, 65.87 µmol, 1.0 eq) were dissolved in toluene (1 mL) and stirred overnight. The precipitate was separated from the solution and dried under vacuum to yield the product as an orange solid (29.9 mg, 23.28 µmol, 70%).

^{1}H NMR (400 MHz, THF-d_8, 300K): δ[ppm] = 6.98 (s, 8H, $C_{Mes}H$), 3.80 (s, 4H, $C_{Cp}H$), 3.60 (s, 4H, $C_{Cp}H$), 2.39 (s, 12H, *p*-$C_{Mes}CH_3$), 1.97 (s, 24H, *o*-$C_{Mes}CH_3$), 1.86 ($NCCH_3$).

^{13}C (101 MHz, THF-d_8, 300K) δ[ppm] = 156.06 (d, $^1J_{C,P}$ = 33.6 Hz, $C_{carbene}P$), 155.64 (d, $^1J_{C,P}$ = 33.8 Hz, $C_{carbene}P$) 141.37 (*p*-$C_{Mes}CH_3$), 136.79 (NC_{Mes}), 131.84 ($NCCH_3$), 131.08 (*o*-$C_{Mes}CH_3$), 129.01 ($C_{Mes}H$), 80.22 (m, $C_{Cp}H$), 72.58 (m, $C_{Cp}H$), 71.58 (broad s, $C_{Cp}P$), 21.55 (*p*-$C_{Mes}CH_3$), 18.75 (*o*-$C_{Mes}CH_3$), 9.35 ($NCCH_3$).

^{31}P (162 Hz, THF-d_8, 300K) δ[ppm] = -49.27 (s, satellites $^1J_{Sn,P}$ = 1116 Hz)

^{119}Sn (149 Hz, THF-d_8, 300K) δ[ppm] = 243.75 (SnCl), -27.39 ($SnCl_3$)

Elemental Analysis: $C_{56}H_{64}Cl_4FeN_4P_2Sn_2$

Calculated [%]: C (52.13), H (5.00), N (4.34)

Observed [%]: C (50.71), H (5.18), N (3.86)

LIFDI-MS:

Calculated for $[C_{56}H_{64}ClFeN_4P_2Sn]^+$:	1065.26661
Observed:	1065.26677

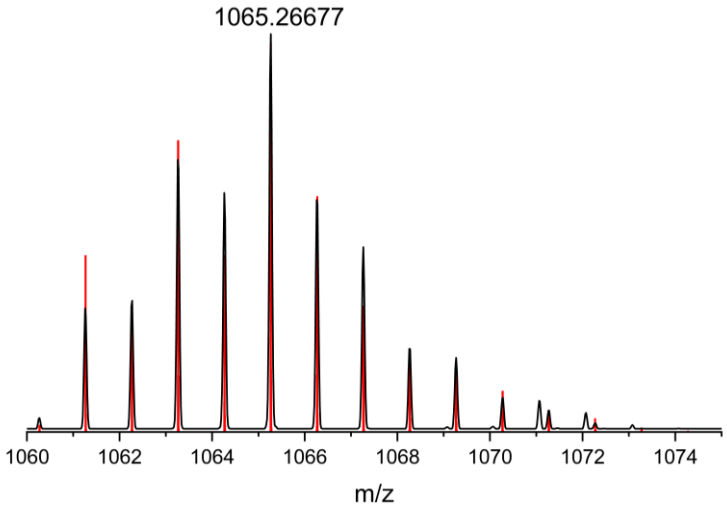


Figure S30 Measured (black) and calculated (red) LIFDI-MS for [**5a**-$SnCl_3$]$^+$.

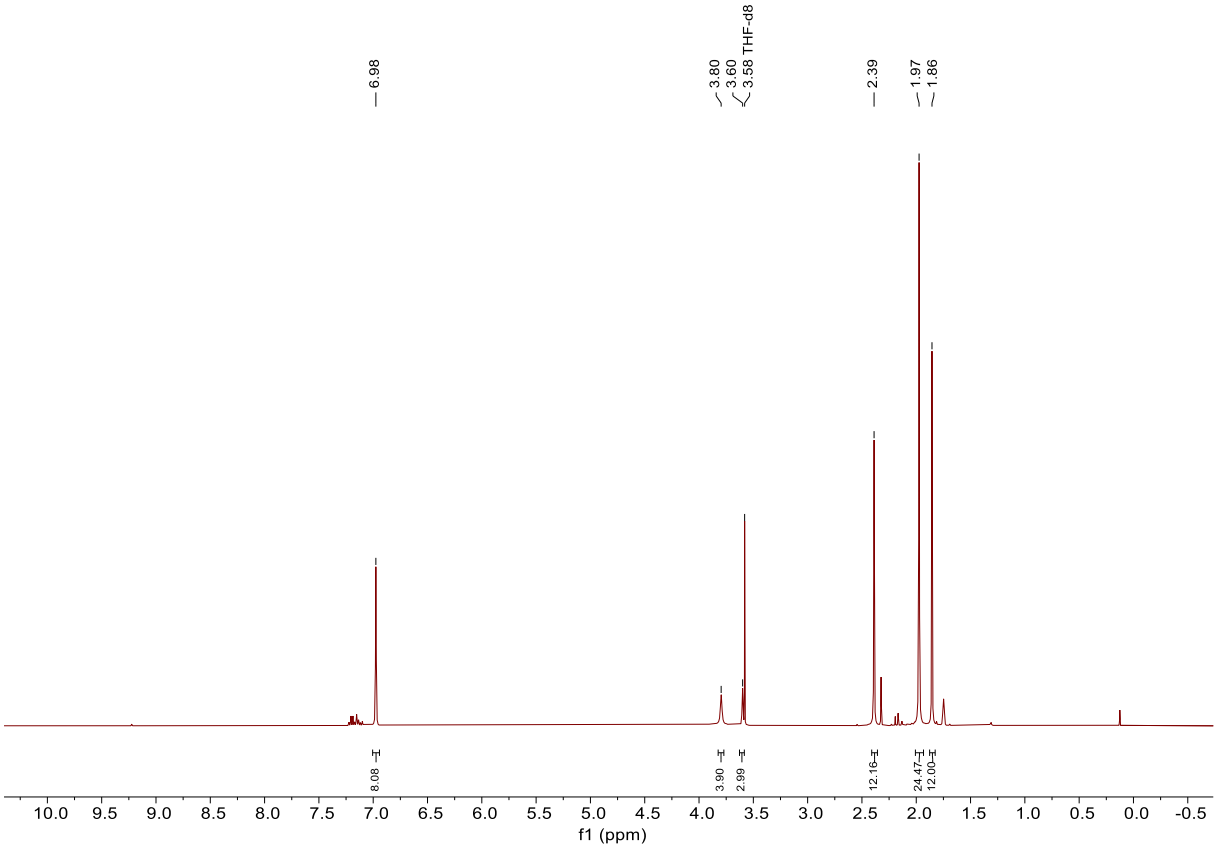


Figure S31 ^{1}H NMR of **5a** in THF-d_8.

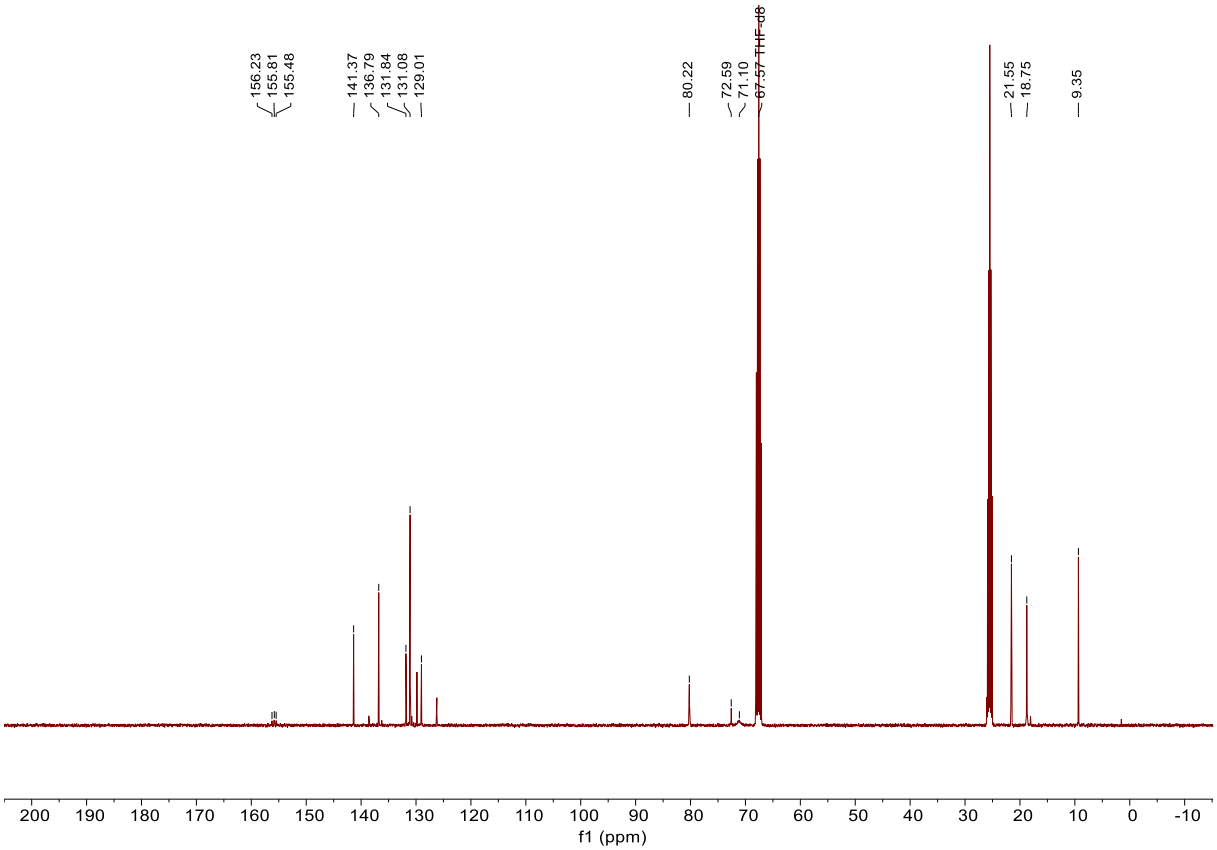


Figure S32 ^{13}C NMR of **5a** in THF-d_8.

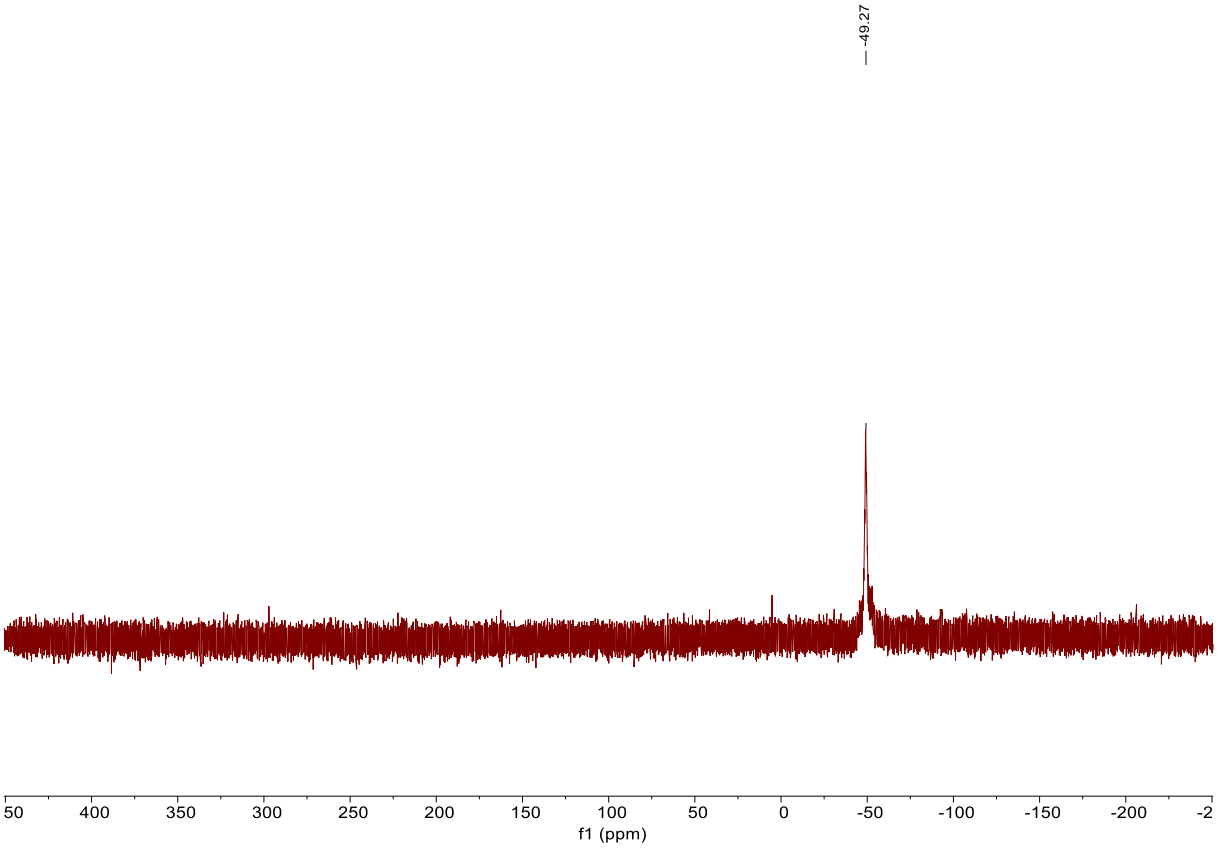


Figure S33 ^{31}P NMR of **5a** in THF-d_8.

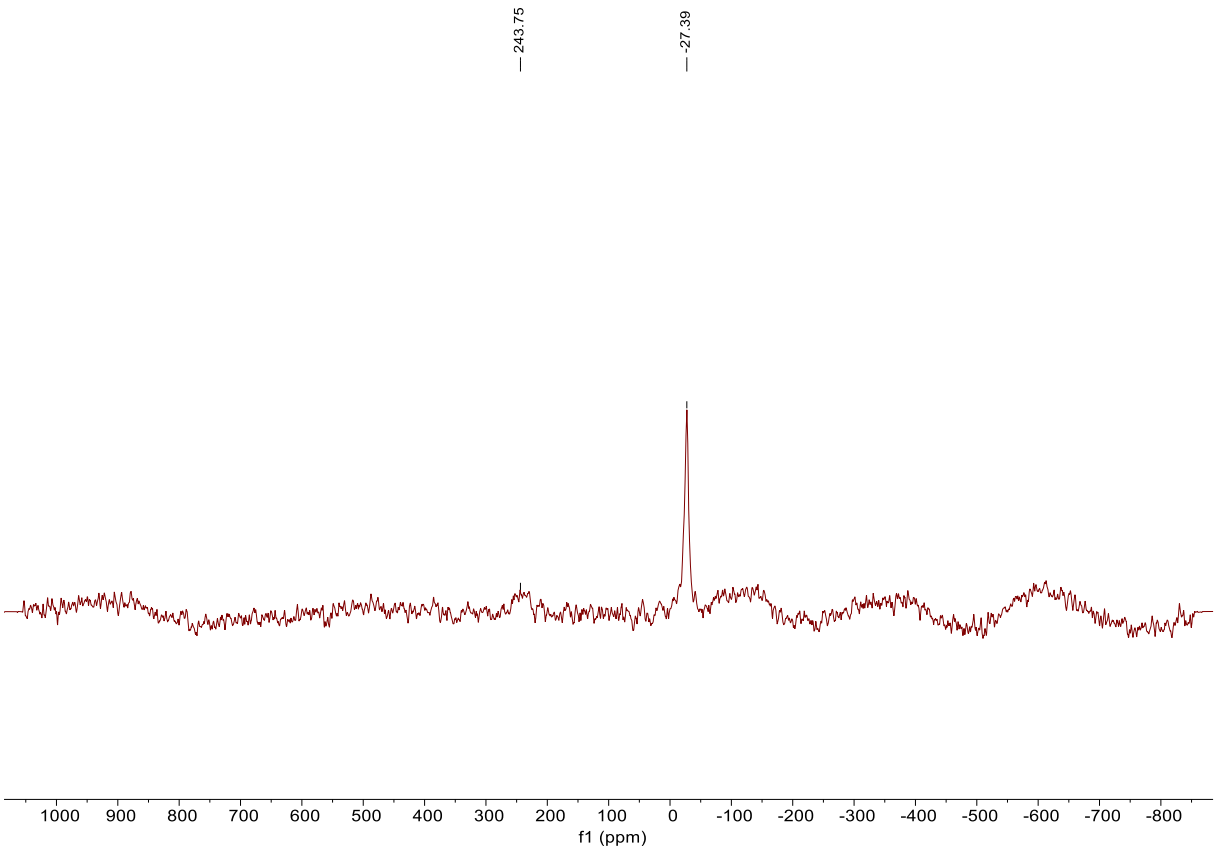
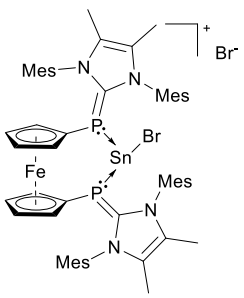


Figure S34 ^{119}Sn NMR of **5a** in THF-d_8.

1.9 Synthesis of BisNHCP $SnBr_2$ Complex 5b (NHC = ^{Me}IMes)



BisNHCP **3b** (30 mg, 32.9 µmol, 1.0 eq) and $SnBr_2$ (10 mg, 35.9 µmol, 1.1 eq) were dissolved in C_6D_6 (0.4 mL) until full conversion was observed in the ^{1}H and ^{31}P NMR. The precipitate was separated from the solution and dried under vacuum to yield the product as an orange solid (12.9 mg, 10.9 µmol, 33%).

^{1}H NMR (400 MHz, THF-d_8, 300K): δ[ppm] = 6.93 (s, 8H, $C_{Mes}H$), 3.94 (s, 4H, $C_{Cp}H$), 3.76 (s, 4H, $C_{Cp}H$), 2.35 (s, 12H, *p*-$C_{Mes}CH_3$), 1.95 (s, 24H, *o*-$C_{Mes}CH_3$), 1.78 ($NCCH_3$).

^{13}C (101 MHz, THF-d_8, 300K) δ[ppm] = 141.36 (*p*-$C_{Mes}CH_3$), 136.69 (NC_{Mes}), 131.74 ($NCCH_3$), 131.13 (*o*-$C_{Mes}CH_3$), 130.83 ($C_{Mes}H$), 80.09 ($C_{Cp}H$), 71.18 ($C_{Cp}H$), 21.63 (*p*-$C_{Mes}CH_3$), 18.95 (*o*-$C_{Mes}CH_3$), 9.47 ($NCCH_3$).

Shifts of carbon atoms directly bound to P were not observed in the ^{13}C NMR spectrum. The signal at 128.66 ppm is from C_6D_6 residuals.

^{31}P (162 Hz, THF-d_8, 300K) δ[ppm] = -49.57 (s, satellites $^{1}J_{Sn,P}$ = 1162 Hz)

^{119}Sn (149 Hz, THF-d_8, 300K) δ[ppm] = 170.47

LIFDI-MS: Calculated for $[C_{56}H_{64}BrFeN_4P_2Sn]^+$: 1109.2161

Observed: 1109.23604

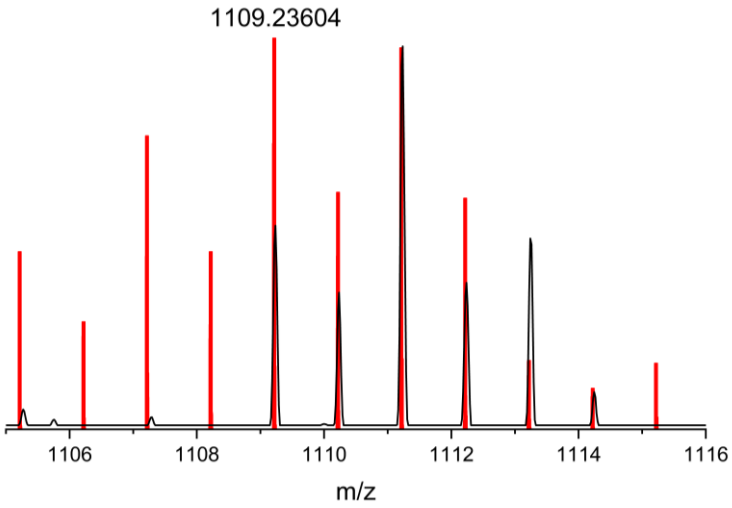


Figure S35 Measured (black) and calculated (red) LIFDI-MS for [**5b**-Br]$^+$.

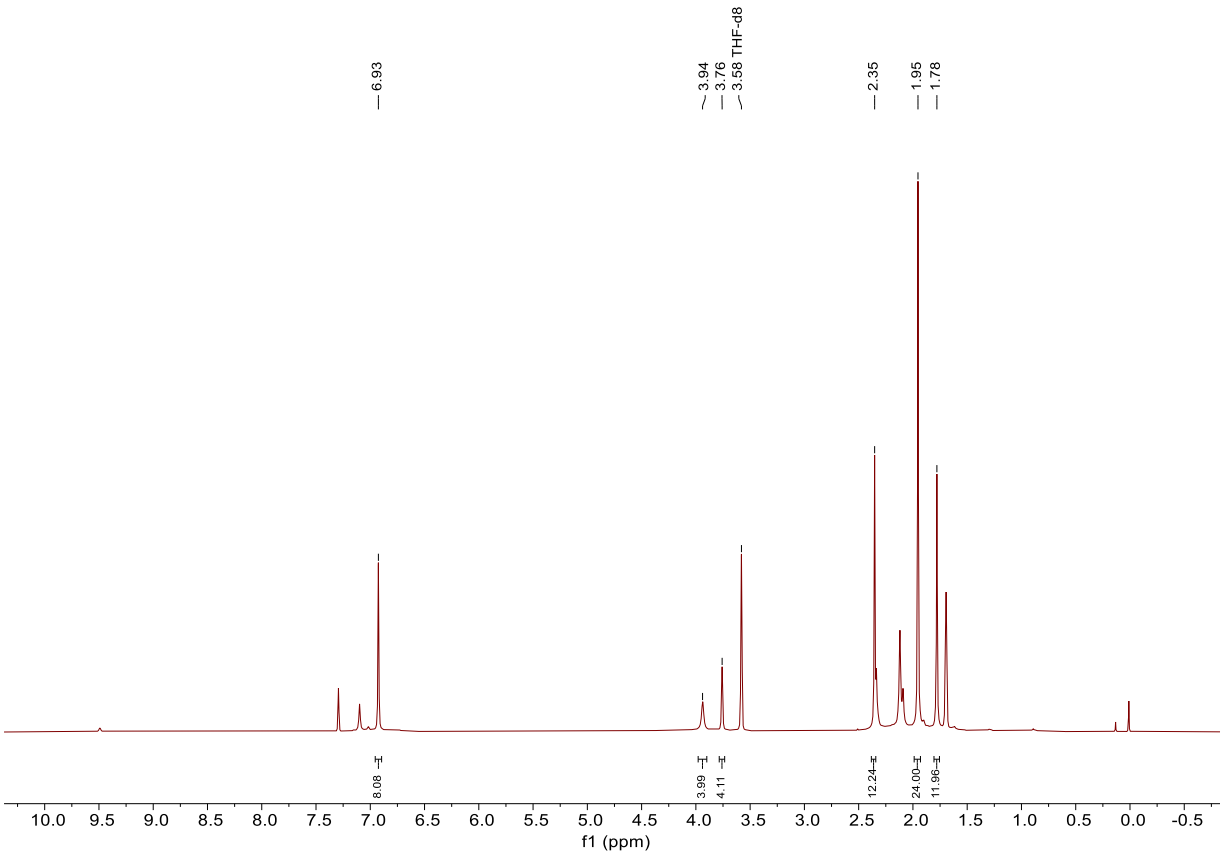


Figure S36 ^{1}H NMR of **5b** in THF-d_8.

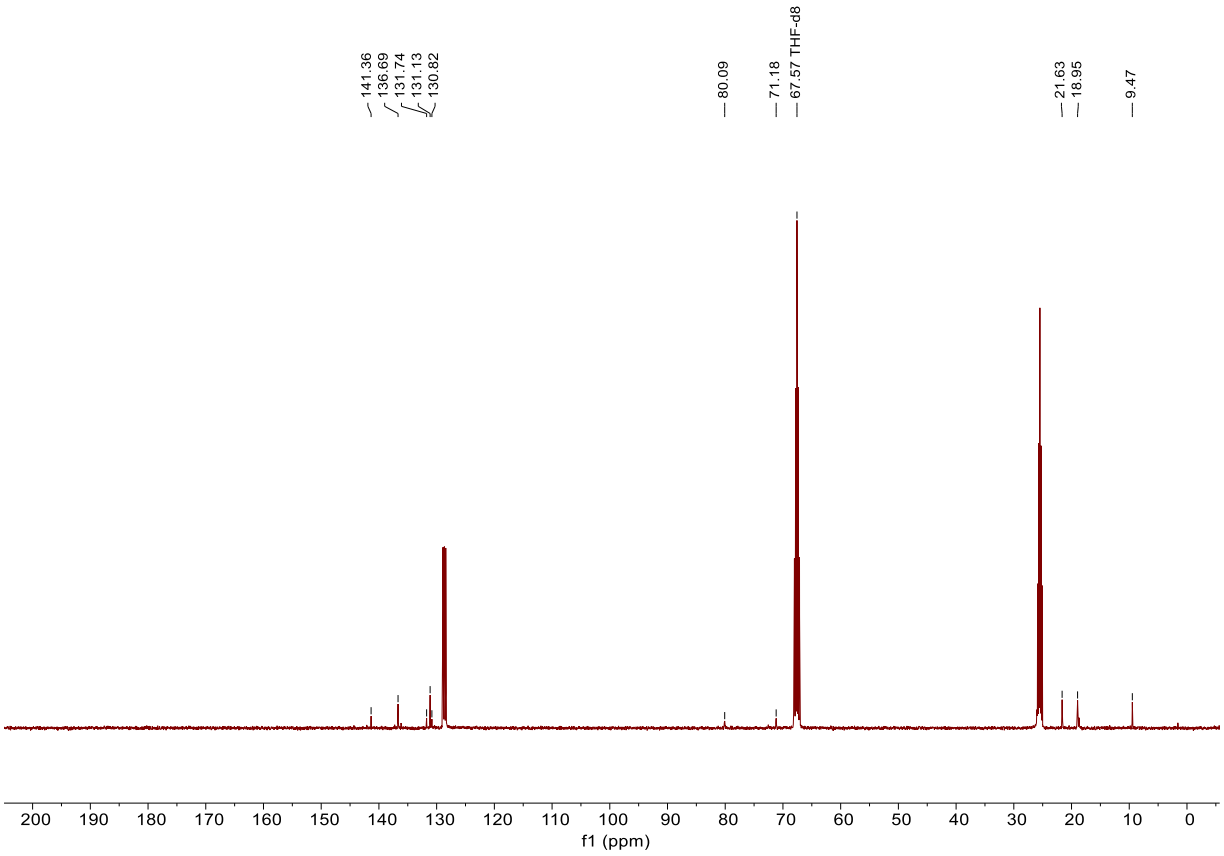


Figure S37 ^{13}C NMR of **5b** in THF-d_8.

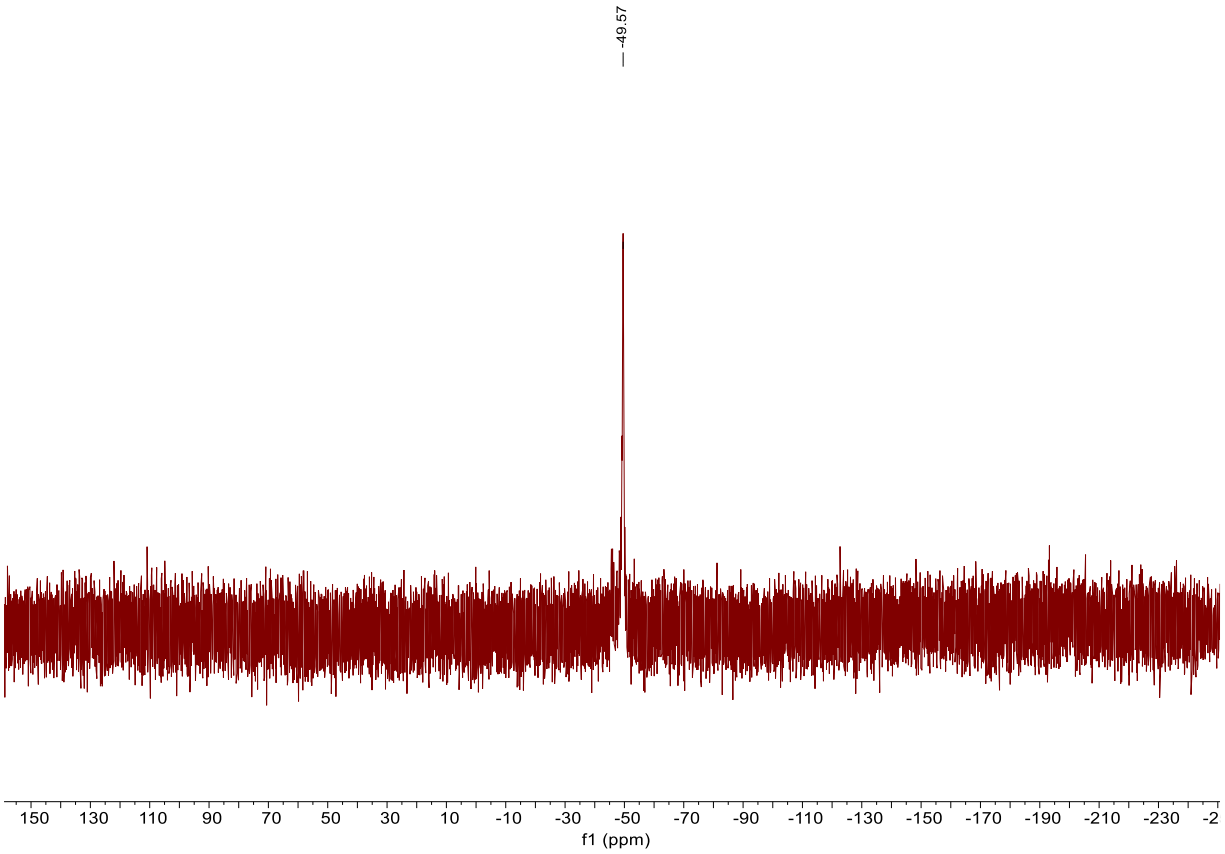


Figure S38 ^{31}P NMR of **5b** in THF-d_8.

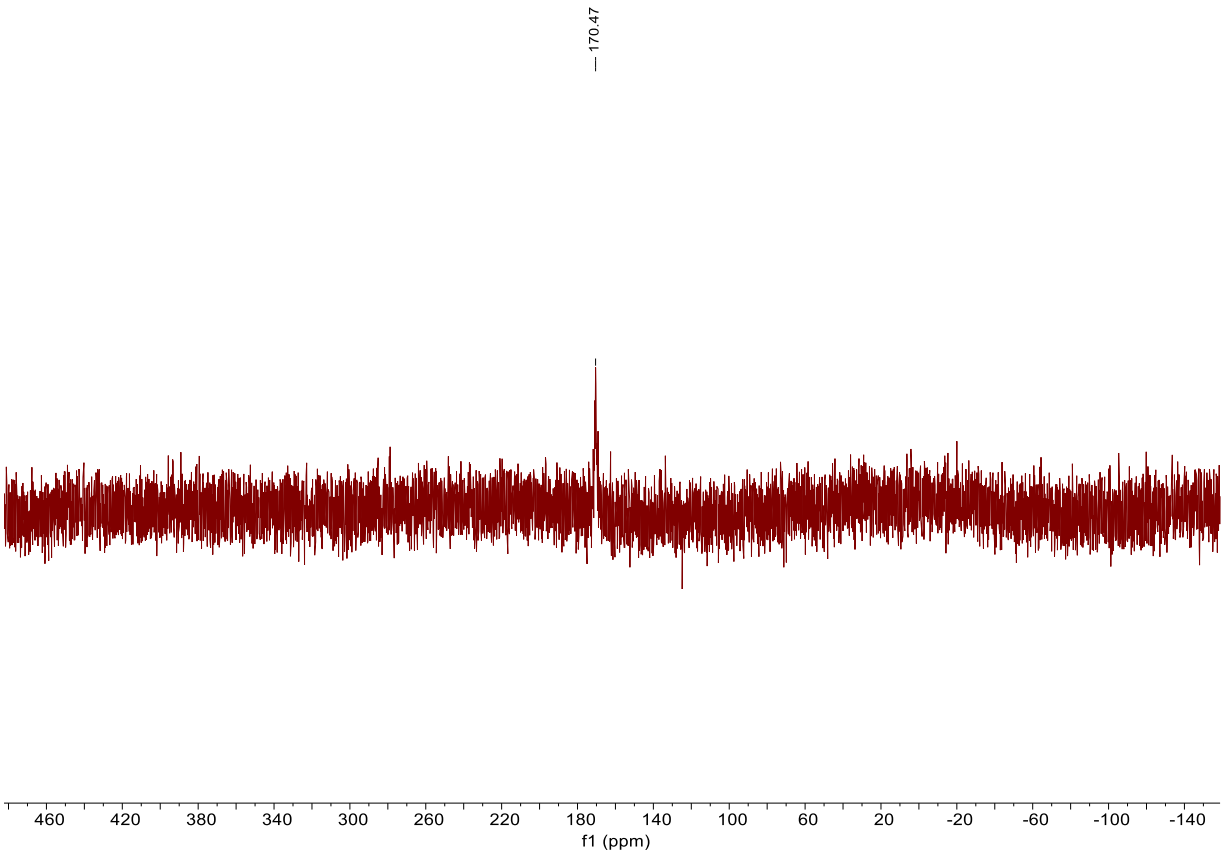
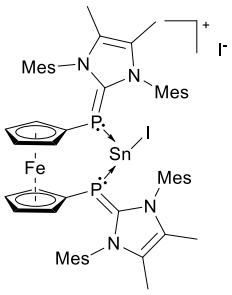


Figure S39 ^{119}Sn NMR of **5b** in THF-d_8.

1.10 Synthesis of BisNHCP SnI_2 Complex 5c (NHC = ^{Me}IMes)



In a J. Young NMR tube, to bisNHCP **3b** (10.0 mg, 10.98 µmol, 1.0 eq) in THF-d_8 (0.4 mL) was added SnI_2 (4.1 mg, 10.98 µmol, 1.0 eq). ^{1}H and ^{31}P NMR showed full conversion. The reaction solution was filtrated and the solvent removed to obtain a yellow product (11.1 mg, 8.65 µmol, 79%).

^{1}H NMR (400 MHz, THF-d_8, 300K): δ[ppm] = 6.97 (s, 8H, $C_{Mes}H$), 4.05 (s, 4H, $C_{Cp}H$), 3.76 (s, 4H, $C_{Cp}H$), 2.38 (s, 12H, *p*-$C_{Mes}CH_3$), 2.02 (s, 24H, *o*-$C_{Mes}CH_3$), 1.85 ($NCCH_3$).

^{13}C (101 MHz, THF-d_8, 300K) δ[ppm] = 156.32(d, $^1J_{C,P}$ = 33.1 Hz, $C_{carbene}$P), 155.97 (d, $^1J_{C,P}$ = 32.6 Hz, $C_{carbene}$P), 141.29 (*p*-$C_{Mes}CH_3$), 136.85 (NC_{Mes}), 131.82 ($NCCH_3$), 131.14 (*o*-$C_{Mes}CH_3$), 130.53 ($C_{Mes}H$), 79.89 (m, $C_{Cp}H$), 72.00 (t, $^1J_{C,P}$ = 12.5 Hz, $C_{Carbene}$P), 71.06 ($C_{Cp}H$), 21.58 (*p*-$C_{Mes}CH_3$), 19.34 (*o*-$C_{Mes}CH_3$), 9.74 ($NCCH_3$).

^{31}P (162 Hz, THF-d_8, 300K) δ[ppm] = -52.12 (s, satellites $^1J_{119Sn,P}$ = 1199 Hz, $^1J_{117Sn,P}$ = 1252 Hz)

^{119}Sn (149 Hz, THF-d_8, 300K) δ[ppm] = 262.20 (t, $^1J_{Sn,P}$ = 1254 Hz)

Elemental Analysis: $C_{56}H_{64}FeI_2N_4P_2Sn$

Calculated [%]: C (52.41), H (5.03), N (4.37)

Observed [%]: C (51.20), H (5.12), N (3.67)

LIFDI-MS: Calculated for $[C_{56}H_{64}FeIN_4P_2Sn]^+$: 1157.20224

Observed: 1157.20661

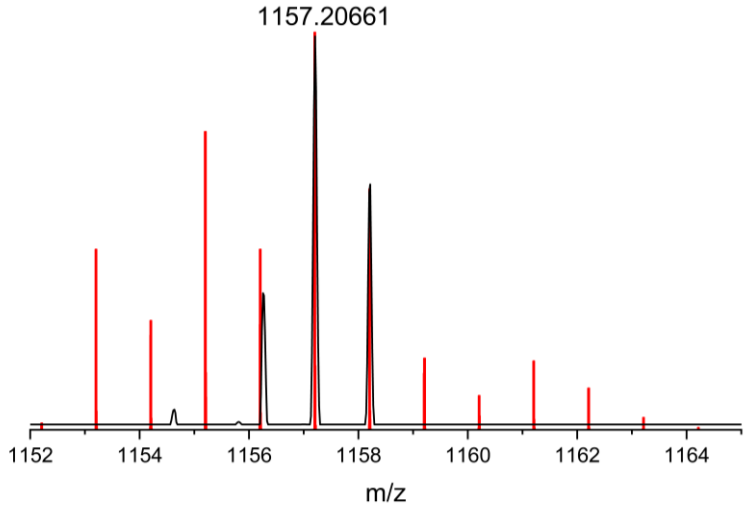


Figure S40 Measured (black) and calculated (red) LIFDI-MS for [**5c**-I]$^{+}$.

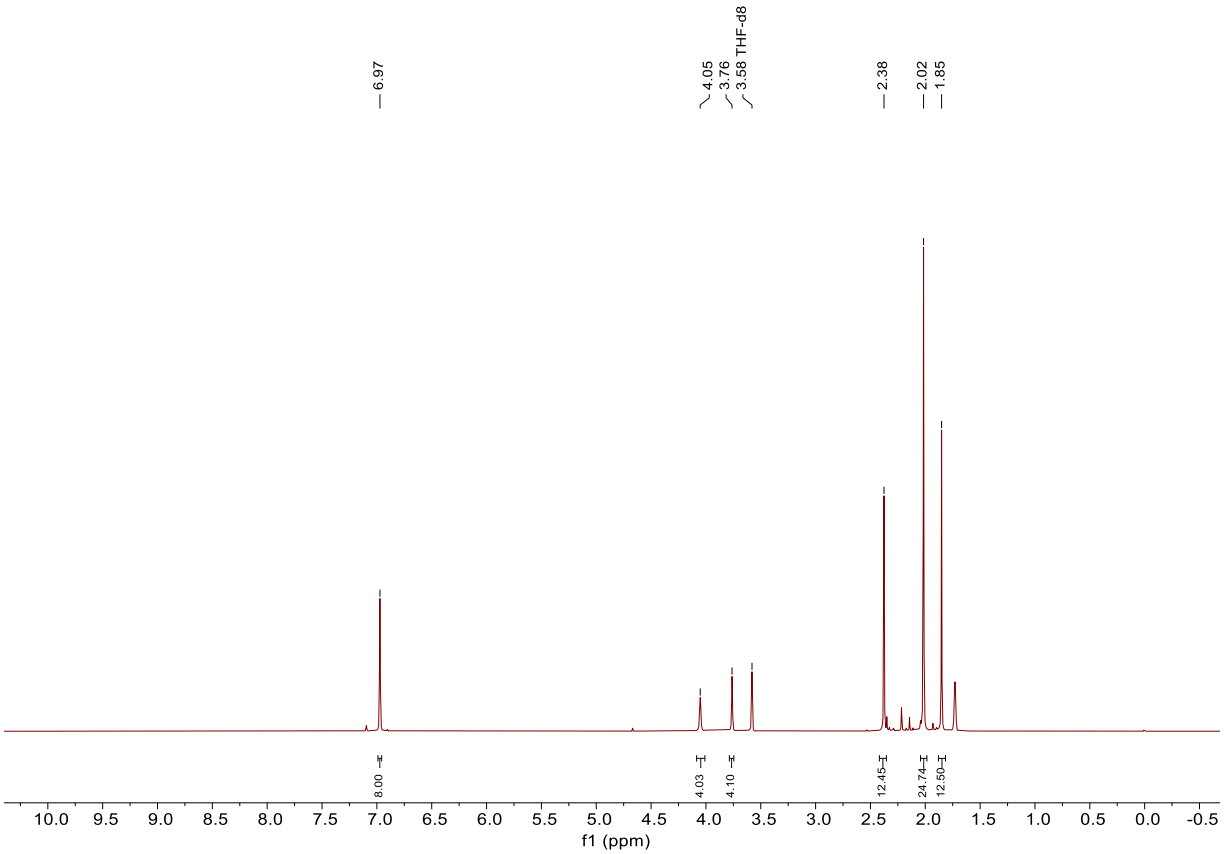


Figure S41 ^{1}H NMR of **5c** in THF-d_8.

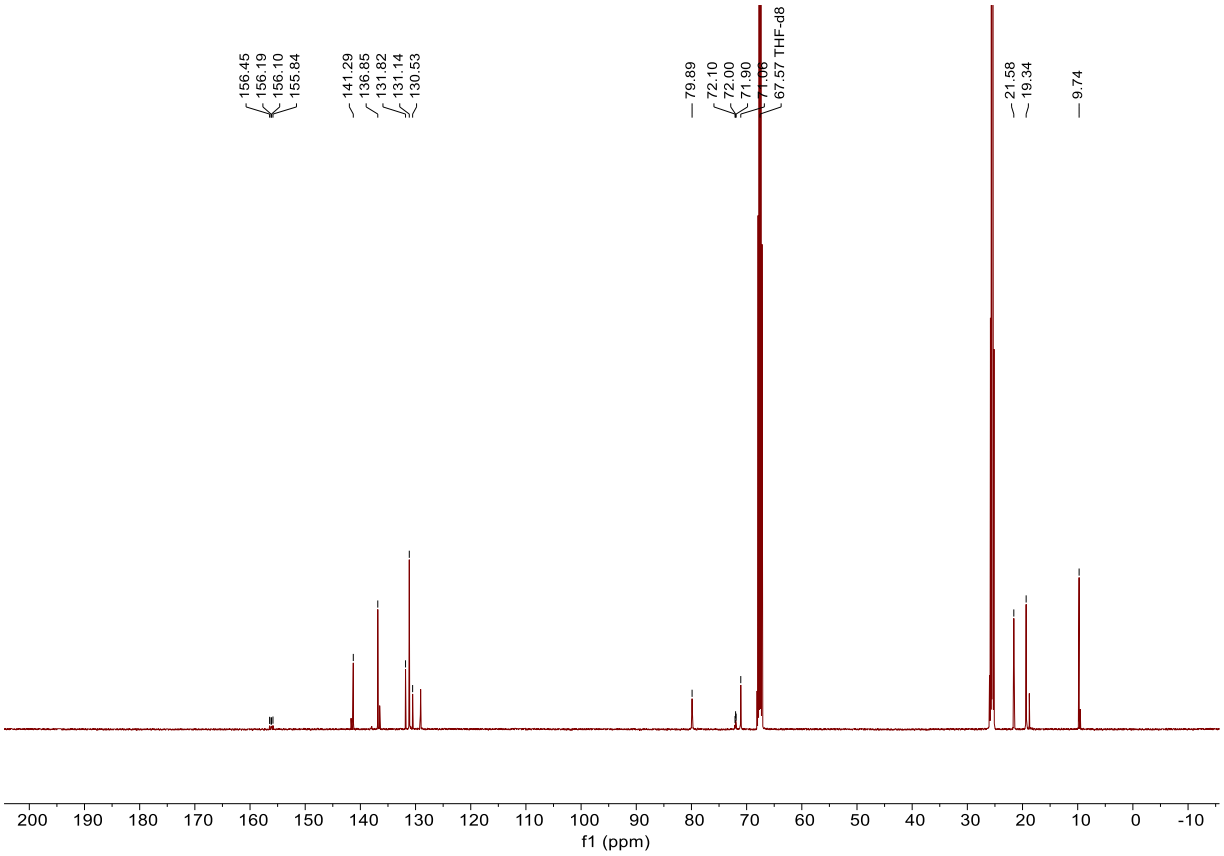


Figure S42 ^{13}C NMR of **5c** in THF-d_8.

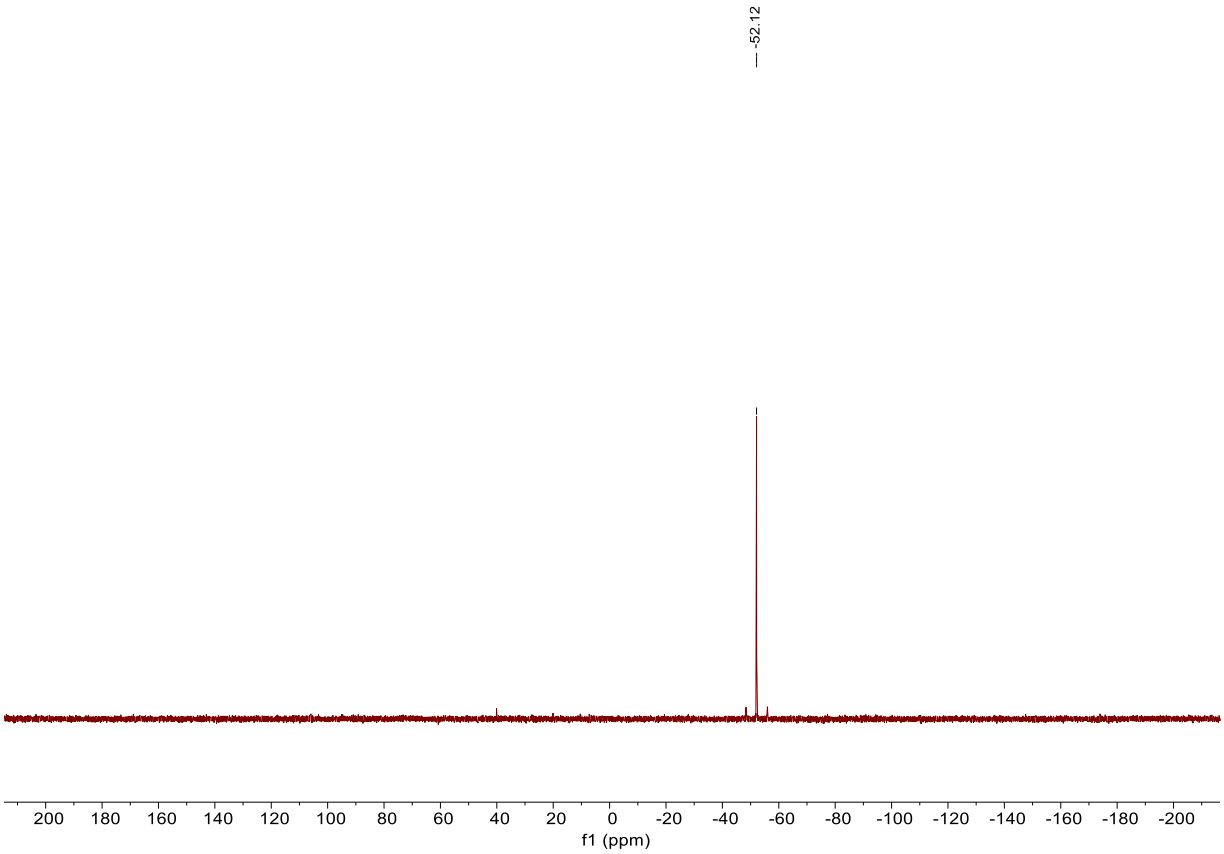


Figure S43 ^{31}P NMR of **5c** in THF-d_8.

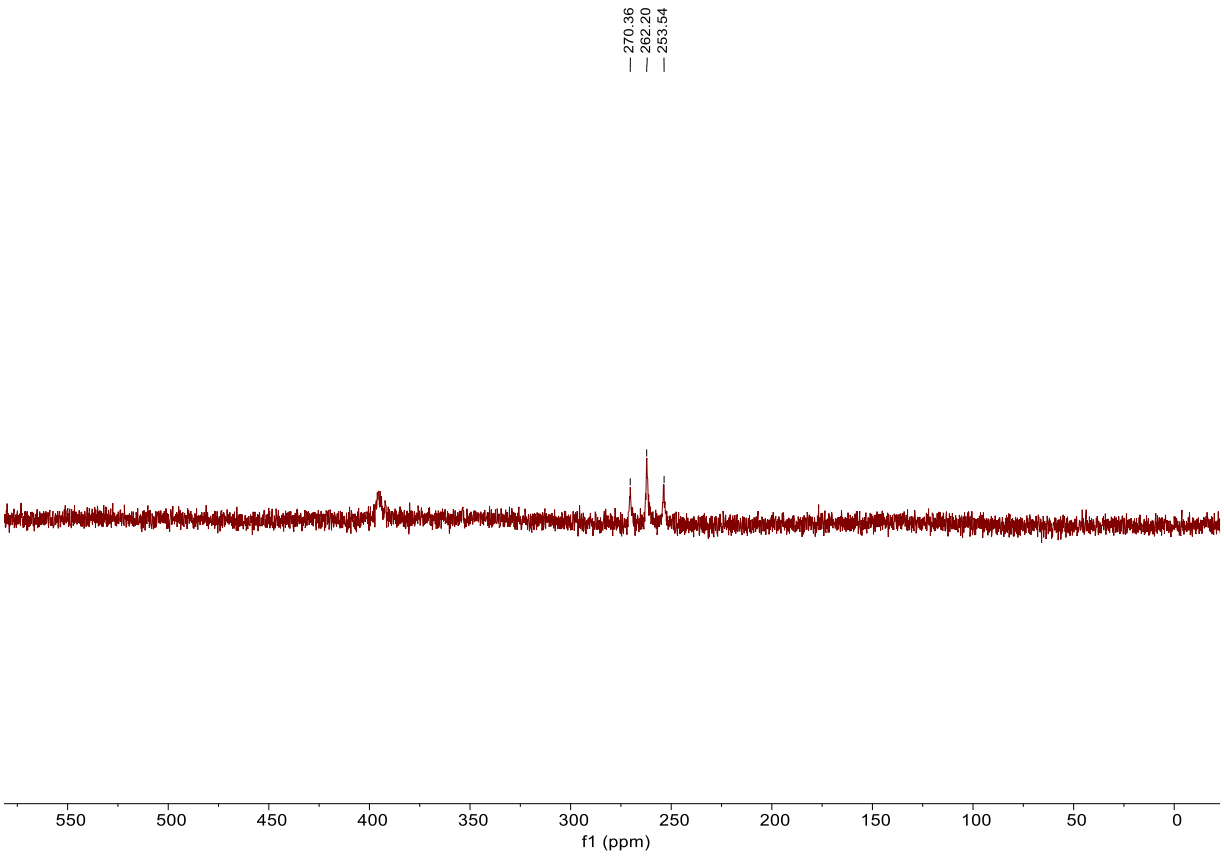
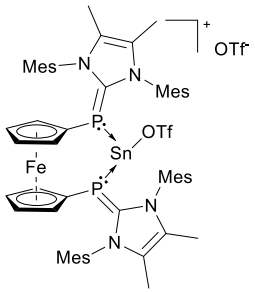


Figure S44 ^{119}Sn NMR of **5c** in THF-d_8.

1.11 Synthesis of BisNHCP Sn(OTf)$_2$ Complex 5d (NHC = ^{Me}IMes)



BisNHCP **3b** (15.0 mg, 16.5 µmol, 1.0 eq) and Sn(OTf)$_2$·dioxane (8.3 mg, 16.5 µmol, 1.0 eq) were dissolved in benzene (0.4 mL) and stirred for 3h. The solvent was removed and the residue extracted with THF. After removal of the solvent a yellow product (21.0 mg, 15.8 µmol, 96%) was isolated.

^{1}H NMR (400 MHz, THF-d_8, 300K): δ[ppm] = 6.99 (s, 8H, C$_{Mes}$H), 3.83 (s, 4H, C$_{Cp}$H), 3.81 (s, 4H, C$_{Cp}$H), 2.39 (s, 12H, *p*-C$_{Mes}$CH$_3$), 1.95 (s, 24H, *o*-C$_{Mes}$CH$_3$), 1.84 (NCCH$_3$).

^{13}C (101 MHz, THF-d_8, 300K) δ[ppm] =153.24 (d, $^1J_{C,P}$ = 31.2 Hz, *C*$_{carbene}$P), 152.87 (d, $^1J_{C,P}$ = 31.0 Hz, *C*$_{carbene}$P), 141.36 (*p*-*C*$_{Mes}$CH$_3$), 136.80 (N*C*$_{Mes}$), 131.49 (N*C*CH$_3$), 131.37 (*o*-*C*$_{Mes}$CH$_3$), 129.62 (*C*$_{Mes}$H), 80.68 (m, *C*$_{Cp}$H), 71.94 (*C*$_{Cp}$H), 69.88 (t, $^1J_{C,P}$ = 10.5 Hz, *C*$_{Cp}$P), 21.54 (*p*-C$_{Mes}$*C*H$_3$), 18.40 (*o*-C$_{Mes}$*C*H$_3$), 9.08 (NC*C*H$_3$).

^{19}F(377 MHz, THF-d_8, 300K) δ[ppm] = -78.56 ppm

^{31}P (162 Hz, THF-d_8, 300K) δ[ppm] = -30.56 (s, $^{1}J_{119Sn,P}$ = 1189 Hz, $^{1}J_{117Sn,P}$ = 1247 Hz)

^{119}Sn (149 Hz, THF-d_8, 300K) δ[ppm] = 465.20 (t, $^{1}J_{Sn,P}$ = 1270 Hz)

Elemental Analysis: $C_{58}H_{64}F_6FeN_4O_6P_2S_2Sn$

Calculated [%]: C (52.47), H (4.86), N (4.22), S (4.83)

Observed [%]: C (52.18), H (5.11), N (4.15), S (4.68)

LIFDI-MS: Calculated for $[C_{57}H_{64}F_3FeN_4O_3P_2SSn]^+$: 1179.24979

Observed: 1179.24543

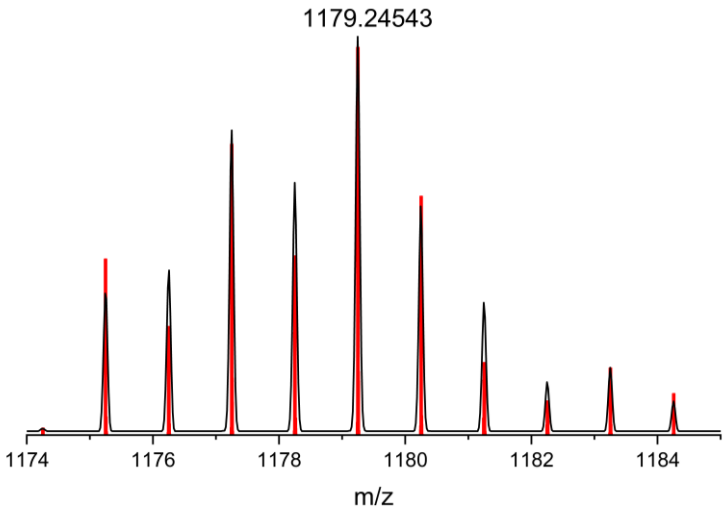


Figure S45 Measured (left) and calculated (right) LIFDI-MS for [**5d**-OTf]$^+$.

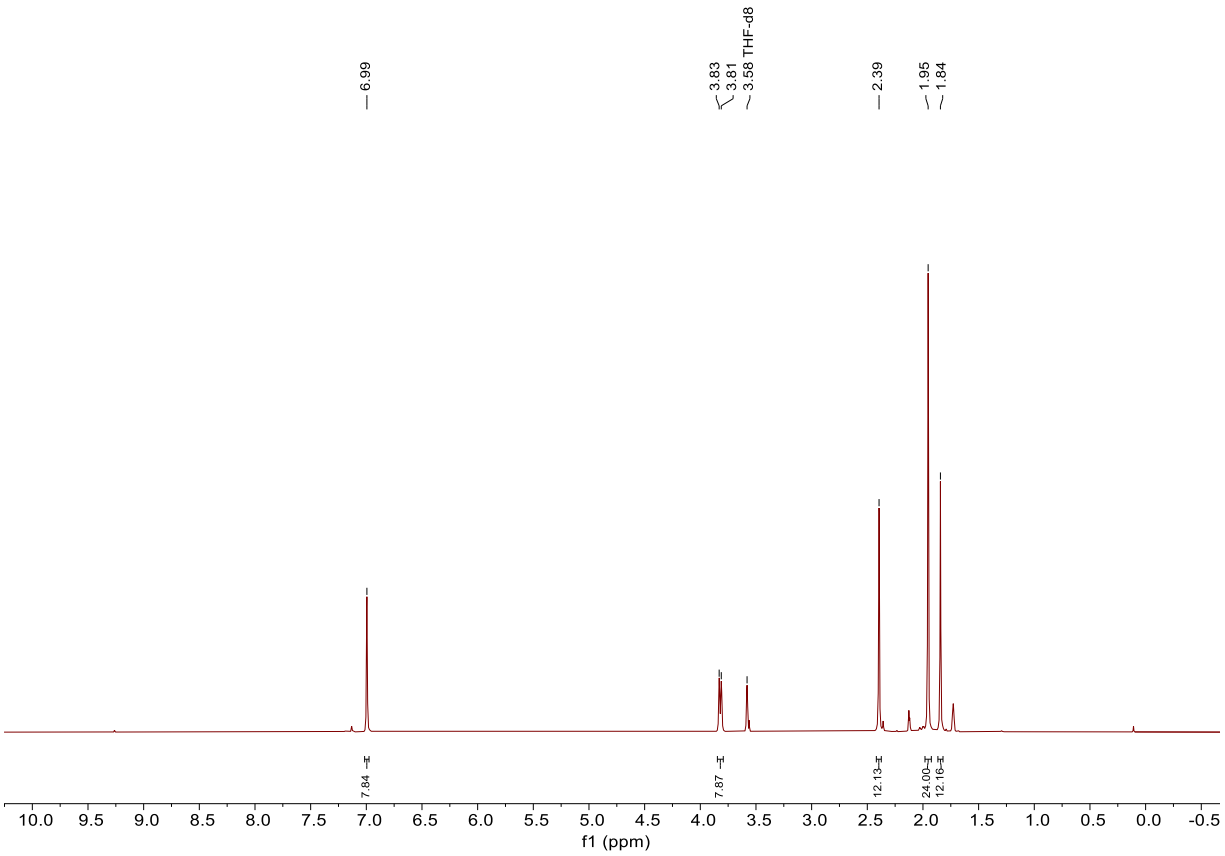


Figure S46 ^{1}H NMR of **5d** in THF-d_8.

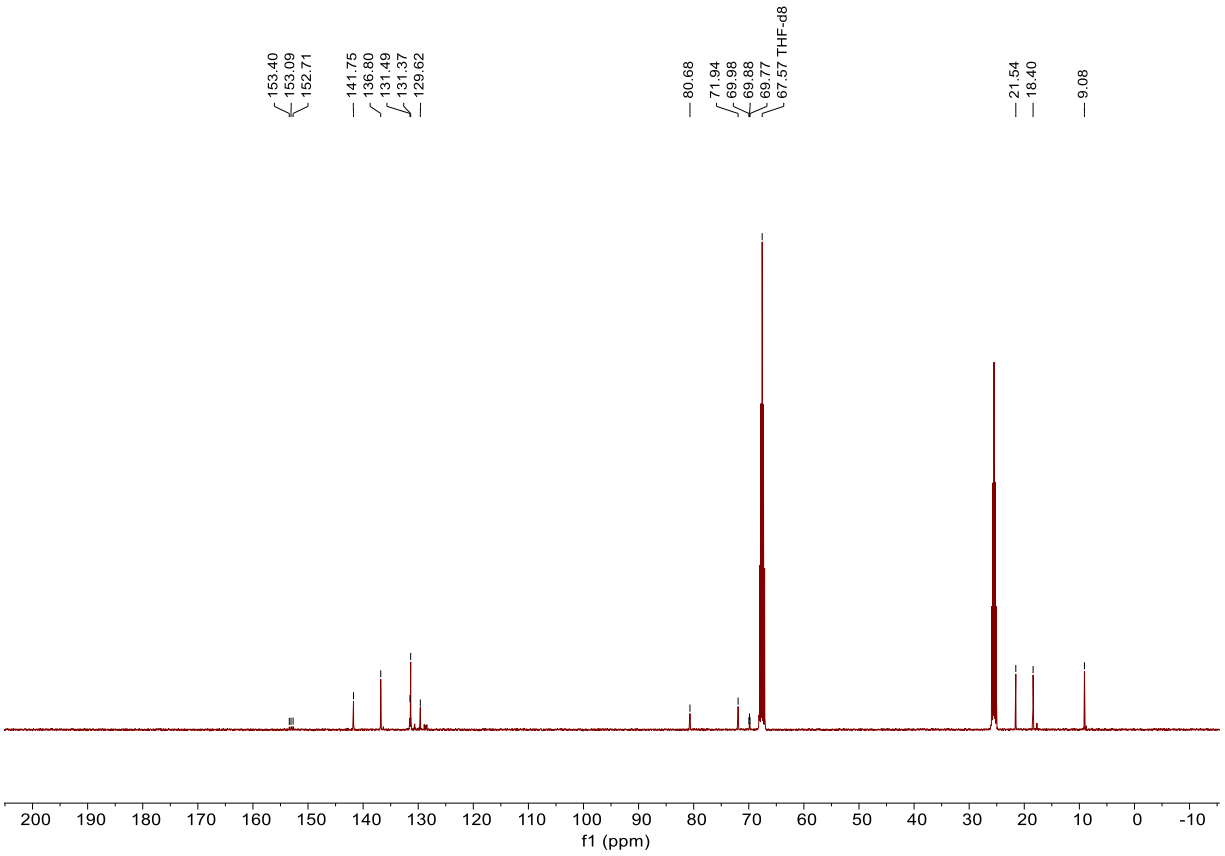


Figure S47 ^{13}C NMR of **5d** in THF-d_8.

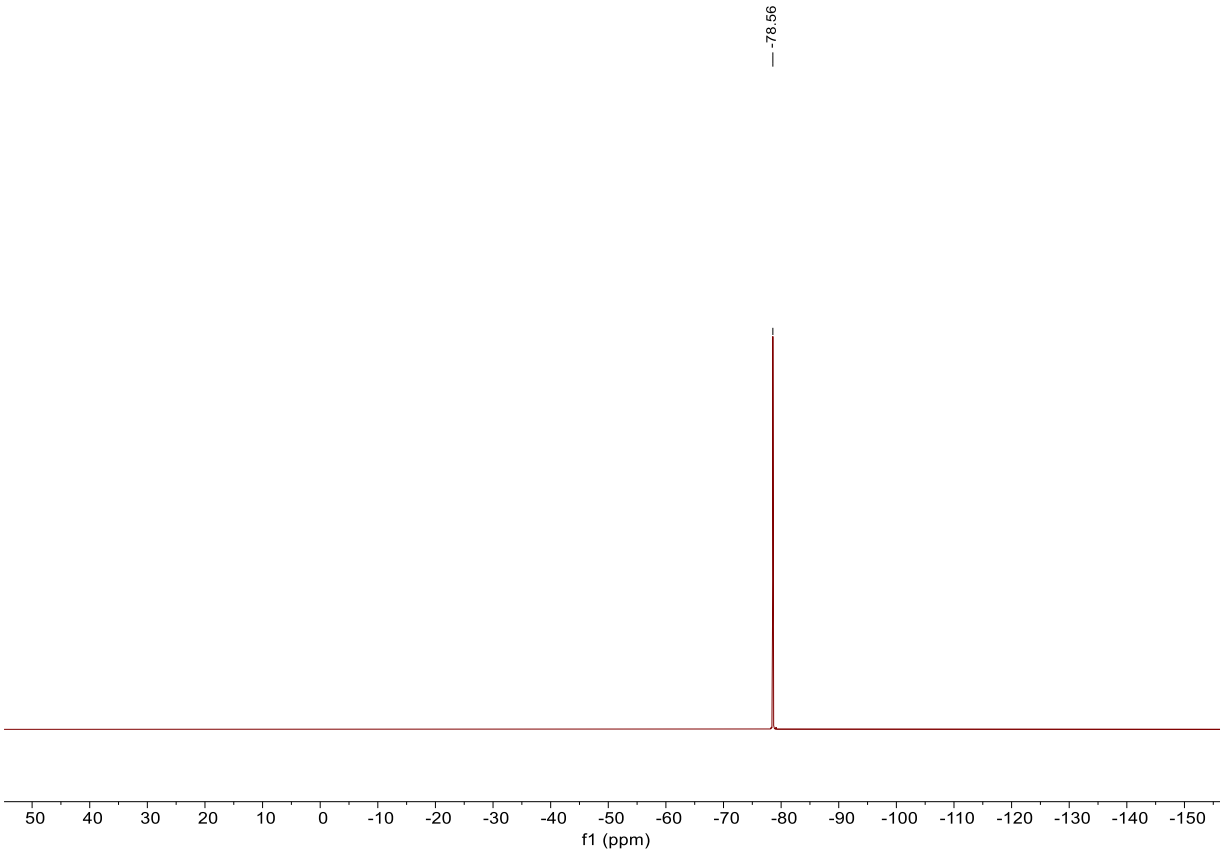


Figure S48 ^{19}F NMR of **5d** in THF-d_8.

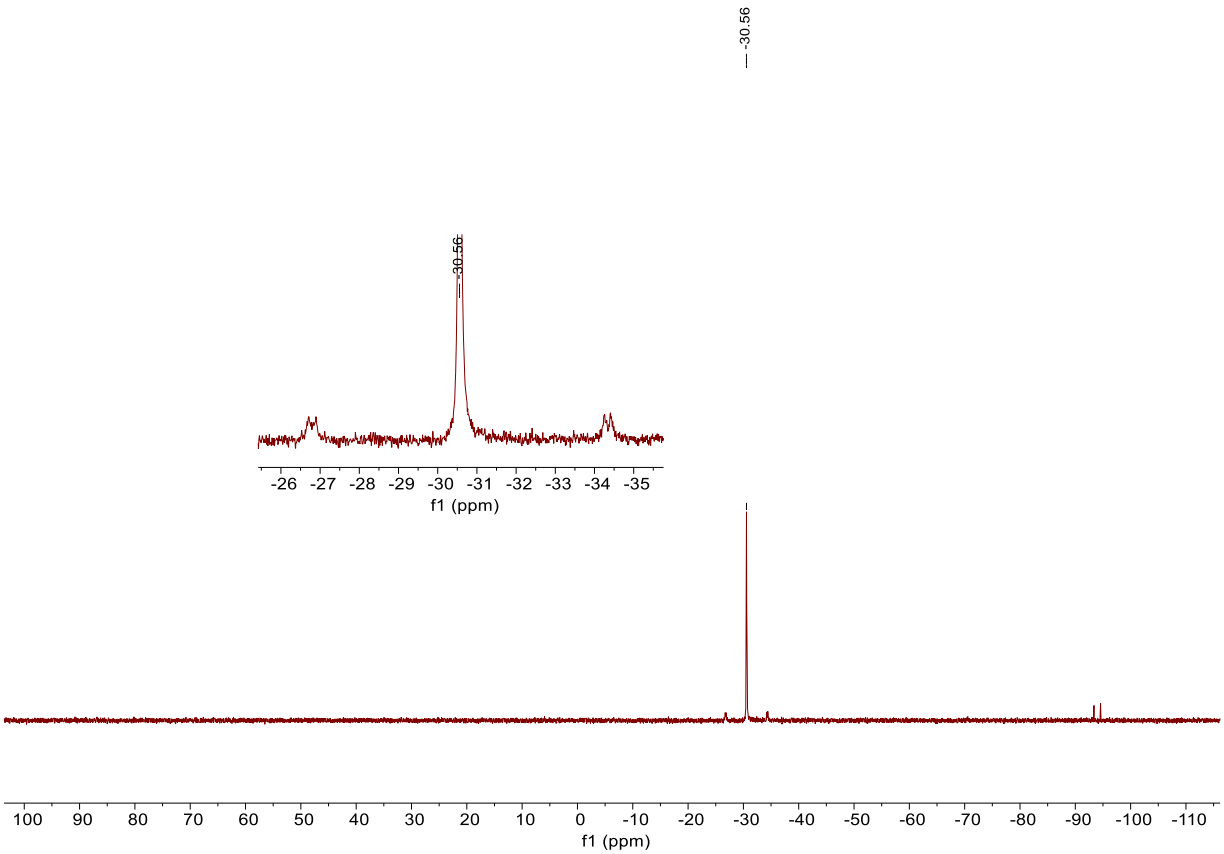


Figure S49 ^{31}P NMR of **5d** in THF-d_8.

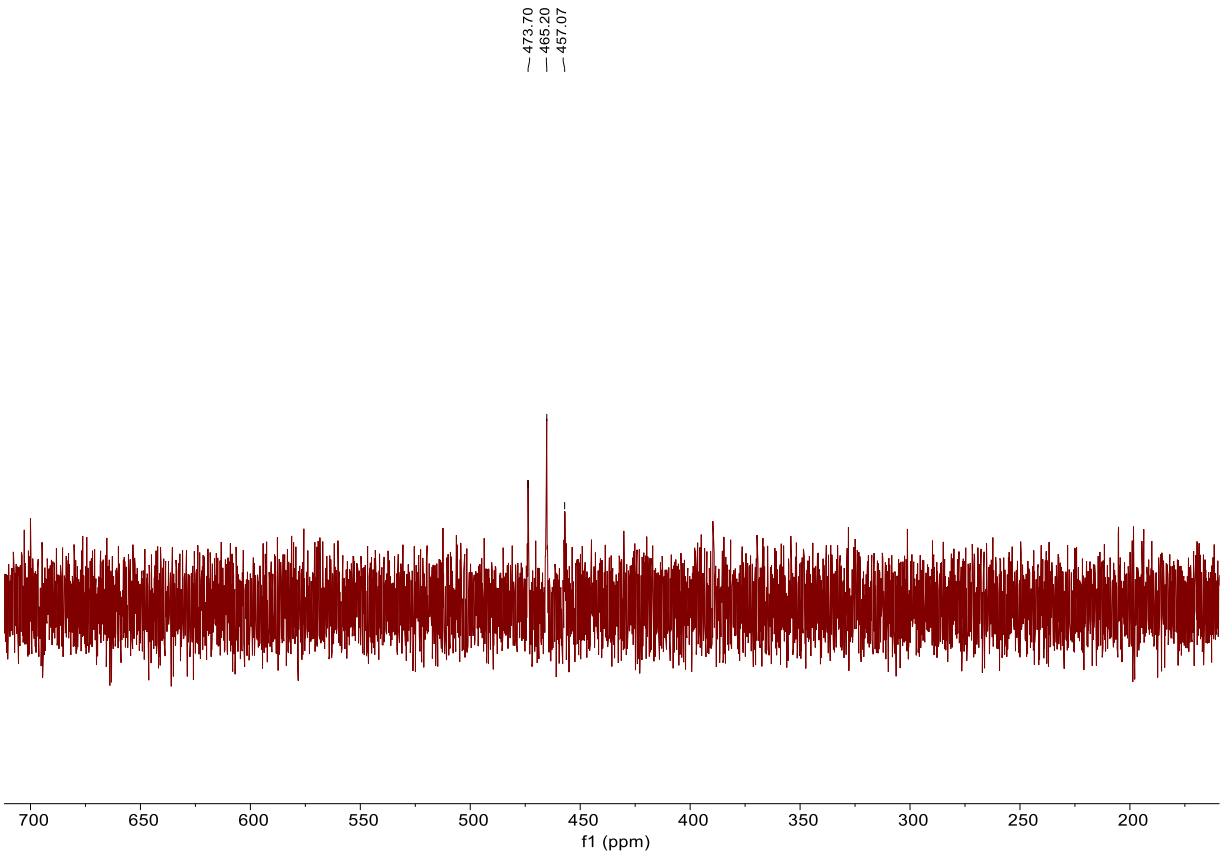
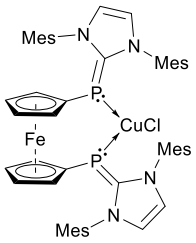


Figure S50 ^{119}Sn NMR of **5d** in THF-d_8.

1.12 Synthesis of BisNHCP CuCl Complex 7a (NHC = IMes)



BisNHCP **3a** (30.0 mg, 35.09 µmol, 1.0 eq) and CuCl (3.5 mg, 35.35 µmol, 1.0 eq) were dissolved in THF-d_8 (0.4 mL). Filtration and removal of the solvent in vacuo yielded the product as yellow solid (17.7 mg, 18.56 µmol, 53%).

^{1}H NMR (400 MHz, THF-d_8, 300K): δ[ppm] = 6.92 (s, 4H, NCH), 6.78 (s, 8H, C_{Mes}H), 3.50 (t, *J* = 1.8 Hz, 4H, C_{Cp}H), 3.13 (s, 4H, C_{Cp}H), 2.30 (s, 12H, *p*-$C_{Mes}CH_3$), 2.11 (s, 24H, *o*-$C_{Mes}CH_3$).

^{13}C (101 MHz, THF-d_8, 300K) δ[ppm] = 167.55 (dd, $^1J_{C,P}$ = 58.7, 37.9 Hz, $C_{Carbene}$P) 139.02 (*p*-$C_{Mes}CH_3$), 137.22 (NC_{Mes}), 135.45 (*p*-$C_{Mes}CH_3$), 129.85 (C_{Mes}H), 122.19 (N*C*H), 81.60 (m, C_{Cp}H), 73.50 (t, $^1J_{C,P}$ = 8.0 Hz, C_{Cp}P), 70.06 (C_{Cp}H), 21.40 (*p*-$C_{Mes}CH_3$), 19.45 (*o*-$C_{Mes}CH_3$).

^{31}P (162 Hz, THF-d_8, 300K) δ[ppm] = -80.45

LIFDI-MS: Calculated for $C_{52}H_{56}ClCuFeN_4P_2$: 952.23141

Observed: 952.23171

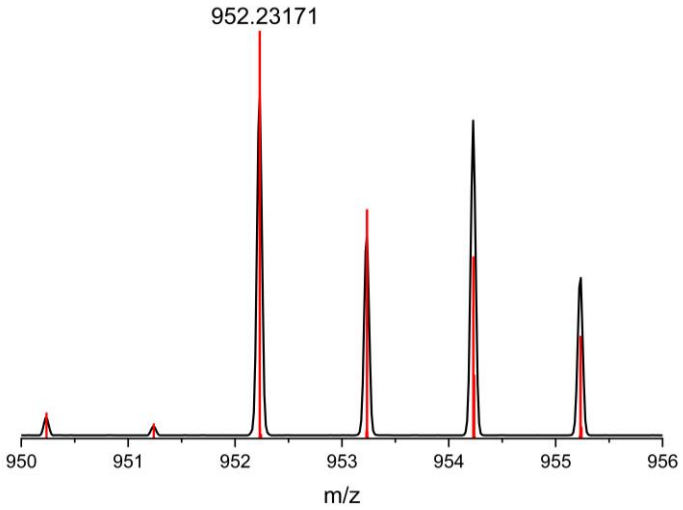


Figure S51 Measured (black) and calculated (red) LIFDI-MS for **7a**.

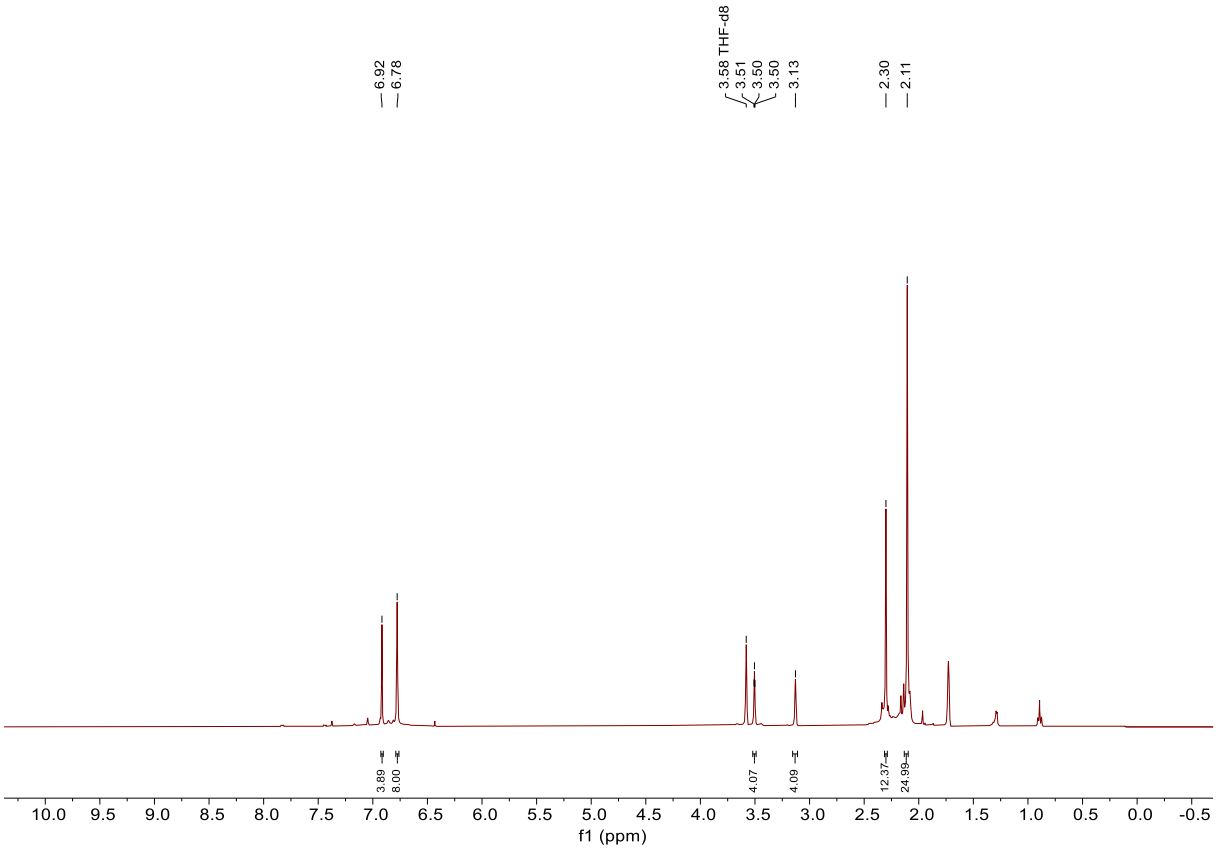


Figure S52 ^{1}H NMR of **7a** in THF-d_8.

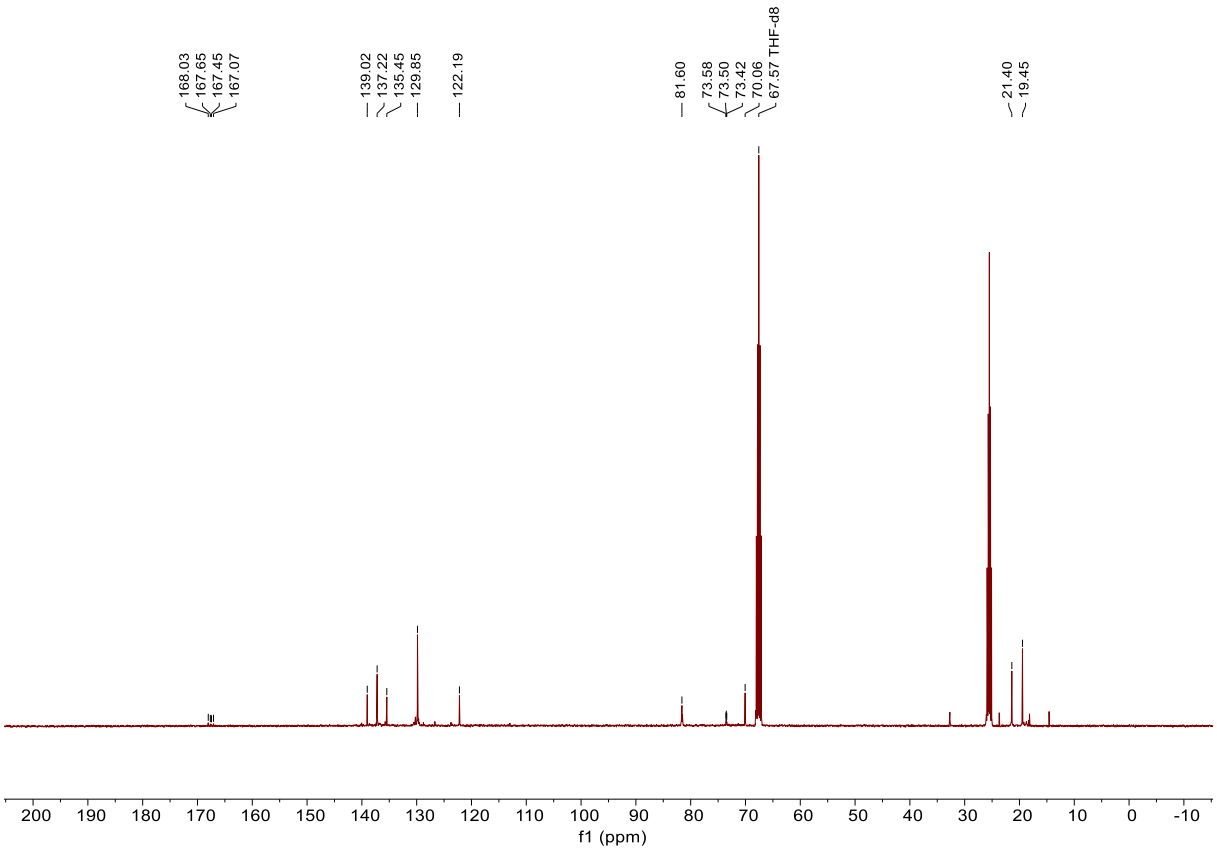


Figure S53 ^{13}C NMR of **7a** in THF-d_8.

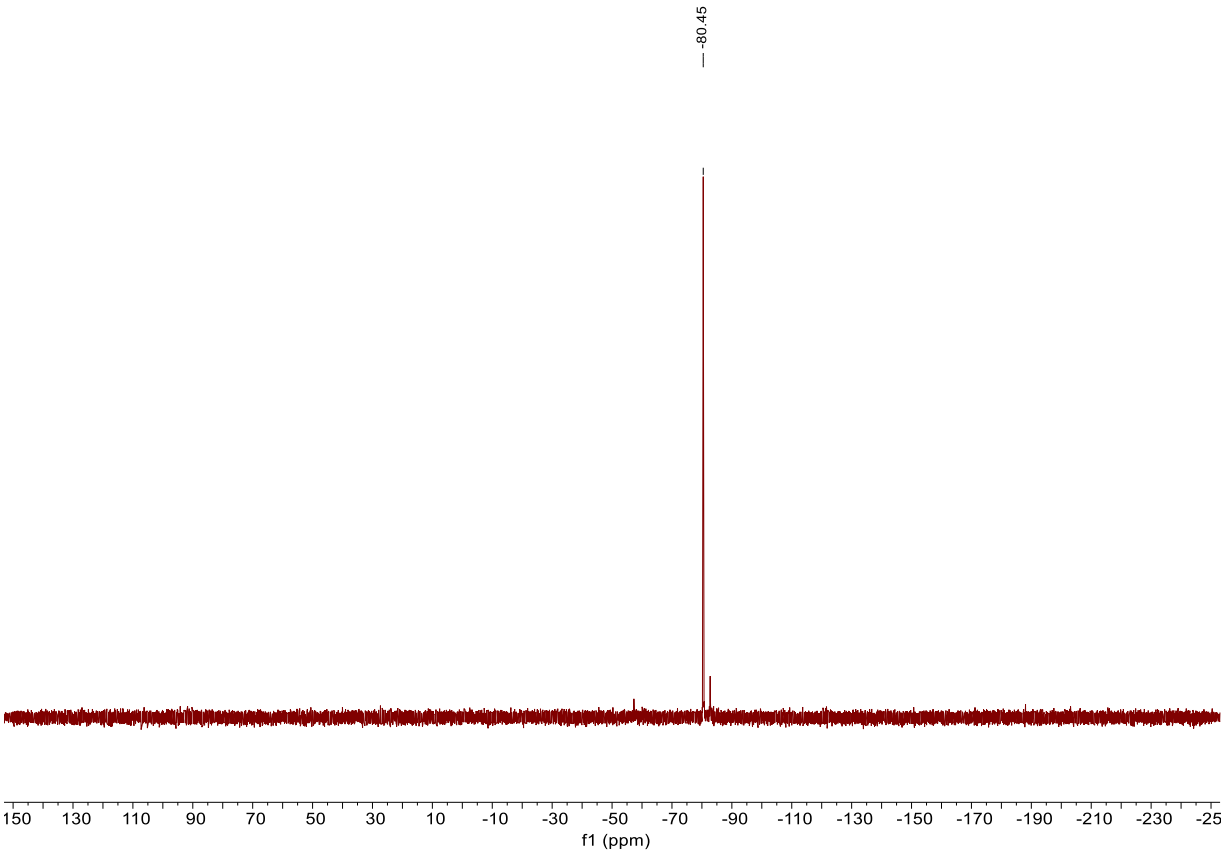
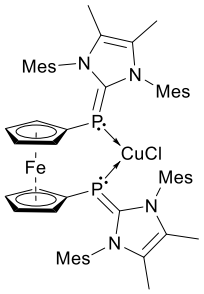


Figure S54 ^{31}P NMR of **7a** in THF-d_8.

1.13 Synthesis of BisNHCP CuCl Complex 7b (NHC = ^{Me}IMes)



Toluene (3 mL) was added to bisNHCP **3b** (30 mg, 32.93 µmol,1.0 eq) and CuCl (3.3 mg, 32.93 µmol, 1.0 eq). The suspension was stirred overnight. The solvent was removed and the residue extracted with THF. After removal of the solvent in vacuo, a yellow product (29.3 mg, 29.01 µmol, 88%) was obtained.

^{1}H NMR (400 MHz, THF-d$_8$, 300K): δ[ppm] = 6.79 (s, 8H, $C_{Mes}H$), 3.49 (t, *J* = 1.8 Hz, 4H, $C_{Cp}H$), 3.06 (s, 4H, $C_{Cp}H$), 2.31 (s, 12H, *p*-$C_{Mes}CH_3$), 2.07 (s, 24H, *o*-$C_{Mes}CH_3$), 1.72 ($NCCH_3$).

^{13}C (101 MHz, THF-d$_8$, 300K) δ[ppm] = 138.97 (*p*-$C_{Mes}CH_3$), 137.71 (NC_{Mes}), 133.71 (N$C$$CH_3$), 129.95 (*o*-$C_{Mes}CH_3$), 124.76 ($C_{Mes}H$), 81.90 (m, $C_{Cp}H$), 69.90 ($C_{Cp}H$), 21.46 (*p*-$C_{Mes}CH_3$), 19.39 (*o*-$C_{Mes}CH_3$), 9.12 ($NCCH_3$).

Shifts of carbon atoms directly bound to P were not observed in the ^{13}C NMR spectrum.

^{31}P (162 Hz, THF-d$_8$, 300K) δ[ppm] = -82.34

Elemental Analysis: $C_{56}H_{64}ClCuFeN_4P_2$

Calculated [%]: C (66.60), H (6.39), N (5.55)

Observed [%]: C (63.94), H (6.33), N (4.65)

LIFDI-MS: Calculated for $C_{56}H_{64}ClCuFeN_4P_2$: 1008.29401

Observed: 1008.29467

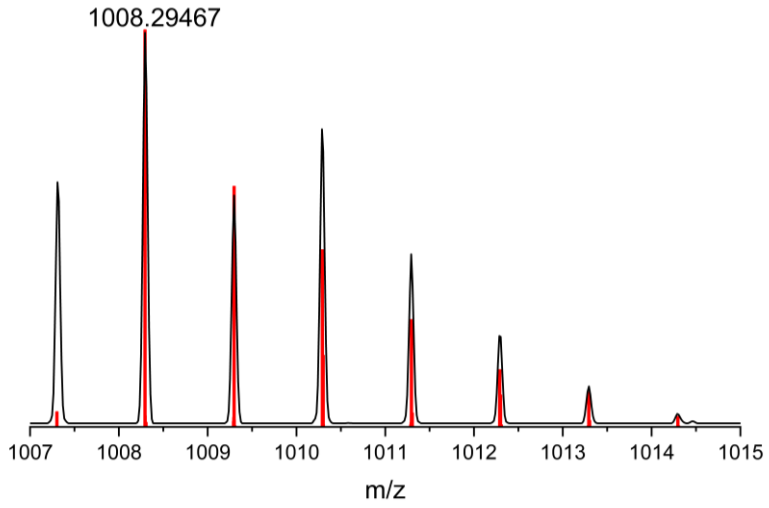


Figure S55 Measured (black) and calculated (red) LIFDI-MS for **7b**.

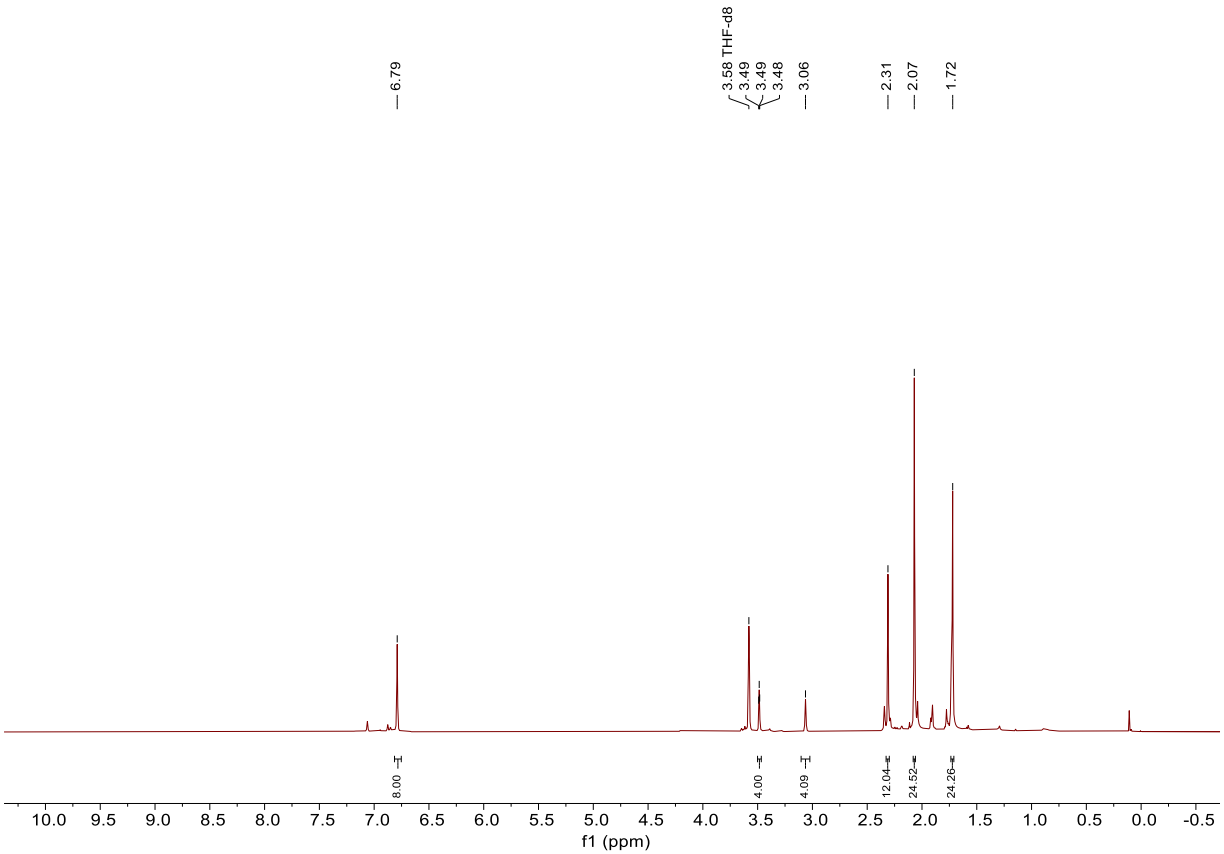


Figure S56 ^{1}H NMR of **7b** in THF-d_8.

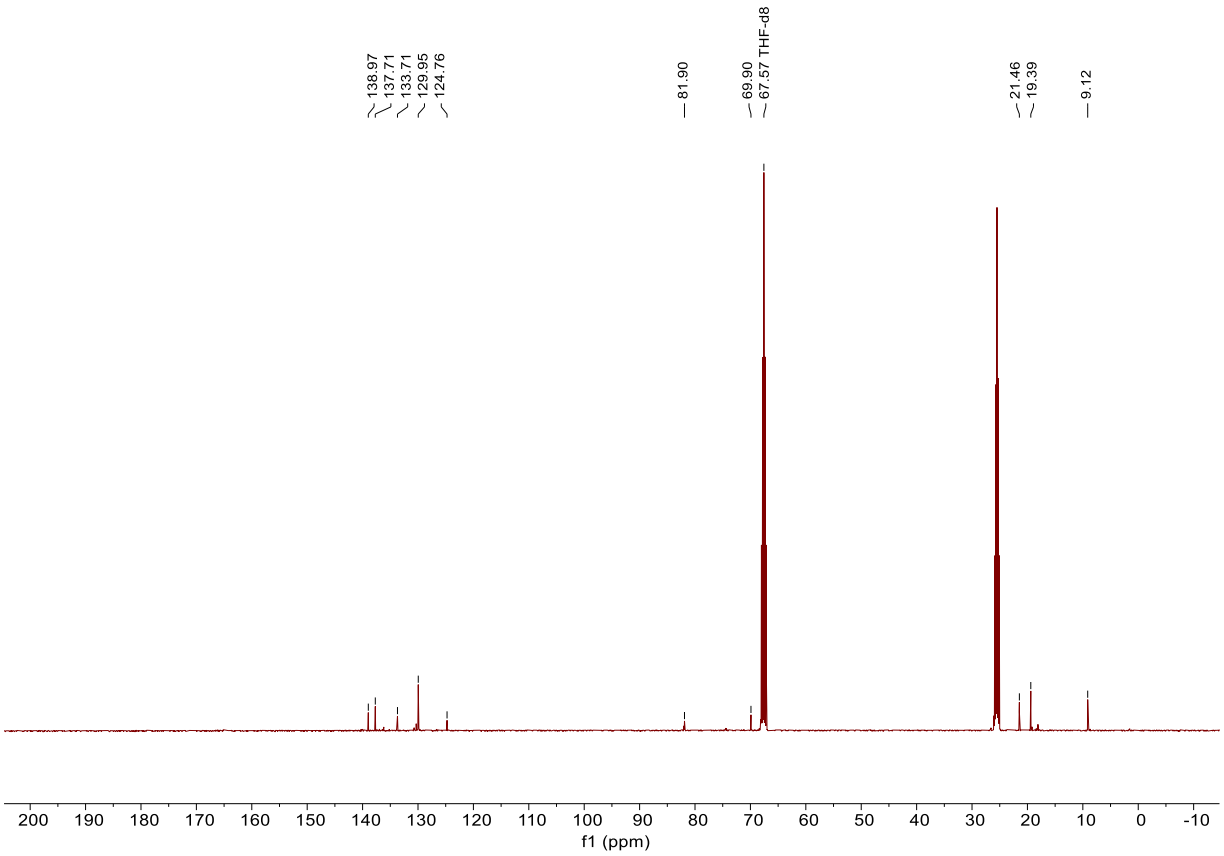


Figure S57 ^{13}C NMR of **7b** in THF-d_8.

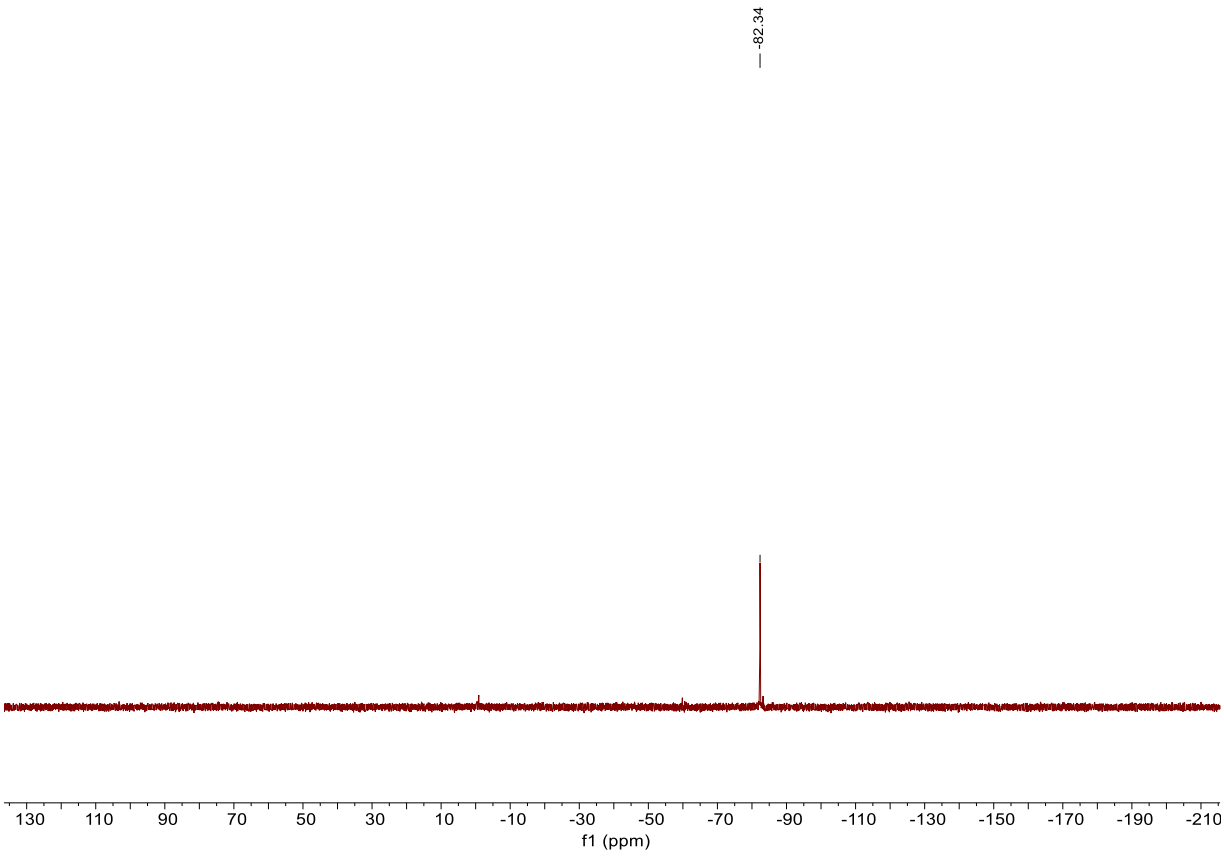


Figure S58 ^{31}P NMR of **7b** in THF-d_8.

1.14 Transmetallation

In a J. Young NMR tube, complex **5c** (9.0 mg, 7.33 µmol, 1.0 eq) was dissolved in THF-d_8 and CuCl (mg, 7.33 µmol, 1.0 eq) was added. Comparison of ^{1}H and ^{31}P NMR shifts to the NMR shifts of **6** showed quantitative conversion to the CuCl complex.

1.15 Sn(II) Transfer to bisNHI

Complex **5a** (30.0 mg, 24.31 µmol, 1.0 eq) was dissolved in THF-d_8 and bisNHI (16.2 mg, 24.31 µmol, 1.0 eq) was added. A crystalline precipitate was formed immediately. ^{31}P NMR showed full conversion of complex **5a** to the free bisNHCP **3b**. The precipitate was dissolved in CD_3CN. Comparing the ^{1}H and ^{119}Sn NMR shifts to the literature confirmed the formation of the bisNHI supported stannyliumylidene.[S8]

2. X-Ray Crystallographic Details

The X-ray intensity data were recorded on a Bruker D8 Venture Duo IMS system equipped with a Helios optic monochromator, a Mo IMS microsource (λ = 0.71073 Å) and a Cu IMS microsource (λ = 1.54178 Å). The data collection was performed, using the APEX III software package[S9] on single crystals coated with Fomblin ® Y as perfluorinated ether. The single crystal was picked on a MiTiGen MicroMount microsampling tool, transferred to the diffractometer and measured frozen under a stream of 100K cold nitrogen. A matrix scan was used to determine the initial lattice parameters. Reflections were merged and corrected for Lorenz and polarization effects, scan speed, and background using SAINT.[S10] Absorption corrections, including odd and even ordered spherical harmonics were performed using SADABS.[S10] Space group assignments were based upon systematic absences, E statistics, and successful refinement of the structures. Structures were solved by direct methods with the aid of successive difference Fourier maps and were refined against all data using the APEX III software in conjunction with SHELXL-2014[S11] and SHELXLE.[S12] H atoms were placed in calculated positions and refined using a riding model, with methylene and aromatic C–H distances of 0.99 and 0.95 Å, respectively, and Uiso(H) =

1.2·Ueq(C). Non-hydrogen atoms were refined with anisotropic displacement parameters. Full-matrix least-squares refinements were carried out by minimizing $\Sigma w(Fo^2-Fc^2)^2$ with the SHELXL weighting scheme.[S13] Neutral atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from International Tables for Crystallography.[S14] The images of the crystal structures were generated by Mercury.[S15] The CCDC numbers CCDC-2105598 (**3a**), CCDC-2105599 (**3b**), and CCDC-2105600 (**5c**) contain the supplementary crystallographic data for the structures **3a**, **3b**, and **5c**. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

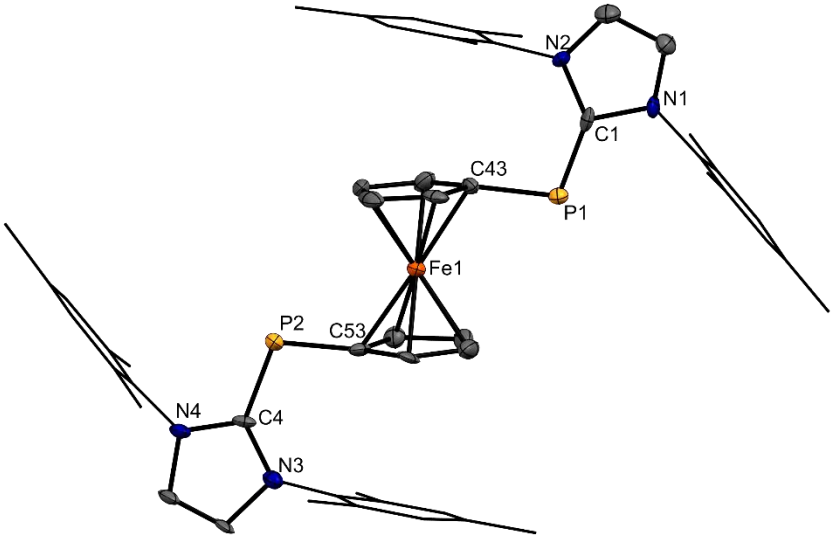


Figure S59 Solid state plot of the molecular structure of bisNHCP **3a**. Translational ellipsoids are set to 50% probability level. For reasons of clarity, hydrogens are omitted and mesityl groups are depicted in wireframe models. Selected bond lengths [Å] and angles [°]: P1–C1 1.731(10), P2–C4 1.808(10), P1–C43 1.863(10), P2–C53 1.803(10), C1–P1–C43 102.6(4), C4–P2–C53 103.6(4).

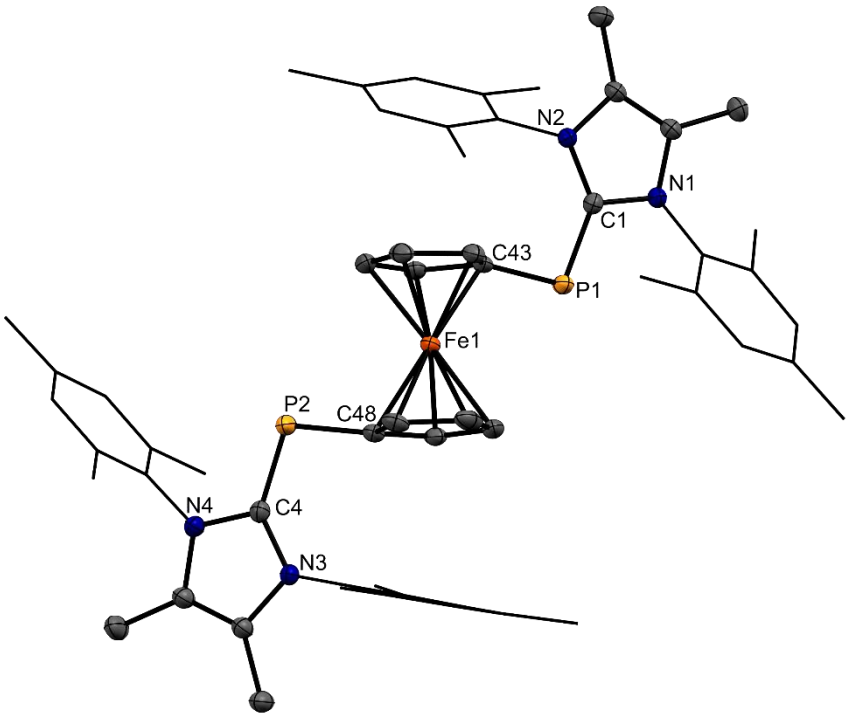


Figure S60 Solid state plot of the molecular structure of bisNHCP **3b**. Translational ellipsoids are set to 50% probability level. For reasons of clarity, hydrogens are omitted and mesityl groups are depicted in wireframe models. Selected bond lengths [Å] and angles [°]: P1–C1 1.7696(18), P2–C4 1.7704(19), P1–C43 1.8319(16), P2–C48 1.8220(17), C1–P1–C43 103.33(8), C4–P2–C48 102.92(8).

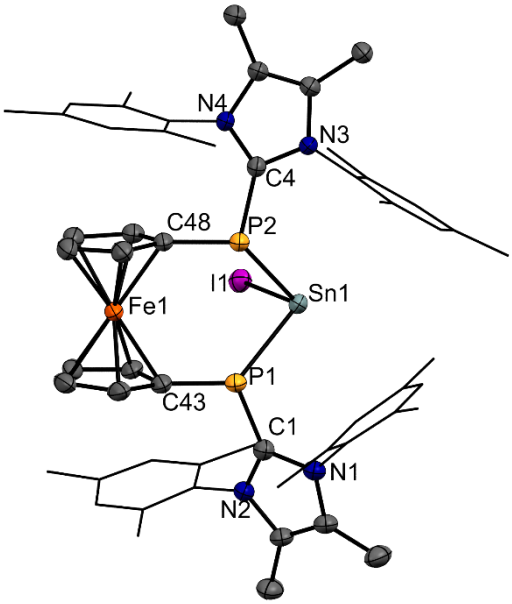


Figure S61 Solid state plot of the molecular structure of stannyliumylidene **5c**. Translational ellipsoids are set to 50% probability level. For reasons of clarity, hydrogens and the counter ion are omitted and mesityl groups are depicted in wireframe models. Selected bond lengths [Å] and angles [°]: P1–Sn1 2.645(5), P2–Sn1 2.659(4), P1–C1 1.824(4), P2–C4 1.828(4), P1–C43 1.809(4), P2–C48 1.817(4), I1–Sn1–P1 104.68(18), I1–Sn1–P2 102.25(14), P1–Sn1–P2 78.73(13).

Table S1 Crystal data and structure refinement for compound **3a**, **3b**, **5c**.

Compound #	3a	3b	5c
Chemical formula	C52 H56 Fe N4 P2, C4 H10 O	C56 H64 Fe N4 P2, 2(C4 H10 O)	C56 H64 Fe I N4 P2 Sn, C4 H8 O, I
Formula weight	928.92 g/mol	1059.14 g/mol	1355.52 g/mol
Temperature	100 K	100 K	100 K
Wavelength	0.71073 Å	0.71073 Å	1.54178 Å
Crystal size	0.319 x 0.276 x 0.092 mm	0.692 x 0.543 x 0.351 mm	0.132 x 0.102 x 0.099 mm
Crystal habit	clear orange fragment	clear orange-yellow fragment	clear yellow fragment
Crystal system	triclinic	triclinic	monoclinic
Space group	P -1	P -1	P 21/c
Unit cell dimensions	a = 9.866(5) Å; α = 101.033(19)°	a = 14.341(5) Å; α = 80.658(13)°	a = 13.8207(4) Å; α = 90°
	b = 10.771(5) Å; β = 101.83(3)°	b = 14.789(4) Å; β = 79.157(15)°	b = 13.9298(4) Å; β = 93.984(2)°
	c = 12.093(6) Å; γ = 91.21(2)°	c = 15.604(6) Å; γ = 66.634(12)°	c = 34.6173(10) Å; γ = 90°
Volume	1232.1(11) Å^3	2969.6(18) Å^3	6648.4(3) Å^3
Z	1	2	4
Density (calculated)	1.252 g/cm^3	1.184 g/cm^3	1.354 g/cm^3
Radiation source	IMS microsource	IMS microsource	IMS microsource
Theta range for data collection	2.11 to 25.34°	1.94 to 25.33°	3.20 to 66.89°
Index ranges	-11<=h<=11, -12<=k<=12, -14<=l<=14	-17<=h<=17, -16<=k<=17, -18<=l<=18	-16<=h<=14, -16<=k<=16, -41<=l<=41
Reflections collected	22312	174163	111370
Independent reflections	8496	10815	11802
Completeness	0.996	0.997	0.997
Absorption correction	Multi-Scan	Multi-Scan	Multi-Scan
Max. and min. transmission	0.7452 and 0.6648	0.7453 and 0.6683	0.7528 and 0.5144
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	$\Sigma\, w(F_o^2 - F_c^2)^2$	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	8496 / 982 / 590	10815 / 0 / 678	11802 / 13 / 675
Goodness-of-fit on F^2	1.010	1.003	1.012
Final R indices [I>2sigma(I)]	R1 = 0.0334, wR2 = 0.0786	R1 = 0.0314, wR2 = 0.0876	R1 = 0.0421, wR2 = 0.1140
R indices (all data)	R1 = 0.0451, wR2 = 0.0851	R1 = 0.0345, wR2 = 0.0899	R1 = 0.0545, wR2 = 0.1251
Largest diff. peak and hole	0.251 and -0.248 eÅ^{-3}	0.528 and -0.308 eÅ^{-3}	1.781 and -1.741 eÅ^{-3}

3. Computational Details

Calculations were carried out using Gaussian 16 software,[S16] at B3PW91[S17]-D3[18] level of theory with [4333111/433111/43] basis set augmented by two d polarization functions (d exponents 0.253 and 0.078) for Sn (see below); [S19] 6-311+G(d,p) basis set for P,[2] s6-31g* basis set for Fe and Cu, 6-311G(d,p) for basis sets for Cl, Br, I , and 6-31G(d,p) basis set for other atoms.[S20] The conductor-like polarizable continuum model (CPCM) was used to account for the solvent effects. The stationary points were verified by analytical frequency calculations. NBO analyses were performed using the NBO 7 software.[S21] QTAIM calculation were done using the Miltiwfn software.[S22]

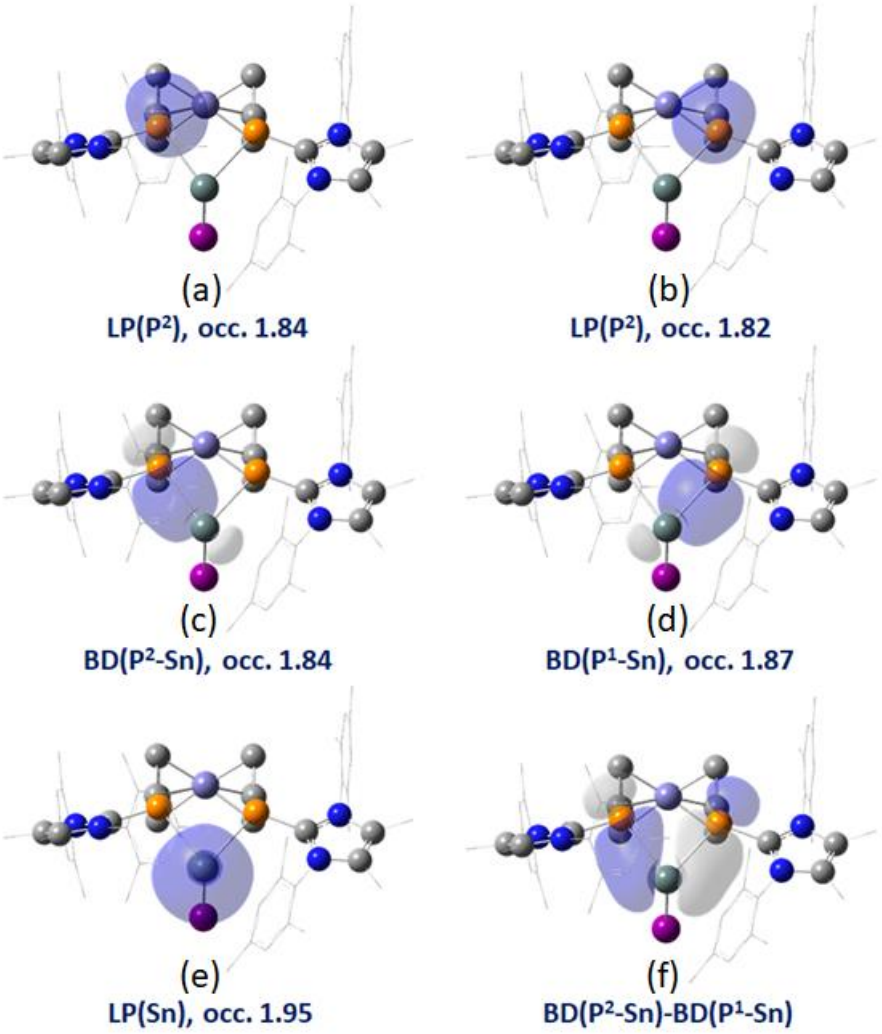


Figure S61. Selected NBO of **6**. (a) and (b) are the lone pairs of the phosphinidene centres. (c) and (d) are the P-Sn bonds. Subtraction of (c) and (d) yields (f) that corresponds to HOMO-1. (e) is the lone pair of Sn.

4333111/433111/43 basis set augmented by two d polarization functions (d exponents 0.253 and 0.078) for Sn in Gaussian format.

Sn 0

s 4 1.00

37472.012 0.16625195E-01

5648.8845 0.11693876

1282.9402 0.43179058

346.45090 0.56561483

s 3 1.00

```
      516.78654      -0.11389480
      59.928116       0.64603107
      26.048741       0.42625579
s  3   1.00
      47.977453      -0.27270744
      8.7546722       0.84987426
      4.0102331       0.30296902
s  3   1.00
      7.5198796       0.34211658
      1.7271022      -0.80241707
     0.77274433      -0.40406798
s  1   1.00
      1.1386522      -0.20454514
s  1   1.00
     0.17346487       0.71113158
s  1   1.00
     0.66274942E-01   0.41257362
p  4   1.00
      1745.5260       0.24426685E-01
      410.51366       0.16656335
      128.31139       0.49415429
      44.903462       0.47526995
p  3   1.00
      140.77605      -0.24768418E-01
      18.242647       0.47906186
      7.1374774       0.58978085
p  3   1.00
      2.9465525       0.42389675
      1.2795029       0.53117256
     0.54560639       0.12762194
```

p 1 1.00

0.25902160 0.33944667

p 1 1.00

0.10239424 0.54968903

p 1 1.00

0.41491833E-01 0.21901539

d 4 1.00

201.37580 0.39987711E-01

58.454606 0.22658972

20.557877 0.52423023

7.4534071 0.42264248

d 3 1.00

4.6147167 0.27827403

1.6488579 0.56541336

0.56081639 0.34880807

d 1 1.00

0.253 1.0

d 1 1.00

0.078 1.0

****

Cartesian coordinates and energies (E_h) of **3a**

E(RB3PW91) = -4179.94244992
Sum of electronic and zero-point Energies= -4178.987830
Sum of electronic and thermal Energies= -4178.927906
Sum of electronic and thermal Enthalpies= -4178.926962
Sum of electronic and thermal Free Energies= -4179.090832

Fe	-0.042433000	-0.279393000	-0.909187000
P	-3.234519000	-0.244304000	0.233352000
P	3.225916000	0.243390000	-0.206537000
N	-5.859324000	0.584046000	0.330467000
N	-4.634867000	2.229155000	-0.397158000
N	4.647588000	-2.201722000	0.479096000
N	5.667264000	-0.332975000	0.929767000
C	-4.553477000	0.916955000	0.023568000

C	-6.712426000	1.654417000	0.100810000
C	-5.955337000	2.674328000	-0.354648000
C	4.492805000	-0.832556000	0.399842000
C	5.878285000	-2.521354000	1.050891000
C	6.510988000	-1.361467000	1.325431000
C	-6.275403000	-0.693047000	0.812043000
C	-6.635032000	-1.678937000	-0.114485000
C	-7.049009000	-2.915534000	0.380619000
C	-7.103487000	-3.175228000	1.753051000
C	-6.725056000	-2.166376000	2.643236000
C	-6.303268000	-0.914612000	2.193982000
C	-6.529749000	-1.402119000	-1.587212000
C	-7.587035000	-4.507181000	2.262942000
C	-5.854534000	0.163277000	3.140821000
C	-3.543976000	3.127008000	-0.611016000
C	-3.147761000	3.414780000	-1.920511000
C	-2.088694000	4.303872000	-2.098755000
C	-1.438729000	4.897542000	-1.014334000
C	-1.882122000	4.601818000	0.276422000
C	-2.933687000	3.714151000	0.503493000
C	-3.837667000	2.758150000	-3.082114000
C	-0.246202000	5.788875000	-1.232598000
C	-3.369252000	3.340887000	1.891574000
C	3.822435000	-3.191217000	-0.138507000
C	3.972565000	-3.425959000	-1.510049000
C	3.172147000	-4.408728000	-2.092689000
C	2.244061000	-5.136028000	-1.344911000
C	2.139427000	-4.881750000	0.024626000
C	2.921967000	-3.913150000	0.651176000
C	4.926575000	-2.597876000	-2.322229000
C	1.331937000	-6.133731000	-2.006095000
C	2.800580000	-3.623497000	2.120179000
C	5.966139000	1.056258000	1.058999000
C	6.626903000	1.702603000	0.007748000
C	6.925865000	3.056637000	0.162395000
C	6.572825000	3.757418000	1.318932000
C	5.907790000	3.074952000	2.341593000
C	5.589540000	1.721271000	2.231928000
C	6.967234000	0.948505000	-1.247376000
C	6.870957000	5.228152000	1.446314000
C	4.838739000	0.987017000	3.305972000
C	-1.872821000	0.603499000	-0.654822000
C	-1.557286000	0.434967000	-2.047695000
C	-0.351765000	1.138639000	-2.335894000
C	0.102575000	1.739579000	-1.124655000
C	-0.819180000	1.401660000	-0.094989000
C	1.372193000	-1.541620000	-1.624532000
C	0.169491000	-2.254746000	-1.356371000

C	-0.143937000	-2.084753000	0.024690000
C	0.867804000	-1.265739000	0.603149000
C	1.832616000	-0.931097000	-0.409559000
H	-7.772632000	1.571600000	0.278283000
H	-6.209445000	3.680615000	-0.646437000
H	6.173441000	-3.548846000	1.190309000
H	7.471382000	-1.156169000	1.770290000
H	-7.328027000	-3.697506000	-0.322396000
H	-6.750781000	-2.360887000	3.713319000
H	-5.484716000	-1.197223000	-1.849543000
H	-7.114459000	-0.521082000	-1.873816000
H	-6.877701000	-2.253784000	-2.176895000
H	-7.132695000	-4.756787000	3.226332000
H	-7.356155000	-5.313191000	1.560101000
H	-8.674722000	-4.499412000	2.406009000
H	-4.798456000	0.399851000	2.966118000
H	-5.972154000	-0.149683000	4.181155000
H	-6.420575000	1.089529000	2.993139000
H	-1.747858000	4.520041000	-3.108645000
H	-1.382709000	5.055382000	1.129904000
H	-3.308629000	2.957265000	-4.017052000
H	-4.869036000	3.114136000	-3.190035000
H	-3.883020000	1.674945000	-2.936339000
H	-0.117018000	6.500909000	-0.412055000
H	-0.328998000	6.354293000	-2.165892000
H	0.669190000	5.187654000	-1.294200000
H	-2.887463000	3.972706000	2.641901000
H	-3.108974000	2.294182000	2.096175000
H	-4.454941000	3.425436000	2.010796000
H	3.262911000	-4.596110000	-3.160541000
H	1.414022000	-5.435247000	0.616416000
H	4.568361000	-1.561531000	-2.377778000
H	5.025131000	-2.988211000	-3.338267000
H	5.921450000	-2.563591000	-1.864933000
H	1.132935000	-6.991804000	-1.356478000
H	1.751339000	-6.506745000	-2.945091000
H	0.365554000	-5.668957000	-2.236737000
H	3.692533000	-3.949483000	2.668317000
H	1.932767000	-4.129223000	2.549871000
H	2.691371000	-2.548603000	2.290704000
H	7.440599000	3.577909000	-0.641923000
H	5.624194000	3.610934000	3.244849000
H	7.507242000	1.581839000	-1.955445000
H	6.050207000	0.591000000	-1.730043000
H	7.582747000	0.067783000	-1.033612000
H	7.029448000	5.517517000	2.489580000
H	6.035502000	5.827212000	1.064230000
H	7.761636000	5.509185000	0.876377000

H	5.387101000	0.102327000	3.647813000
H	3.876631000	0.639684000	2.910243000
H	4.649725000	1.630437000	4.168743000
H	-2.132990000	-0.162038000	-2.743246000
H	0.155882000	1.175605000	-3.291075000
H	1.019263000	2.300997000	-0.997340000
H	-0.738199000	1.682275000	0.946085000
H	1.863709000	-1.456283000	-2.584275000
H	-0.426994000	-2.796329000	-2.078935000
H	-1.027802000	-2.458506000	0.525907000
H	0.893235000	-0.911118000	1.625217000

Cartesian coordinates and energies (E_h) of **3b**

E(RB3PW91) = -4337.20355951
Sum of electronic and zero-point Energies= -4336.137227
Sum of electronic and thermal Energies= -4336.070422
Sum of electronic and thermal Enthalpies= -4336.069478
Sum of electronic and thermal Free Energies= -4336.247372

Fe	0.000017000	0.000040000	-1.169311000
P	3.194138000	0.451108000	-0.153558000
P	-3.194154000	-0.451069000	-0.153687000
N	5.825020000	-0.161799000	0.346077000
N	4.730605000	-2.014719000	0.079596000
N	-4.730641000	2.014727000	0.079830000
N	-5.824985000	0.161760000	0.346235000
C	4.564573000	-0.648602000	0.073523000
C	6.745107000	-1.198593000	0.527150000
C	6.063953000	-2.357748000	0.361285000
C	-4.564575000	0.648616000	0.073606000
C	-6.063977000	2.357699000	0.361645000
C	-6.745086000	1.198512000	0.527465000
C	6.153110000	1.221714000	0.443042000
C	6.556720000	1.903473000	-0.711332000
C	6.901324000	3.249262000	-0.586402000
C	6.848311000	3.908235000	0.645372000
C	6.430547000	3.194048000	1.771753000
C	6.074786000	1.847130000	1.693160000
C	6.568265000	1.194603000	-2.035724000
C	7.260353000	5.352243000	0.760443000
C	5.582601000	1.080837000	2.889039000
C	3.692601000	-2.992977000	0.048221000
C	3.358758000	-3.595455000	-1.167980000

C	2.352884000	-4.560831000	-1.160887000
C	1.696944000	-4.928094000	0.016470000
C	2.075734000	-4.317788000	1.214351000
C	3.069609000	-3.340297000	1.252175000
C	4.053531000	-3.177285000	-2.432317000
C	0.560562000	-5.913773000	-0.018890000
C	3.432954000	-2.620941000	2.520334000
C	-3.692683000	2.993024000	0.048281000
C	-3.359009000	3.595433000	-1.168004000
C	-2.353160000	4.560829000	-1.161099000
C	-1.697086000	4.928185000	0.016160000
C	-2.075738000	4.317980000	1.214132000
C	-3.069582000	3.340458000	1.252139000
C	-4.053934000	3.177135000	-2.432214000
C	-0.560666000	5.913807000	-0.019449000
C	-3.432794000	2.621192000	2.520389000
C	-6.153052000	-1.221770000	0.443037000
C	-6.556717000	-1.903377000	-0.711388000
C	-6.901278000	-3.249210000	-0.586611000
C	-6.848159000	-3.908339000	0.645054000
C	-6.430329000	-3.194283000	1.771516000
C	-6.074625000	-1.847359000	1.693081000
C	-6.568381000	-1.194345000	-2.035691000
C	-7.260153000	-5.352361000	0.760124000
C	-5.582340000	-1.081218000	2.889016000
C	1.880967000	-0.687850000	-0.738569000
C	1.534393000	-0.924679000	-2.114269000
C	0.365136000	-1.738154000	-2.162873000
C	-0.036717000	-2.004876000	-0.820464000
C	0.880729000	-1.351921000	0.049165000
C	-1.880969000	0.687906000	-0.738640000
C	-0.880772000	1.351987000	0.049133000
C	0.036706000	2.004949000	-0.820458000
C	-0.365092000	1.738228000	-2.162885000
C	-1.534338000	0.924737000	-2.114328000
C	8.173003000	-0.914955000	0.824019000
C	6.490520000	-3.778224000	0.448328000
C	-6.490570000	3.778159000	0.448830000
C	-8.172948000	0.914814000	0.824440000
H	7.212064000	3.798327000	-1.472788000
H	6.372666000	3.699413000	2.733508000
H	6.951185000	1.840763000	-2.829479000
H	5.548776000	0.884848000	-2.295210000
H	7.181142000	0.286995000	-2.002481000
H	7.044736000	5.904840000	-0.158935000

H	8.337909000	5.437913000	0.948077000
H	6.744343000	5.852276000	1.585385000
H	4.541851000	0.774534000	2.731469000
H	5.633796000	1.686649000	3.797115000
H	6.163777000	0.166248000	3.050869000
H	2.058112000	-5.020943000	-2.101207000
H	1.566791000	-4.589241000	2.136779000
H	3.584242000	-3.631230000	-3.308336000
H	5.111873000	-3.463521000	-2.424086000
H	4.015153000	-2.089831000	-2.545396000
H	-0.378858000	-5.398682000	-0.253961000
H	0.428572000	-6.415269000	0.944431000
H	0.713387000	-6.680087000	-0.785153000
H	4.511268000	-2.656231000	2.712782000
H	2.913351000	-3.046890000	3.382194000
H	3.162923000	-1.560530000	2.438386000
H	-2.058527000	5.020912000	-2.101477000
H	-1.566710000	4.589526000	2.136485000
H	-3.585090000	3.631405000	-3.308302000
H	-5.112405000	3.462876000	-2.423645000
H	-4.015100000	2.089709000	-2.545440000
H	-0.713859000	6.680445000	-0.785314000
H	0.378564000	5.398710000	-0.255286000
H	-0.428062000	6.414890000	0.944000000
H	-3.163004000	1.560722000	2.438407000
H	-4.511058000	2.656712000	2.713078000
H	-2.912914000	3.047049000	3.382127000
H	-7.212060000	-3.798158000	-1.473053000
H	-6.372363000	-3.699784000	2.733196000
H	-5.548930000	-0.884490000	-2.295203000
H	-7.181317000	-0.286781000	-2.002300000
H	-6.951307000	-1.840431000	-2.829503000
H	-7.048290000	-5.904039000	-0.160665000
H	-8.336978000	-5.437934000	0.951957000
H	-6.741056000	-5.853410000	1.582522000
H	-4.541508000	-0.775159000	2.731506000
H	-5.633734000	-1.687044000	3.797072000
H	-6.163296000	-0.166490000	3.050830000
H	2.065586000	-0.515228000	-2.963901000
H	-0.154435000	-2.060764000	-3.055918000
H	-0.919949000	-2.552712000	-0.517835000
H	0.829100000	-1.336023000	1.129021000
H	-0.829178000	1.336093000	1.128991000
H	0.919899000	2.552832000	-0.517800000
H	0.154496000	2.060865000	-3.055911000

H	-2.065508000	0.515284000	-2.963973000
H	8.640614000	-0.333343000	0.021377000
H	8.731036000	-1.845947000	0.942078000
H	8.279756000	-0.330131000	1.744536000
H	6.316263000	-4.310015000	-0.493736000
H	5.932472000	-4.314672000	1.224007000
H	7.554817000	-3.841296000	0.684534000
H	-6.316361000	4.310035000	-0.493196000
H	-5.932501000	4.314558000	1.224529000
H	-7.554857000	3.841189000	0.685091000
H	-8.731046000	1.845785000	0.942360000
H	-8.279633000	0.330138000	1.745062000
H	-8.640536000	0.333030000	0.021911000

Cartesian coordinates and energies (E_h) of **3b**, scrf=(cpcm,solvent=thf)

E(RB3PW91) = -4337.22795778
Sum of electronic and zero-point Energies= -4336.162337
Sum of electronic and thermal Energies= -4336.095499
Sum of electronic and thermal Enthalpies= -4336.094555
Sum of electronic and thermal Free Energies= -4336.271594

Fe	0.000028000	0.000029000	-1.162557000
P	-3.202270000	-0.461640000	-0.149906000
P	3.202307000	0.461652000	-0.149852000
N	-5.840015000	0.140216000	0.377055000
N	-4.752620000	1.993680000	0.131021000
N	4.752587000	-1.993696000	0.131229000
N	5.840019000	-0.140249000	0.377226000
C	-4.589775000	0.634887000	0.104943000
C	-6.764117000	1.170678000	0.575010000
C	-6.085216000	2.333859000	0.419134000
C	4.589776000	-0.634900000	0.105089000
C	6.085165000	-2.333896000	0.419396000
C	6.764083000	-1.170726000	0.575280000
C	-6.160462000	-1.247816000	0.456168000
C	-6.578487000	-1.910898000	-0.704689000
C	-6.899737000	-3.265147000	-0.600098000
C	-6.816066000	-3.947079000	0.618825000
C	-6.395317000	-3.246240000	1.753962000
C	-6.062547000	-1.891433000	1.696274000
C	-6.650466000	-1.172131000	-2.011569000
C	-7.204214000	-5.398988000	0.712890000
C	-5.596949000	-1.133108000	2.908413000

C	-3.722938000	2.980201000	0.053253000
C	-3.428071000	3.559159000	-1.184466000
C	-2.438271000	4.541315000	-1.221579000
C	-1.762347000	4.945998000	-0.066963000
C	-2.103428000	4.355981000	1.153276000
C	-3.081215000	3.364238000	1.235846000
C	-4.150823000	3.107855000	-2.421638000
C	-0.651323000	5.958111000	-0.147512000
C	-3.415873000	2.680971000	2.531786000
C	3.722882000	-2.980194000	0.053469000
C	3.428029000	-3.559186000	-1.184238000
C	2.438209000	-4.541322000	-1.221339000
C	1.762251000	-4.945953000	-0.066725000
C	2.103316000	-4.355901000	1.153502000
C	3.081122000	-3.364177000	1.236061000
C	4.150813000	-3.107934000	-2.421410000
C	0.651206000	-5.958042000	-0.147265000
C	3.415766000	-2.680872000	2.531985000
C	6.160497000	1.247777000	0.456296000
C	6.578623000	1.910796000	-0.704553000
C	6.899899000	3.265049000	-0.599996000
C	6.816152000	3.947033000	0.618886000
C	6.395298000	3.246249000	1.754026000
C	6.062504000	1.891454000	1.696372000
C	6.650691000	1.171976000	-2.011398000
C	7.204323000	5.398934000	0.712974000
C	5.596788000	1.133188000	2.908503000
C	-1.889944000	0.675799000	-0.738382000
C	-1.542589000	0.913298000	-2.113480000
C	-0.380616000	1.735934000	-2.161474000
C	0.014327000	2.010116000	-0.818756000
C	-0.898929000	1.352002000	0.050449000
C	1.889996000	-0.675764000	-0.738406000
C	0.898975000	-1.352015000	0.050377000
C	-0.014273000	-2.010079000	-0.818874000
C	0.380680000	-1.735818000	-2.161573000
C	1.542652000	-0.913184000	-2.113522000
C	-8.188628000	0.882041000	0.882690000
C	-6.515909000	3.752246000	0.518475000
C	6.515822000	-3.752291000	0.518800000
C	8.188583000	-0.882112000	0.883031000
H	-7.222076000	-3.800869000	-1.490264000
H	-6.323490000	-3.766609000	2.706489000
H	-6.978085000	-1.829389000	-2.820251000
H	-5.667507000	-0.761804000	-2.270522000

H	-7.344499000	-0.326226000	-1.954946000
H	-7.001904000	-5.929099000	-0.222291000
H	-8.276507000	-5.500485000	0.920141000
H	-6.666597000	-5.906526000	1.518895000
H	-4.590013000	-0.732291000	2.745773000
H	-5.576883000	-1.774837000	3.792190000
H	-6.248683000	-0.278279000	3.120208000
H	-2.178670000	4.991380000	-2.177087000
H	-1.583039000	4.660610000	2.058674000
H	-3.731478000	3.574362000	-3.316001000
H	-5.217586000	3.355126000	-2.375643000
H	-4.078067000	2.021452000	-2.532560000
H	0.298597000	5.460920000	-0.379626000
H	-0.519779000	6.490570000	0.798877000
H	-0.833242000	6.695346000	-0.935253000
H	-4.485921000	2.744389000	2.758926000
H	-2.860127000	3.116867000	3.365165000
H	-3.170092000	1.613683000	2.470668000
H	2.178619000	-4.991414000	-2.176838000
H	1.582899000	-4.660488000	2.058899000
H	3.731477000	-3.574460000	-3.315766000
H	5.217571000	-3.355222000	-2.375387000
H	4.078080000	-2.021532000	-2.532366000
H	0.833132000	-6.695315000	-0.934970000
H	-0.298695000	-5.460838000	-0.379429000
H	0.519620000	-6.490458000	0.799143000
H	3.170007000	-1.613580000	2.470824000
H	4.485808000	-2.744303000	2.759150000
H	2.859993000	-3.116728000	3.365366000
H	7.222321000	3.800720000	-1.490161000
H	6.323408000	3.766666000	2.706523000
H	5.667743000	0.761664000	-2.270415000
H	7.344699000	0.326057000	-1.954685000
H	6.978393000	1.829194000	-2.820079000
H	7.003385000	5.928748000	-0.222666000
H	8.276327000	5.500389000	0.921735000
H	6.665624000	5.906802000	1.518055000
H	4.589849000	0.732404000	2.745802000
H	5.576680000	1.774949000	3.792256000
H	6.248474000	0.278342000	3.120375000
H	-2.071904000	0.507350000	-2.966278000
H	0.132816000	2.066932000	-3.055308000
H	0.882891000	2.580588000	-0.515453000
H	-0.858265000	1.350862000	1.131220000
H	0.858302000	-1.350937000	1.131149000

H	-0.882839000	-2.580570000	-0.515611000
H	-0.132744000	-2.066766000	-3.055430000
H	2.071974000	-0.507186000	-2.966292000
H	-8.664097000	0.310842000	0.077874000
H	-8.744239000	1.811844000	1.015496000
H	-8.285296000	0.290938000	1.799818000
H	-6.341824000	4.291393000	-0.418964000
H	-5.964737000	4.282014000	1.303119000
H	-7.580814000	3.807567000	0.751100000
H	6.341766000	-4.291466000	-0.418627000
H	5.964602000	-4.282019000	1.303438000
H	7.580715000	-3.807628000	0.751476000
H	8.744166000	-1.811924000	1.015895000
H	8.285214000	-0.290983000	1.800147000
H	8.664108000	-0.310948000	0.078224000

Cartesian coordinates and energies (E_h) of **3b**, scrf=(cpcm,solvent=acetonitrile)

E(RB3PW91) = -4337.23224772
Sum of electronic and zero-point Energies= -4336.166696
Sum of electronic and thermal Energies= -4336.099846
Sum of electronic and thermal Enthalpies= -4336.098902
Sum of electronic and thermal Free Energies= -4336.275914

Fe	0.000009000	-0.000041000	-1.151608000
P	-3.204956000	-0.463860000	-0.140507000
P	3.204915000	0.463825000	-0.140367000
N	-5.847489000	0.136167000	0.374850000
N	-4.760155000	1.989429000	0.135125000
N	4.760188000	-1.989414000	0.135350000
N	5.847454000	-0.136109000	0.375050000
C	-4.597696000	0.631924000	0.108977000
C	-6.773418000	1.165718000	0.568924000
C	-6.094153000	2.329444000	0.416408000
C	4.597682000	-0.631915000	0.109169000
C	6.094194000	-2.329376000	0.416659000
C	6.773416000	-1.165624000	0.569158000
C	-6.166600000	-1.252538000	0.452226000
C	-6.579039000	-1.915577000	-0.710807000
C	-6.896840000	-3.270948000	-0.608316000
C	-6.816294000	-3.953499000	0.610710000
C	-6.402615000	-3.251986000	1.748278000
C	-6.073568000	-1.896019000	1.692908000
C	-6.652647000	-1.175355000	-2.016920000
C	-7.201282000	-5.406318000	0.702422000

C	-5.621761000	-1.135841000	2.909257000
C	-3.731349000	2.977045000	0.054450000
C	-3.437336000	3.552278000	-1.185264000
C	-2.450177000	4.537125000	-1.224966000
C	-1.776470000	4.947983000	-0.071083000
C	-2.116723000	4.361079000	1.151047000
C	-3.092095000	3.367073000	1.236416000
C	-4.159335000	3.096550000	-2.421294000
C	-0.670018000	5.964998000	-0.153883000
C	-3.428596000	2.690491000	2.535416000
C	3.731420000	-2.977071000	0.054681000
C	3.437438000	-3.552332000	-1.185027000
C	2.450325000	-4.537225000	-1.224721000
C	1.776634000	-4.948101000	-0.070835000
C	2.116857000	-4.361168000	1.151289000
C	3.092181000	-3.367115000	1.236650000
C	4.159419000	-3.096582000	-2.421060000
C	0.670230000	-5.965169000	-0.153627000
C	3.428648000	-2.690505000	2.535643000
C	6.166516000	1.252609000	0.452400000
C	6.578950000	1.915634000	-0.710636000
C	6.896703000	3.271024000	-0.608169000
C	6.816113000	3.953596000	0.610837000
C	6.402437000	3.252090000	1.748417000
C	6.073440000	1.896116000	1.693072000
C	6.652605000	1.175391000	-2.016734000
C	7.201045000	5.406429000	0.702569000
C	5.621636000	1.135945000	2.909427000
C	-1.892122000	0.672704000	-0.729361000
C	-1.544077000	0.910450000	-2.104134000
C	-0.383938000	1.735386000	-2.151490000
C	0.008997000	2.011066000	-0.808581000
C	-0.903671000	1.351734000	0.060136000
C	1.892120000	-0.672771000	-0.729249000
C	0.903631000	-1.351778000	0.060221000
C	-0.008994000	-2.011138000	-0.808520000
C	0.384006000	-1.735499000	-2.151419000
C	1.544142000	-0.910560000	-2.104031000
C	-8.199149000	0.876714000	0.870382000
C	-6.526264000	3.747518000	0.513376000
C	6.526353000	-3.747433000	0.513662000
C	8.199134000	-0.876564000	0.870626000
H	-7.215308000	-3.806728000	-1.499807000
H	-6.335059000	-3.772354000	2.701083000
H	-6.962513000	-1.836521000	-2.829327000

H	-5.675955000	-0.745952000	-2.268281000
H	-7.362623000	-0.342575000	-1.964038000
H	-6.995119000	-5.935264000	-0.232530000
H	-8.274054000	-5.509604000	0.905933000
H	-6.665735000	-5.913093000	1.510233000
H	-4.625053000	-0.709564000	2.749040000
H	-5.585745000	-1.783146000	3.788377000
H	-6.293263000	-0.298390000	3.128570000
H	-2.192268000	4.985756000	-2.181610000
H	-1.599159000	4.671493000	2.056084000
H	-3.739009000	3.559340000	-3.317081000
H	-5.225770000	3.345305000	-2.377105000
H	-4.088078000	2.009626000	-2.528349000
H	0.282684000	5.471946000	-0.383604000
H	-0.541934000	6.500971000	0.790947000
H	-0.854751000	6.698659000	-0.944235000
H	-4.498226000	2.759266000	2.762733000
H	-2.871074000	3.128163000	3.366595000
H	-3.187058000	1.621991000	2.479614000
H	2.192439000	-4.985879000	-2.181360000
H	1.599304000	-4.671596000	2.056328000
H	3.739122000	-3.559408000	-3.316842000
H	5.225867000	-3.345279000	-2.376863000
H	4.088103000	-2.009664000	-2.528131000
H	0.855004000	-6.698835000	-0.943966000
H	-0.282493000	-5.472166000	-0.383364000
H	0.542164000	-6.501133000	0.791211000
H	3.187058000	-1.622016000	2.479831000
H	4.498281000	-2.759226000	2.762962000
H	2.871146000	-3.128196000	3.366826000
H	7.215168000	3.806792000	-1.499666000
H	6.334845000	3.772480000	2.701208000
H	5.675931000	0.745954000	-2.268105000
H	7.362605000	0.342633000	-1.963823000
H	6.962467000	1.836552000	-2.829147000
H	6.995857000	5.935151000	-0.232721000
H	8.273604000	5.509738000	0.907185000
H	6.664680000	5.913414000	1.509708000
H	4.624941000	0.709641000	2.749202000
H	5.585591000	1.783264000	3.788536000
H	6.293156000	0.298514000	3.128762000
H	-2.072342000	0.504962000	-2.957835000
H	0.128340000	2.068289000	-3.045315000
H	0.874239000	2.586347000	-0.504857000
H	-0.866057000	1.353907000	1.141093000

H	0.865964000	-1.353916000	1.141176000
H	-0.874249000	-2.586411000	-0.504820000
H	-0.128227000	-2.068432000	-3.045258000
H	2.072448000	-0.505098000	-2.957720000
H	-8.671287000	0.306621000	0.062961000
H	-8.754937000	1.806520000	1.001472000
H	-8.299733000	0.285463000	1.786878000
H	-6.348478000	4.286311000	-0.423473000
H	-5.979674000	4.277591000	1.300909000
H	-7.592232000	3.801662000	0.740794000
H	6.348598000	-4.286252000	-0.423179000
H	5.979771000	-4.277509000	1.301198000
H	7.592320000	-3.801535000	0.741095000
H	8.754953000	-1.806348000	1.001742000
H	8.299687000	-0.285290000	1.787110000
H	8.671261000	-0.306471000	0.063198000

Cartesian coordinates and energies (E_h) of **5a [$FcP_2SnCl]^+$**

E(RB3PW91) = -10818.4274008
Sum of electronic and zero-point Energies= -10817.355685
Sum of electronic and thermal Energies= -10817.285737
Sum of electronic and thermal Enthalpies= -10817.284793
Sum of electronic and thermal Free Energies= -10817.463826

Fe	-0.079972000	-3.038686000	0.116434000
P	1.618356000	-0.258177000	0.862838000
P	-1.679612000	0.027498000	0.523571000
N	3.710544000	1.552621000	1.150159000
N	4.474214000	-0.272235000	0.285123000
N	-3.639179000	1.721772000	-0.655220000
N	-4.494342000	-0.130328000	0.044462000
C	3.330507000	0.330813000	0.685692000
C	5.092112000	1.712329000	1.049005000
C	5.574829000	0.562098000	0.503306000
C	-3.310414000	0.512322000	-0.132293000
C	-5.022495000	1.844560000	-0.798108000
C	-5.560793000	0.674017000	-0.360183000
C	2.815896000	2.560330000	1.641112000
C	2.446597000	3.608752000	0.788562000
C	1.556216000	4.563625000	1.288071000
C	1.044440000	4.489348000	2.582369000
C	1.463140000	3.439131000	3.408556000
C	2.360764000	2.469427000	2.967456000
C	2.983265000	3.745541000	-0.610755000

C	0.093065000	5.531342000	3.105089000
C	2.822319000	1.361610000	3.871659000
C	4.592022000	-1.536393000	-0.380239000
C	4.491964000	-1.557350000	-1.774232000
C	4.643610000	-2.791965000	-2.408105000
C	4.877266000	-3.963836000	-1.685385000
C	4.977095000	-3.887975000	-0.291985000
C	4.842426000	-2.679015000	0.386571000
C	4.172449000	-0.307199000	-2.544926000
C	4.981682000	-5.293754000	-2.380611000
C	4.932575000	-2.589870000	1.883826000
C	-2.735427000	2.737023000	-1.103709000
C	-2.292415000	3.709241000	-0.200313000
C	-1.455569000	4.711199000	-0.697669000
C	-1.056321000	4.742691000	-2.034469000
C	-1.526651000	3.748842000	-2.902021000
C	-2.378688000	2.736625000	-2.462920000
C	-2.646911000	3.647372000	1.258814000
C	-0.141034000	5.821527000	-2.545642000
C	-2.869736000	1.654010000	-3.382690000
C	-4.694950000	-1.414650000	0.650243000
C	-4.760360000	-1.483926000	2.047876000
C	-4.989005000	-2.735165000	2.619086000
C	-5.156207000	-3.881522000	1.836218000
C	-5.107238000	-3.756142000	0.446468000
C	-4.880129000	-2.528148000	-0.175498000
C	-4.577464000	-0.253299000	2.892457000
C	-5.347197000	-5.228902000	2.477438000
C	-4.844230000	-2.414740000	-1.674054000
C	1.652598000	-2.003879000	0.383945000
C	1.524703000	-3.054297000	1.359431000
C	1.434692000	-4.292840000	0.668121000
C	1.496138000	-4.021170000	-0.730604000
C	1.615580000	-2.618267000	-0.911351000
C	-1.681561000	-1.765872000	0.202610000
C	-1.759208000	-2.766805000	1.229906000
C	-1.783396000	-4.042689000	0.606077000
C	-1.703591000	-3.847282000	-0.805119000
C	-1.628299000	-2.448992000	-1.058226000
C	5.767806000	2.951887000	1.510328000
C	6.949061000	0.141417000	0.127862000
C	-5.641449000	3.088436000	-1.324101000
C	-6.969244000	0.217360000	-0.240325000
H	1.254595000	5.379807000	0.637222000
H	1.088902000	3.381835000	4.428040000

H	3.386947000	2.806955000	-0.997858000
H	3.783040000	4.495205000	-0.647365000
H	2.191388000	4.073112000	-1.289548000
H	-0.294899000	6.164664000	2.302717000
H	0.591266000	6.185764000	3.829416000
H	-0.757057000	5.070504000	3.617665000
H	3.903791000	1.206634000	3.797252000
H	2.337532000	0.418325000	3.593827000
H	2.578828000	1.579744000	4.913754000
H	4.561626000	-2.838869000	-3.491178000
H	5.156627000	-4.795075000	0.279795000
H	4.322659000	-0.454904000	-3.616278000
H	4.788828000	0.540427000	-2.226169000
H	3.122918000	-0.023353000	-2.400027000
H	5.179773000	-5.178680000	-3.449346000
H	4.044814000	-5.853697000	-2.274932000
H	5.777028000	-5.909889000	-1.950371000
H	5.753933000	-1.938237000	2.202929000
H	5.090959000	-3.574739000	2.327765000
H	4.010236000	-2.173982000	2.302792000
H	-1.100002000	5.477534000	-0.014795000
H	-1.210870000	3.753428000	-3.941977000
H	-2.581489000	4.635818000	1.718938000
H	-1.949163000	2.986843000	1.788313000
H	-3.654619000	3.255081000	1.422933000
H	0.666777000	5.397162000	-3.150260000
H	0.308026000	6.392340000	-1.728360000
H	-0.684928000	6.527573000	-3.183382000
H	-2.451188000	1.771675000	-4.383267000
H	-3.962637000	1.654353000	-3.461083000
H	-2.564430000	0.668116000	-3.016811000
H	-5.039759000	-2.816647000	3.702345000
H	-5.236623000	-4.639785000	-0.173567000
H	-5.213168000	0.570286000	2.548121000
H	-3.540107000	0.099535000	2.843384000
H	-4.821308000	-0.455189000	3.937763000
H	-4.379271000	-5.724284000	2.621124000
H	-5.961225000	-5.887378000	1.856700000
H	-5.820773000	-5.145968000	3.459558000
H	-4.505122000	-3.351089000	-2.122115000
H	-4.168988000	-1.622252000	-2.004590000
H	-5.839143000	-2.195458000	-2.080207000
H	1.477737000	-2.910084000	2.430943000
H	1.299190000	-5.265709000	1.121822000
H	1.416955000	-4.753187000	-1.523211000

H	1.643682000	-2.095528000	-1.854850000
H	-1.803448000	-2.568382000	2.291653000
H	-1.817734000	-4.997033000	1.114228000
H	-1.658354000	-4.628638000	-1.552460000
H	-1.510188000	-1.972277000	-2.021236000
H	5.487806000	3.814889000	0.898167000
H	6.851319000	2.834580000	1.457480000
H	5.496850000	3.183314000	2.545323000
H	7.020756000	-0.052082000	-0.947544000
H	7.239575000	-0.780412000	0.641446000
H	7.667999000	0.920769000	0.385516000
H	-5.310988000	3.302668000	-2.345535000
H	-5.370057000	3.952060000	-0.708172000
H	-6.728700000	2.997249000	-1.329130000
H	-7.167629000	-0.645715000	-0.882957000
H	-7.652193000	1.018971000	-0.525949000
H	-7.197901000	-0.083165000	0.787046000
Cl	0.258535000	-0.091069000	-2.921815000
Sn	0.252138000	1.276885000	-0.832228000

Cartesian coordinates and energies (E_h) of **5a [FcP_2SnCl]$^+$**, scrf=(cpcm,solvent=thf)

E(RB3PW91) = -10818.4724827
Sum of electronic and zero-point Energies= -10817.401714
Sum of electronic and thermal Energies= -10817.331720
Sum of electronic and thermal Enthalpies= -10817.330776
Sum of electronic and thermal Free Energies= -10817.509527

Fe	-0.027474000	-3.038391000	0.102921000
P	1.617432000	-0.226615000	0.821973000
P	-1.666357000	0.008114000	0.479923000
N	3.675132000	1.608649000	1.172130000
N	4.481710000	-0.182218000	0.279254000
N	-3.665296000	1.672698000	-0.673717000
N	-4.488973000	-0.179184000	0.059787000
C	3.324966000	0.390785000	0.681688000
C	5.052532000	1.800189000	1.084099000
C	5.563299000	0.669788000	0.520648000
C	-3.316844000	0.472306000	-0.147631000
C	-5.051827000	1.782800000	-0.789571000
C	-5.570680000	0.611033000	-0.330340000
C	2.751380000	2.573656000	1.693948000
C	2.335997000	3.629131000	0.872707000
C	1.411358000	4.534054000	1.405264000

C	0.914737000	4.404436000	2.701789000
C	1.384542000	3.351229000	3.498219000
C	2.316003000	2.430849000	3.022783000
C	2.869929000	3.830399000	-0.519495000
C	-0.076615000	5.390041000	3.258336000
C	2.844692000	1.324980000	3.892506000
C	4.626701000	-1.441638000	-0.388634000
C	4.529364000	-1.461806000	-1.783078000
C	4.700860000	-2.692056000	-2.419951000
C	4.951602000	-3.861964000	-1.698028000
C	5.051126000	-3.787063000	-0.304771000
C	4.894997000	-2.581005000	0.376592000
C	4.196817000	-0.211906000	-2.548363000
C	5.067677000	-5.188630000	-2.398149000
C	4.982685000	-2.493872000	1.874030000
C	-2.778758000	2.699352000	-1.130136000
C	-2.336976000	3.674050000	-0.228907000
C	-1.521782000	4.691222000	-0.734474000
C	-1.145239000	4.735691000	-2.077724000
C	-1.616420000	3.739660000	-2.943703000
C	-2.444726000	2.711918000	-2.495258000
C	-2.675959000	3.607945000	1.233639000
C	-0.252669000	5.829319000	-2.597836000
C	-2.939330000	1.629002000	-3.413012000
C	-4.661805000	-1.461912000	0.676848000
C	-4.703443000	-1.522464000	2.075465000
C	-4.897217000	-2.774783000	2.658811000
C	-5.053480000	-3.928869000	1.884971000
C	-5.033599000	-3.811799000	0.493113000
C	-4.840651000	-2.583455000	-0.139877000
C	-4.533342000	-0.281983000	2.908042000
C	-5.198998000	-5.277341000	2.536371000
C	-4.831558000	-2.474629000	-1.638934000
C	1.688626000	-1.976773000	0.366370000
C	1.574303000	-3.020043000	1.350849000
C	1.504124000	-4.265935000	0.670003000
C	1.566094000	-4.006529000	-0.731257000
C	1.666810000	-2.603435000	-0.922986000
C	-1.646935000	-1.788008000	0.180032000
C	-1.707446000	-2.778725000	1.218344000
C	-1.716395000	-4.061452000	0.608473000
C	-1.645315000	-3.880564000	-0.804940000
C	-1.590771000	-2.484385000	-1.072838000
C	5.699038000	3.044522000	1.571822000
C	6.949256000	0.285829000	0.150819000

C	-5.694174000	3.017542000	-1.307494000
C	-6.972220000	0.145772000	-0.174611000
H	1.076556000	5.358436000	0.781965000
H	1.024508000	3.254509000	4.519786000
H	3.269573000	2.909563000	-0.950947000
H	3.675038000	4.574775000	-0.517500000
H	2.081861000	4.200291000	-1.180347000
H	-0.458393000	6.060129000	2.483892000
H	0.385397000	6.007830000	4.036728000
H	-0.927577000	4.876674000	3.716790000
H	3.938559000	1.281994000	3.860726000
H	2.472335000	0.352693000	3.549222000
H	2.536457000	1.463637000	4.930913000
H	4.620832000	-2.738539000	-3.503305000
H	5.245651000	-4.691893000	0.265813000
H	4.300418000	-0.369995000	-3.623818000
H	4.837783000	0.627988000	-2.260193000
H	3.160456000	0.090726000	-2.355648000
H	5.355006000	-5.068798000	-3.446248000
H	4.104882000	-5.713370000	-2.377417000
H	5.801428000	-5.837327000	-1.910674000
H	5.796526000	-1.833606000	2.193662000
H	5.151152000	-3.478459000	2.314957000
H	4.056362000	-2.087569000	2.293468000
H	-1.172445000	5.463369000	-0.055236000
H	-1.325376000	3.760833000	-3.990871000
H	-2.648108000	4.601858000	1.685048000
H	-1.944538000	2.984335000	1.762284000
H	-3.663706000	3.173691000	1.410251000
H	0.587645000	5.411843000	-3.161984000
H	0.150664000	6.440891000	-1.786804000
H	-0.800741000	6.490610000	-3.278363000
H	-2.561088000	1.774869000	-4.426296000
H	-4.033393000	1.601454000	-3.454379000
H	-2.601534000	0.645699000	-3.068588000
H	-4.925601000	-2.850326000	3.743298000
H	-5.155730000	-4.701932000	-0.119070000
H	-5.196129000	0.523024000	2.572029000
H	-3.507085000	0.097284000	2.833383000
H	-4.747095000	-0.484249000	3.959739000
H	-4.217605000	-5.755175000	2.643618000
H	-5.823463000	-5.947456000	1.938558000
H	-5.635808000	-5.198043000	3.535768000
H	-4.542329000	-3.425484000	-2.091406000
H	-4.132016000	-1.709621000	-1.983829000

H	-5.824049000	-2.211145000	-2.023468000
H	1.526710000	-2.868299000	2.421398000
H	1.381122000	-5.236649000	1.132077000
H	1.502593000	-4.748102000	-1.516537000
H	1.700714000	-2.086755000	-1.869477000
H	-1.754538000	-2.570678000	2.278277000
H	-1.737747000	-5.010451000	1.127384000
H	-1.596712000	-4.669651000	-1.543905000
H	-1.494912000	-2.014370000	-2.041274000
H	5.399592000	3.911961000	0.975784000
H	6.784407000	2.951600000	1.516437000
H	5.423130000	3.246172000	2.611567000
H	7.033843000	0.110781000	-0.926681000
H	7.257375000	-0.634171000	0.657179000
H	7.645556000	1.079405000	0.425243000
H	-5.383450000	3.233212000	-2.334584000
H	-5.425156000	3.883798000	-0.694517000
H	-6.779506000	2.910001000	-1.294582000
H	-7.173714000	-0.734728000	-0.791813000
H	-7.664719000	0.935104000	-0.469824000
H	-7.180229000	-0.126243000	0.864975000
Cl	0.266694000	-0.137388000	-3.021750000
Sn	0.237214000	1.257137000	-0.900739000

Cartesian coordinates and energies (E_h) of **5a [FcP_2SnCl]$^+$**, scrf=(cpcm,solvent=acetonitrile)

E(RB3PW91) = -10818.4785180
Sum of electronic and zero-point Energies= -10817.407839
Sum of electronic and thermal Energies= -10817.337855
Sum of electronic and thermal Enthalpies= -10817.336911
Sum of electronic and thermal Free Energies= -10817.515595

Fe	-0.020667000	-3.038413000	0.102152000
P	1.617322000	-0.222083000	0.815866000
P	-1.665052000	0.005310000	0.472881000
N	3.670588000	1.615791000	1.174889000
N	4.482829000	-0.170800000	0.279180000
N	-3.669073000	1.665833000	-0.677316000
N	-4.488576000	-0.185968000	0.060550000
C	3.324383000	0.398632000	0.681066000
C	5.047444000	1.811055000	1.089696000
C	5.561974000	0.683109000	0.524346000
C	-3.318123000	0.466672000	-0.150885000
C	-5.055935000	1.774302000	-0.789737000
C	-5.572207000	0.602313000	-0.327808000

C	2.743027000	2.575656000	1.699386000
C	2.322191000	3.631103000	0.881044000
C	1.393985000	4.530643000	1.416934000
C	0.899717000	4.395831000	2.713905000
C	1.375444000	3.342905000	3.507560000
C	2.310477000	2.427925000	3.028674000
C	2.855759000	3.838942000	-0.510284000
C	-0.095859000	5.375230000	3.273799000
C	2.848134000	1.323837000	3.895274000
C	4.631148000	-1.429328000	-0.389457000
C	4.534423000	-1.448792000	-1.783960000
C	4.708378000	-2.678253000	-2.421750000
C	4.960957000	-3.848217000	-1.700395000
C	5.060130000	-3.774033000	-0.307065000
C	4.901439000	-2.568662000	0.375158000
C	4.200423000	-0.198613000	-2.548182000
C	5.079097000	-5.174284000	-2.401407000
C	4.988817000	-2.482424000	1.872640000
C	-2.784559000	2.694617000	-1.132710000
C	-2.342946000	3.667779000	-0.229684000
C	-1.530150000	4.687660000	-0.734028000
C	-1.156616000	4.736709000	-2.078007000
C	-1.627961000	3.742233000	-2.945885000
C	-2.453256000	2.711595000	-2.498446000
C	-2.680935000	3.598929000	1.232965000
C	-0.268073000	5.834239000	-2.596867000
C	-2.948506000	1.630623000	-3.418213000
C	-4.657628000	-1.468007000	0.680021000
C	-4.696222000	-1.526062000	2.078829000
C	-4.885049000	-2.777969000	2.664870000
C	-5.039534000	-3.933818000	1.893256000
C	-5.023558000	-3.819170000	0.501079000
C	-4.835426000	-2.591357000	-0.134470000
C	-4.528619000	-0.283406000	2.908657000
C	-5.178673000	-5.281761000	2.547223000
C	-4.830149000	-2.484739000	-1.633670000
C	1.693109000	-1.973112000	0.364977000
C	1.580377000	-3.014869000	1.351166000
C	1.513025000	-4.262067000	0.672395000
C	1.575464000	-4.005112000	-0.729325000
C	1.673761000	-2.602109000	-0.923196000
C	-1.642652000	-1.791295000	0.177278000
C	-1.700578000	-2.779703000	1.217939000
C	-1.707369000	-4.063861000	0.611165000
C	-1.637838000	-3.886242000	-0.802693000

C	-1.586402000	-2.490612000	-1.073850000
C	5.689980000	3.055763000	1.581390000
C	6.949563000	0.303706000	0.156259000
C	-5.701393000	3.008087000	-1.305809000
C	-6.972755000	0.135858000	-0.167747000
H	1.055742000	5.355725000	0.796515000
H	1.017684000	3.242781000	4.529597000
H	3.254299000	2.919895000	-0.946596000
H	3.662205000	4.581760000	-0.503991000
H	2.068463000	4.214574000	-1.168807000
H	-0.471682000	6.053812000	2.503917000
H	0.360131000	5.983583000	4.063055000
H	-0.950250000	4.856464000	3.719675000
H	3.942839000	1.298909000	3.873207000
H	2.495457000	0.347768000	3.542210000
H	2.528283000	1.450239000	4.931714000
H	4.629123000	-2.724165000	-3.505218000
H	5.256324000	-4.678830000	0.263016000
H	4.301441000	-0.356762000	-3.623921000
H	4.842216000	0.641044000	-2.261430000
H	3.164940000	0.104698000	-2.351689000
H	5.369153000	-5.053315000	-3.448662000
H	4.116217000	-5.699000000	-2.383755000
H	5.811406000	-5.823378000	-1.912286000
H	5.802449000	-1.822136000	2.192570000
H	5.157410000	-3.467320000	2.312818000
H	4.062545000	-2.076319000	2.292301000
H	-1.181833000	5.459127000	-0.053575000
H	-1.340473000	3.767990000	-3.993989000
H	-2.660463000	4.593069000	1.684169000
H	-1.944377000	2.981338000	1.761502000
H	-3.665156000	3.157139000	1.410066000
H	0.570760000	5.420902000	-3.166228000
H	0.137251000	6.442742000	-1.784608000
H	-0.820392000	6.497215000	-3.272331000
H	-2.572805000	1.780278000	-4.431980000
H	-4.042541000	1.602084000	-3.457689000
H	-2.610078000	0.646534000	-3.076570000
H	-4.910536000	-2.851688000	3.749551000
H	-5.144566000	-4.710723000	-0.109266000
H	-5.195746000	0.518214000	2.573324000
H	-3.504360000	0.100338000	2.829973000
H	-4.737839000	-0.484903000	3.961391000
H	-4.195371000	-5.756373000	2.651244000
H	-5.803252000	-5.954585000	1.952532000

H	-5.611717000	-5.202091000	3.548244000
H	-4.543989000	-3.436861000	-2.085454000
H	-4.130419000	-1.721159000	-1.981391000
H	-5.823146000	-2.219620000	-2.015641000
H	1.532596000	-2.861624000	2.421504000
H	1.391542000	-5.232195000	1.136115000
H	1.514490000	-4.748496000	-1.513126000
H	1.709257000	-2.086446000	-1.870160000
H	-1.747895000	-2.569481000	2.277456000
H	-1.726675000	-5.011635000	1.132384000
H	-1.588990000	-4.677084000	-1.539765000
H	-1.494244000	-2.022353000	-2.043446000
H	5.390013000	3.923512000	0.986123000
H	6.775580000	2.965144000	1.528236000
H	5.411201000	3.254320000	2.620928000
H	7.036676000	0.131746000	-0.921522000
H	7.259289000	-0.616316000	0.661541000
H	7.642814000	1.098759000	0.433868000
H	-5.392761000	3.225084000	-2.333202000
H	-5.433441000	3.874090000	-0.692062000
H	-6.786381000	2.897966000	-1.291312000
H	-7.174463000	-0.746478000	-0.782206000
H	-7.666461000	0.923727000	-0.463793000
H	-7.178129000	-0.132876000	0.873195000
Cl	0.266985000	-0.147605000	-3.039721000
Sn	0.234858000	1.252576000	-0.911636000

Cartesian coordinates and energies (E_h) of **5a [$FcP_2SnCl]^+[SnCl_3]^-$**, scrf=(cpcm,solvent=THF)

E(RB3PW91) = -18220.3853502
Sum of electronic and zero-point Energies= -18219.311281
Sum of electronic and thermal Energies= -18219.232743
Sum of electronic and thermal Enthalpies= -18219.231798
Sum of electronic and thermal Free Energies= -18219.434503

Fe	-1.925862000	3.044776000	-0.252544000
P	0.307367000	0.569511000	-0.113829000
P	-2.841955000	-0.292889000	-0.625189000
Cl	-2.081583000	0.540387000	3.210229000
Sn	-1.231670000	-1.001017000	1.373876000
Sn	8.211371000	-0.246467000	-1.847242000
Cl	8.499839000	-0.617401000	0.627781000
Cl	5.984435000	0.865673000	-1.582588000
Cl	7.190772000	-2.507679000	-2.256645000
N	2.661902000	-0.833123000	0.333413000

N	2.863648000	1.144091000	1.169426000
N	-4.778058000	-2.220907000	0.168899000
N	-5.653282000	-0.644999000	-1.012962000
C	1.985149000	0.323624000	0.550878000
C	3.966342000	-0.742386000	0.811104000
C	4.096892000	0.507642000	1.336725000
C	-4.499619000	-1.024809000	-0.406854000
C	-6.098127000	-2.599422000	-0.080656000
C	-6.651369000	-1.601472000	-0.822683000
C	2.104399000	-1.996274000	-0.291647000
C	1.644018000	-3.045038000	0.513422000
C	1.072420000	-4.148258000	-0.130075000
C	0.965309000	-4.217499000	-1.518641000
C	1.476463000	-3.161373000	-2.285010000
C	2.066436000	-2.045122000	-1.695771000
C	1.786133000	-3.036191000	2.011337000
C	0.350553000	-5.413705000	-2.193817000
C	2.655330000	-0.934700000	-2.518365000
C	2.588899000	2.449958000	1.690056000
C	2.096497000	2.545886000	2.995191000
C	1.857068000	3.825120000	3.499826000
C	2.090056000	4.969561000	2.732564000
C	2.591839000	4.821360000	1.435699000
C	2.853743000	3.565496000	0.889247000
C	1.789665000	1.308913000	3.791639000
C	1.764269000	6.336722000	3.270441000
C	3.378026000	3.398430000	-0.507842000
C	-3.904211000	-3.004593000	0.988045000
C	-3.061212000	-3.945409000	0.387089000
C	-2.273043000	-4.731897000	1.232997000
C	-2.305920000	-4.583489000	2.620249000
C	-3.170641000	-3.631171000	3.176652000
C	-3.989160000	-2.832323000	2.380235000
C	-2.961444000	-4.074960000	-1.106726000
C	-1.429093000	-5.419069000	3.512571000
C	-4.905522000	-1.795264000	2.966880000
C	-5.852866000	0.516890000	-1.828850000
C	-5.493526000	0.445302000	-3.180676000
C	-5.717335000	1.576541000	-3.965749000
C	-6.285352000	2.738374000	-3.434269000
C	-6.653824000	2.749963000	-2.086928000
C	-6.449503000	1.646235000	-1.258299000
C	-4.879668000	-0.802744000	-3.751929000
C	-6.459012000	3.967693000	-4.284329000
C	-6.860295000	1.673242000	0.187244000

C	-0.053480000	2.330427000	0.102664000
C	-0.051398000	3.245934000	-1.006940000
C	-0.525434000	4.503777000	-0.544660000
C	-0.830349000	4.376795000	0.842978000
C	-0.553043000	3.042842000	1.241737000
C	-3.215062000	1.489608000	-0.589430000
C	-3.133664000	2.353087000	-1.734475000
C	-3.538460000	3.655901000	-1.338702000
C	-3.857293000	3.617518000	0.051478000
C	-3.648452000	2.290158000	0.519376000
C	4.932182000	-1.853574000	0.648537000
C	5.250760000	1.193399000	1.967615000
C	-6.643311000	-3.889809000	0.412356000
C	-8.004207000	-1.444534000	-1.414651000
H	0.707351000	-4.970690000	0.478696000
H	1.426123000	-3.217342000	-3.369916000
H	1.883273000	-2.026096000	2.416337000
H	2.676626000	-3.600618000	2.312646000
H	0.920194000	-3.509457000	2.481068000
H	-0.117348000	-6.088427000	-1.472342000
H	1.109495000	-5.983465000	-2.741885000
H	-0.410203000	-5.108806000	-2.919443000
H	3.683975000	-0.715486000	-2.212905000
H	2.078816000	-0.010725000	-2.392022000
H	2.658053000	-1.194626000	-3.579196000
H	1.466054000	3.927523000	4.509327000
H	2.774884000	5.705682000	0.830110000
H	1.556609000	1.556317000	4.829460000
H	2.624920000	0.600830000	3.783776000
H	0.920521000	0.788918000	3.370755000
H	1.765141000	6.351693000	4.363829000
H	0.767028000	6.648518000	2.936898000
H	2.475157000	7.088327000	2.914439000
H	4.367035000	2.928448000	-0.515907000
H	3.451373000	4.361898000	-1.016736000
H	2.718914000	2.751845000	-1.096271000
H	-1.615465000	-5.474337000	0.789993000
H	-3.201483000	-3.504266000	4.255894000
H	-2.638424000	-5.078853000	-1.390053000
H	-2.219807000	-3.367399000	-1.497361000
H	-3.911087000	-3.861733000	-1.604978000
H	-0.791341000	-4.782117000	4.134804000
H	-0.782986000	-6.084985000	2.935279000
H	-2.030734000	-6.032898000	4.191794000
H	-4.821304000	-1.772122000	4.054804000

H	-5.952257000	-1.985146000	2.706212000
H	-4.651089000	-0.798472000	2.591142000
H	-5.439193000	1.549802000	-5.016718000
H	-7.097794000	3.647253000	-1.662772000
H	-5.467607000	-1.692493000	-3.500872000
H	-3.873156000	-0.960000000	-3.345946000
H	-4.803323000	-0.738853000	-4.839505000
H	-5.589649000	4.628042000	-4.179035000
H	-7.341198000	4.541595000	-3.986100000
H	-6.552946000	3.715782000	-5.344323000
H	-6.873296000	2.698229000	0.563753000
H	-6.177172000	1.092903000	0.811700000
H	-7.865325000	1.255885000	0.321577000
H	0.242111000	3.001436000	-2.019512000
H	-0.670228000	5.389569000	-1.149146000
H	-1.243157000	5.152169000	1.474711000
H	-0.706307000	2.621824000	2.223210000
H	-2.829841000	2.047959000	-2.726238000
H	-3.566151000	4.531696000	-1.973203000
H	-4.162720000	4.461495000	0.656119000
H	-3.764271000	1.936055000	1.533903000
H	4.601382000	-2.755931000	1.171860000
H	5.909210000	-1.561201000	1.033071000
H	5.061313000	-2.100814000	-0.409322000
H	5.032997000	1.470633000	3.004474000
H	5.506230000	2.106339000	1.421387000
H	6.124636000	0.540823000	1.948829000
H	-6.616838000	-3.947338000	1.505042000
H	-6.060442000	-4.731988000	0.025635000
H	-7.678099000	-4.009099000	0.088852000
H	-8.523612000	-0.573720000	-1.003642000
H	-8.608308000	-2.329657000	-1.211006000
H	-7.942727000	-1.309563000	-2.499110000

Cartesian coordinates and energies (E_h) of **5a** **$[FcP_2SnCl]^+[SnCl_3]^-$**, scrf=(cpcm,solvent=acetonitrile)

E(RB3PW91) = -18220.3917008
Sum of electronic and zero-point Energies= -18219.317797
Sum of electronic and thermal Energies= -18219.239213
Sum of electronic and thermal Enthalpies= -18219.238269
Sum of electronic and thermal Free Energies= -18219.441054

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symmetry c1

Fe	-1.935032000	3.044359000	-0.252698000
P	0.298556000	0.570054000	-0.118105000
P	-2.853617000	-0.292707000	-0.625705000
Cl	-2.080388000	0.542324000	3.217147000
Sn	-1.242904000	-1.001771000	1.368937000
Sn	8.259395000	-0.238861000	-1.825475000
Cl	8.517823000	-0.620981000	0.655084000
Cl	6.017455000	0.845737000	-1.582769000
Cl	7.263427000	-2.515882000	-2.241240000
N	2.654362000	-0.832962000	0.324125000
N	2.855624000	1.142670000	1.164432000
N	-4.788428000	-2.220502000	0.174933000
N	-5.664328000	-0.648467000	-1.011156000
C	1.977233000	0.323280000	0.544135000
C	3.958883000	-0.742441000	0.801696000
C	4.088818000	0.506097000	1.330637000
C	-4.511037000	-1.026363000	-0.404417000
C	-6.108548000	-2.599940000	-0.072461000
C	-6.662310000	-1.604061000	-0.817370000
C	2.097614000	-1.994082000	-0.305621000
C	1.635367000	-3.045841000	0.494461000
C	1.064139000	-4.146205000	-0.154796000
C	0.959672000	-4.210018000	-1.543928000
C	1.473274000	-3.151002000	-2.305297000
C	2.061918000	-2.037339000	-1.710101000
C	1.776049000	-3.043531000	1.992522000
C	0.341624000	-5.400779000	-2.225485000
C	2.651467000	-0.922619000	-2.526939000
C	2.583521000	2.449888000	1.683130000
C	2.092889000	2.549503000	2.988594000
C	1.856712000	3.830435000	3.490496000
C	2.091147000	4.972793000	2.720272000
C	2.592185000	4.820778000	1.423405000
C	2.850819000	3.562989000	0.879854000
C	1.785351000	1.314474000	3.787766000
C	1.767697000	6.341564000	3.255267000
C	3.372949000	3.390724000	-0.517633000
C	-3.912879000	-3.002209000	0.994050000
C	-3.072031000	-3.945135000	0.393128000
C	-2.282287000	-4.730298000	1.238934000
C	-2.312655000	-4.579502000	2.626134000
C	-3.175665000	-3.625497000	3.182521000
C	-3.995243000	-2.827435000	2.386121000
C	-2.978711000	-4.079819000	-1.100676000
C	-1.436500000	-5.416081000	3.518214000

C	-4.912173000	-1.790782000	2.972617000
C	-5.863902000	0.512818000	-1.828136000
C	-5.505638000	0.439284000	-3.180117000
C	-5.727603000	1.570495000	-3.965916000
C	-6.293357000	2.733715000	-3.434871000
C	-6.661611000	2.746835000	-2.087384000
C	-6.458750000	1.643387000	-1.257956000
C	-4.896829000	-0.811310000	-3.751324000
C	-6.465565000	3.962768000	-4.285635000
C	-6.869807000	1.672042000	0.187453000
C	-0.061536000	2.330984000	0.096723000
C	-0.063462000	3.245846000	-1.013680000
C	-0.536193000	4.503931000	-0.550539000
C	-0.836302000	4.377952000	0.838236000
C	-0.557478000	3.044260000	1.236928000
C	-3.225521000	1.489747000	-0.586921000
C	-3.147504000	2.353813000	-1.731713000
C	-3.551309000	3.656235000	-1.334079000
C	-3.866361000	3.617056000	0.056792000
C	-3.656292000	2.289493000	0.523293000
C	4.925932000	-1.852638000	0.637196000
C	5.240676000	1.189857000	1.967530000
C	-6.653439000	-3.888924000	0.424238000
C	-8.015636000	-1.448784000	-1.408362000
H	0.697127000	-4.970737000	0.449873000
H	1.424694000	-3.202794000	-3.390512000
H	1.868933000	-2.035024000	2.402498000
H	2.668257000	-3.606300000	2.291904000
H	0.912021000	-3.523108000	2.459228000
H	-0.089420000	-6.100076000	-1.504678000
H	1.089205000	-5.943203000	-2.815070000
H	-0.449786000	-5.091164000	-2.915596000
H	3.678882000	-0.703078000	-2.217228000
H	2.073602000	0.000260000	-2.398305000
H	2.657080000	-1.178073000	-3.588868000
H	1.467065000	3.936168000	4.500169000
H	2.776869000	5.703443000	0.815923000
H	1.545812000	1.565050000	4.823335000
H	2.622760000	0.608862000	3.787438000
H	0.920935000	0.789714000	3.363112000
H	1.776856000	6.360731000	4.348534000
H	0.767274000	6.649983000	2.928275000
H	2.474290000	7.092876000	2.890366000
H	4.350893000	2.897877000	-0.526713000
H	3.468868000	4.354616000	-1.021902000

H	2.698476000	2.762913000	-1.109225000
H	-1.627308000	-5.475130000	0.796244000
H	-3.205971000	-3.498346000	4.261780000
H	-2.649293000	-5.082296000	-1.381377000
H	-2.245125000	-3.367902000	-1.498587000
H	-3.932657000	-3.876406000	-1.594744000
H	-0.802141000	-4.780186000	4.144966000
H	-0.787504000	-6.078556000	2.940280000
H	-2.039276000	-6.033417000	4.193252000
H	-4.823728000	-1.763675000	4.060154000
H	-5.959302000	-1.985404000	2.717426000
H	-4.663795000	-0.794696000	2.591047000
H	-5.450487000	1.542297000	-5.017099000
H	-7.104459000	3.644983000	-1.663897000
H	-5.490615000	-1.698019000	-3.503521000
H	-3.892510000	-0.975460000	-3.342754000
H	-4.816862000	-0.745976000	-4.838528000
H	-5.597140000	4.623910000	-4.177605000
H	-7.349088000	4.535862000	-3.989837000
H	-6.555979000	3.710494000	-5.345838000
H	-6.880440000	2.697278000	0.563372000
H	-6.188933000	1.089777000	0.812572000
H	-7.875950000	1.257365000	0.321166000
H	0.226447000	3.001178000	-2.027305000
H	-0.683818000	5.389163000	-1.155162000
H	-1.247038000	5.153949000	1.470570000
H	-0.706207000	2.623847000	2.219333000
H	-2.847865000	2.049397000	-2.724980000
H	-3.581348000	4.532259000	-1.968114000
H	-4.171170000	4.460580000	0.662341000
H	-3.771833000	1.934158000	1.537373000
H	4.590816000	-2.759166000	1.150275000
H	5.899471000	-1.563265000	1.032928000
H	5.063598000	-2.090851000	-0.421798000
H	5.018629000	1.464325000	3.004161000
H	5.498786000	2.104711000	1.425607000
H	6.113795000	0.536202000	1.952117000
H	-6.627118000	-3.943343000	1.517039000
H	-6.070837000	-4.731983000	0.039166000
H	-7.688207000	-4.008773000	0.101199000
H	-8.534878000	-0.577547000	-0.998178000
H	-8.618935000	-2.333783000	-1.202285000
H	-7.955005000	-1.316389000	-2.493131000

Cartesian coordinates and energies (E_h) of **5c [$FcP_2SnI]^+I^-$**, scrf=(cpcm,solvent=thf)

E(RB3PW91) = -24197.7589891
Sum of electronic and zero-point Energies= -24196.688333
Sum of electronic and thermal Energies= -24196.615647
Sum of electronic and thermal Enthalpies= -24196.614703
Sum of electronic and thermal Free Energies= -24196.802897

I	1.115560000	-0.207291000	3.486555000
Sn	0.565408000	1.245878000	0.995264000
I	-7.088507000	0.209710000	-2.607611000
Fe	0.684214000	-3.044406000	-0.175857000
P	-1.141016000	-0.247644000	-0.376729000
P	2.122749000	0.048631000	-0.799255000
N	-3.285933000	1.512258000	-0.220425000
N	-3.830939000	-0.335871000	0.747997000
N	4.300652000	1.774398000	-0.196414000
N	4.963508000	-0.057174000	-1.120050000
C	-2.802085000	0.295226000	0.138343000
C	-4.617322000	1.648950000	0.162558000
C	-4.963659000	0.481073000	0.772489000
C	3.865167000	0.559264000	-0.614010000
C	5.664917000	1.928529000	-0.446794000
C	6.083659000	0.769986000	-1.025218000
C	-2.521762000	2.534866000	-0.872009000
C	-1.979504000	3.567353000	-0.095998000
C	-1.230678000	4.546156000	-0.757016000
C	-1.022472000	4.506537000	-2.135987000
C	-1.602025000	3.466070000	-2.873390000
C	-2.372562000	2.474536000	-2.267495000
C	-2.212702000	3.663113000	1.387644000
C	-0.231235000	5.579061000	-2.834813000
C	-3.025168000	1.382801000	-3.065760000
C	-3.791123000	-1.620511000	1.380979000
C	-3.412999000	-1.675938000	2.725922000
C	-3.399476000	-2.929871000	3.338560000
C	-3.747382000	-4.088621000	2.638765000
C	-4.136966000	-3.977596000	1.300314000
C	-4.171027000	-2.746945000	0.644719000
C	-3.004151000	-0.428218000	3.456087000
C	-3.664183000	-5.439184000	3.297262000
C	-4.574175000	-2.619554000	-0.795428000
C	3.533889000	2.770545000	0.487753000
C	2.840039000	3.733330000	-0.252556000
C	2.153061000	4.718325000	0.463828000

C	2.136594000	4.739728000	1.858900000
C	2.855884000	3.760304000	2.557215000
C	3.575656000	2.769234000	1.892743000
C	2.784040000	3.689302000	-1.753514000
C	1.358824000	5.785045000	2.610750000
C	4.355887000	1.718985000	2.632005000
C	5.016630000	-1.338403000	-1.761420000
C	4.721258000	-1.408165000	-3.128077000
C	4.813457000	-2.657752000	-3.742024000
C	5.190452000	-3.799695000	-3.029220000
C	5.498886000	-3.673611000	-1.672203000
C	5.422149000	-2.447588000	-1.011492000
C	4.302441000	-0.182324000	-3.891201000
C	5.222379000	-5.147513000	-3.697217000
C	5.763026000	-2.322058000	0.446834000
C	-1.065423000	-2.017391000	-0.003832000
C	-1.152868000	-3.014707000	-1.036805000
C	-0.914621000	-4.285652000	-0.446275000
C	-0.669762000	-4.086515000	0.944734000
C	-0.751384000	-2.696020000	1.218055000
C	2.221209000	-1.754380000	-0.574353000
C	2.053327000	-2.706068000	-1.637253000
C	2.224470000	-4.008826000	-1.097927000
C	2.481736000	-3.879830000	0.299439000
C	2.469849000	-2.495804000	0.627821000
C	-5.406408000	2.859125000	-0.171916000
C	-6.244552000	0.018352000	1.359725000
C	6.377882000	3.189590000	-0.119963000
C	7.409959000	0.347067000	-1.542283000
H	-0.803388000	5.355501000	-0.171400000
H	-1.463265000	3.436293000	-3.951617000
H	-2.397558000	2.687395000	1.844192000
H	-3.082935000	4.294768000	1.602403000
H	-1.347826000	4.112119000	1.882198000
H	0.340966000	6.186160000	-2.128477000
H	-0.897062000	6.252842000	-3.386428000
H	0.465600000	5.148359000	-3.560176000
H	-4.085213000	1.271538000	-2.809320000
H	-2.544113000	0.418591000	-2.862538000
H	-2.949071000	1.584134000	-4.136655000
H	-3.099558000	-3.002868000	4.381233000
H	-4.412723000	-4.873122000	0.748739000
H	-2.831348000	-0.629681000	4.515257000
H	-3.762913000	0.357444000	3.372324000
H	-2.073269000	-0.025813000	3.039883000

H	-3.739160000	-5.363582000	4.385582000
H	-2.704441000	-5.916587000	3.065013000
H	-4.453641000	-6.108446000	2.942532000
H	-5.442927000	-1.963865000	-0.924421000
H	-4.812961000	-3.595356000	-1.223887000
H	-3.764583000	-2.178666000	-1.386327000
H	1.610896000	5.479851000	-0.088678000
H	2.850430000	3.766375000	3.644236000
H	2.656888000	4.691972000	-2.167345000
H	1.927947000	3.086760000	-2.080857000
H	3.683127000	3.245211000	-2.188741000
H	0.616040000	5.317177000	3.265803000
H	0.834112000	6.463197000	1.933157000
H	2.017966000	6.383813000	3.248647000
H	4.205574000	1.808496000	3.709015000
H	5.429123000	1.796469000	2.425724000
H	4.038172000	0.714525000	2.334300000
H	4.581101000	-2.741011000	-4.801112000
H	5.793094000	-4.554977000	-1.107678000
H	4.994216000	0.651403000	-3.728439000
H	3.311962000	0.156594000	-3.564140000
H	4.256834000	-0.384801000	-4.963378000
H	4.266418000	-5.665454000	-3.553026000
H	6.004715000	-5.786176000	-3.276951000
H	5.389051000	-5.060475000	-4.774462000
H	5.697255000	-3.292429000	0.943211000
H	5.085399000	-1.633981000	0.958224000
H	6.782078000	-1.942487000	0.587075000
H	-1.345287000	-2.816926000	-2.083215000
H	-0.880843000	-5.232638000	-0.968810000
H	-0.423485000	-4.857976000	1.662231000
H	-0.592998000	-2.219847000	2.173359000
H	1.844789000	-2.459617000	-2.669116000
H	2.136815000	-4.938064000	-1.644873000
H	2.618855000	-4.695218000	0.997575000
H	2.600162000	-2.064200000	1.610148000
H	-4.888673000	3.774392000	0.128231000
H	-6.374815000	2.824690000	0.328490000
H	-5.591745000	2.900538000	-1.250287000
H	-6.097590000	-0.378800000	2.368910000
H	-6.692903000	-0.765644000	0.741316000
H	-6.952127000	0.846945000	1.408537000
H	6.335814000	3.411435000	0.950923000
H	5.930141000	4.037605000	-0.648223000
H	7.425917000	3.115845000	-0.412934000

H	7.779801000	-0.539938000	-1.019470000
H	8.137446000	1.149135000	-1.410908000
H	7.354596000	0.101170000	-2.607513000

Cartesian coordinates and energies (E_h) of **5c [$FcP_2SnI]^+$**

E(RB3PW91) = -17277.8905110
Sum of electronic and zero-point Energies= -17276.819252
Sum of electronic and thermal Energies= -17276.749018
Sum of electronic and thermal Enthalpies= -17276.748074
Sum of electronic and thermal Free Energies= -17276.928751

I	0.326609000	0.001770000	-3.170890000
Sn	0.203098000	1.319968000	-0.611290000
Fe	-0.078611000	-3.044650000	0.294944000
P	1.591673000	-0.237389000	1.042210000
P	-1.705565000	-0.007033000	0.696666000
N	3.677170000	1.578563000	1.358072000
N	4.463483000	-0.264389000	0.554189000
N	-3.703667000	1.711001000	-0.376304000
N	-4.529517000	-0.171141000	0.277261000
C	3.308080000	0.350139000	0.902586000
C	5.061964000	1.731762000	1.302174000
C	5.558823000	0.569866000	0.795668000
C	-3.354308000	0.484902000	0.092615000
C	-5.090889000	1.829951000	-0.477301000
C	-5.610915000	0.640857000	-0.068597000
C	2.777558000	2.596677000	1.816546000
C	2.431450000	3.634824000	0.942350000
C	1.552503000	4.612617000	1.417394000
C	1.028031000	4.567971000	2.708073000
C	1.416039000	3.520908000	3.553160000
C	2.303165000	2.530602000	3.137376000
C	2.982383000	3.733965000	-0.454724000
C	0.097412000	5.638569000	3.209941000
C	2.737038000	1.429008000	4.062725000
C	4.602025000	-1.540864000	-0.083211000
C	4.566022000	-1.581214000	-1.479988000
C	4.732305000	-2.825924000	-2.088971000
C	4.923378000	-3.988855000	-1.338970000
C	4.965428000	-3.892535000	0.055906000
C	4.811557000	-2.672402000	0.710782000
C	4.310375000	-0.332892000	-2.275823000
C	5.042636000	-5.329948000	-2.009881000
C	4.847194000	-2.560193000	2.208829000

C	-2.817095000	2.738056000	-0.832643000
C	-2.344734000	3.694368000	0.072483000
C	-1.523509000	4.704540000	-0.434949000
C	-1.162283000	4.754881000	-1.781701000
C	-1.664849000	3.778913000	-2.651877000
C	-2.510193000	2.765633000	-2.204088000
C	-2.644330000	3.606989000	1.542336000
C	-0.248062000	5.829997000	-2.302150000
C	-3.061218000	1.720154000	-3.132240000
C	-4.710253000	-1.479581000	0.835536000
C	-4.765375000	-1.603517000	2.229038000
C	-4.981800000	-2.878155000	2.752160000
C	-5.144600000	-3.993834000	1.925789000
C	-5.102293000	-3.814476000	0.541114000
C	-4.888911000	-2.561455000	-0.032918000
C	-4.579631000	-0.405402000	3.118492000
C	-5.323548000	-5.366985000	2.513591000
C	-4.856378000	-2.381580000	-1.524837000
C	1.638813000	-1.989110000	0.587001000
C	1.498325000	-3.029953000	1.570875000
C	1.435869000	-4.276591000	0.890838000
C	1.525361000	-4.019062000	-0.509038000
C	1.637419000	-2.617244000	-0.701034000
C	-1.699179000	-1.796631000	0.363856000
C	-1.774572000	-2.802988000	1.386022000
C	-1.773606000	-4.076024000	0.756143000
C	-1.679108000	-3.873196000	-0.652972000
C	-1.621389000	-2.473162000	-0.898527000
C	5.725867000	2.977712000	1.763365000
C	6.944388000	0.135958000	0.481949000
C	-5.730702000	3.089606000	-0.936428000
C	-7.012956000	0.171181000	0.074553000
H	1.270379000	5.422741000	0.750337000
H	1.028899000	3.485046000	4.568806000
H	3.356715000	2.776738000	-0.825862000
H	3.808112000	4.454576000	-0.497180000
H	2.207463000	4.079567000	-1.144118000
H	-0.272023000	6.270052000	2.397523000
H	0.607478000	6.291632000	3.927225000
H	-0.765106000	5.204990000	3.725427000
H	3.819472000	1.269084000	4.016642000
H	2.255658000	0.484973000	3.781647000
H	2.469035000	1.657549000	5.096509000
H	4.698153000	-2.888127000	-3.173782000
H	5.113503000	-4.792170000	0.648095000

H	4.401204000	-0.520190000	-3.347345000
H	5.004831000	0.471427000	-2.007959000
H	3.294769000	0.039066000	-2.096800000
H	5.313033000	-5.233459000	-3.064551000
H	4.087805000	-5.866963000	-1.960359000
H	5.793136000	-5.958227000	-1.520893000
H	5.686834000	-1.942588000	2.547977000
H	4.942346000	-3.543145000	2.674538000
H	3.931424000	-2.093783000	2.586439000
H	-1.144273000	5.457788000	0.249289000
H	-1.381787000	3.799565000	-3.700925000
H	-2.620756000	4.596546000	2.004546000
H	-1.888884000	2.988202000	2.042527000
H	-3.620115000	3.155045000	1.740480000
H	0.592412000	5.393839000	-2.852060000
H	0.155667000	6.445445000	-1.493805000
H	-0.775723000	6.494482000	-2.995263000
H	-2.625015000	1.812659000	-4.127674000
H	-4.150932000	1.797334000	-3.221693000
H	-2.830940000	0.713838000	-2.768242000
H	-5.024762000	-3.002633000	3.831648000
H	-5.227163000	-4.674645000	-0.111895000
H	-5.232637000	0.423090000	2.821534000
H	-3.548067000	-0.036788000	3.061267000
H	-4.797709000	-0.651736000	4.159932000
H	-4.354318000	-5.871459000	2.608389000
H	-5.957201000	-5.996007000	1.881999000
H	-5.769742000	-5.325303000	3.510938000
H	-4.613384000	-3.322626000	-2.022421000
H	-4.109894000	-1.641859000	-1.824080000
H	-5.826826000	-2.044177000	-1.908369000
H	1.426394000	-2.875118000	2.639474000
H	1.299061000	-5.245854000	1.351859000
H	1.471502000	-4.759781000	-1.295604000
H	1.690181000	-2.103633000	-1.648771000
H	-1.832384000	-2.610274000	2.448113000
H	-1.799562000	-5.033054000	1.259733000
H	-1.613796000	-4.650088000	-1.403367000
H	-1.502608000	-1.991163000	-1.858973000
H	5.461536000	3.831653000	1.131829000
H	6.810332000	2.859836000	1.739842000
H	5.428550000	3.224238000	2.787604000
H	7.056576000	-0.084348000	-0.584736000
H	7.211490000	-0.773767000	1.028739000
H	7.656236000	0.919068000	0.747697000

H	-5.424215000	3.350424000	-1.954392000
H	-5.452623000	3.928275000	-0.289748000
H	-6.817070000	2.989478000	-0.921899000
H	-7.217351000	-0.686234000	-0.573761000
H	-7.708017000	0.970379000	-0.187535000
H	-7.218816000	-0.143667000	1.102546000

Cartesian coordinates and energies (E_h) of **XantP$_2$**

E(RB3PW91) = -2260.46227557
Sum of electronic and zero-point Energies= -2259.743422
Sum of electronic and thermal Energies= -2259.702523
Sum of electronic and thermal Enthalpies= -2259.701579
Sum of electronic and thermal Free Energies= -2259.816242

P	1.452014000	-0.213227000	-0.952133000
P	-1.884750000	2.726868000	-1.247881000
O	-1.450070000	-0.266169000	-0.777597000
C	2.855613000	-0.799348000	0.003433000
N	4.162698000	-0.800071000	-0.412858000
C	-1.007960000	-1.558617000	-0.705093000
C	0.398090000	-1.700038000	-0.728917000
N	2.903865000	-1.234414000	1.306438000
C	0.898752000	-3.011046000	-0.683809000
H	1.973202000	-3.166043000	-0.742198000
C	-1.881011000	-2.643168000	-0.602384000
N	-0.855269000	2.001685000	1.371717000
C	-2.786274000	0.011746000	-0.853918000
C	4.992718000	-1.242125000	0.598965000
C	-3.757818000	-0.986481000	-0.761016000
C	-3.393987000	-2.457061000	-0.580242000
C	-1.323030000	-3.924837000	-0.516075000
H	-1.977455000	-4.787327000	-0.430230000
C	4.205478000	-1.525824000	1.664689000
C	-0.739924000	2.512477000	0.101556000
C	1.784327000	-1.159689000	2.254940000
H	0.997525000	-0.639973000	1.696512000
C	5.177599000	-1.780103000	-2.422678000
H	6.090550000	-2.109391000	-1.914477000
H	5.427843000	-1.584868000	-3.469371000
H	4.447071000	-2.593213000	-2.389361000
C	0.311525000	2.226160000	2.081745000
N	0.532412000	3.035781000	0.049541000
C	0.054015000	-4.110756000	-0.559573000
H	0.470311000	-5.113725000	-0.514613000

C	2.184651000	-0.308168000	3.458633000
H	2.944089000	-0.801361000	4.074665000
H	1.309176000	-0.145883000	4.094396000
H	2.568784000	0.663036000	3.137041000
C	4.599448000	-0.519350000	-1.785308000
H	3.672213000	-0.251083000	-2.306559000
C	-3.107436000	1.382919000	-0.995463000
C	-5.101828000	-0.598292000	-0.839849000
H	-5.878485000	-1.354004000	-0.762734000
C	-1.851825000	0.081158000	2.537790000
H	-1.501049000	-0.578926000	1.741541000
H	-2.789693000	-0.317646000	2.934824000
H	-1.116100000	0.068891000	3.350681000
C	-2.073470000	1.494546000	2.005990000
H	-2.826270000	1.456109000	1.220279000
C	-4.468950000	1.709239000	-1.081887000
H	-4.742348000	2.756178000	-1.186865000
C	1.299588000	-2.543343000	2.670746000
H	1.003332000	-3.131205000	1.801245000
H	0.431569000	-2.443679000	3.329417000
H	2.079396000	-3.083837000	3.220241000
C	-4.020364000	-3.279564000	-1.727671000
H	-5.109639000	-3.178657000	-1.736506000
H	-3.788900000	-4.343778000	-1.623468000
H	-3.637035000	-2.937811000	-2.692986000
C	-3.944262000	-2.953045000	0.774776000
H	-3.502078000	-2.383701000	1.597220000
H	-3.711789000	-4.011669000	0.928775000
H	-5.031459000	-2.835968000	0.823239000
C	-5.459330000	0.733034000	-1.010627000
H	-6.507429000	1.012930000	-1.071089000
C	5.564100000	0.661182000	-1.810757000
H	5.115922000	1.541933000	-1.343621000
H	5.817520000	0.911179000	-2.845059000
H	6.497866000	0.429297000	-1.285629000
C	-2.555073000	2.469782000	3.078560000
H	-1.840672000	2.546925000	3.905784000
H	-3.510807000	2.130045000	3.488919000
H	-2.696559000	3.465399000	2.648798000
C	1.169602000	2.873649000	1.262914000
C	0.784894000	5.107315000	-1.250843000
H	-0.297312000	5.260672000	-1.220817000
H	1.164968000	5.522176000	-2.189697000
H	1.240535000	5.657965000	-0.419938000
C	1.122820000	3.619978000	-1.155675000

H	0.635756000	3.083762000	-1.981728000
C	2.624749000	3.363892000	-1.217058000
H	3.175432000	3.954976000	-0.476048000
H	2.995217000	3.652988000	-2.204411000
H	2.835465000	2.302302000	-1.064524000
H	6.060131000	-1.326688000	0.474040000
H	4.464386000	-1.899410000	2.642147000
H	0.422966000	1.918025000	3.107091000
H	2.176933000	3.211597000	1.436817000

Cartesian coordinates and energies (E_h) of **[XantP$_2$SnI]$^+$**

E(RB3PW91) = -15201.1266463
Sum of electronic and zero-point Energies= -15200.403908
Sum of electronic and thermal Energies= -15200.358641
Sum of electronic and thermal Enthalpies= -15200.357697
Sum of electronic and thermal Free Energies= -15200.485639

Sn	-0.000009000	-0.277902000	0.832205000
P	1.912876000	-0.000647000	-1.029560000
P	-1.912874000	-0.000668000	-1.029578000
I	0.000000000	-3.124026000	0.611984000
O	-0.000010000	1.988615000	-0.958155000
N	-3.937974000	-0.615864000	0.992964000
N	4.017361000	-1.823940000	-0.808394000
N	-4.017340000	-1.823988000	-0.808382000
N	3.937986000	-0.615866000	0.992984000
C	-3.348137000	-0.800977000	-0.218005000
C	-3.679420000	3.750371000	-0.517956000
H	-4.663802000	4.201595000	-0.437871000
C	-4.965814000	-1.516994000	1.149425000
H	-5.569379000	-1.551859000	2.041702000
C	3.563153000	2.367302000	-0.660648000
H	4.454746000	1.747115000	-0.692716000
C	2.300230000	1.778972000	-0.766133000
C	3.348148000	-0.800950000	-0.217991000
C	-2.300250000	1.778945000	-0.766141000
C	-3.563180000	2.367259000	-0.660635000
H	-4.454766000	1.747062000	-0.692681000
C	-3.746600000	-2.392211000	-2.149394000
H	-2.926153000	-1.785392000	-2.543913000
C	3.679380000	3.750416000	-0.517991000
H	4.663758000	4.201653000	-0.437940000
C	1.259905000	4.018873000	-0.610408000
C	-1.190802000	2.640297000	-0.770968000

C	-3.499769000	0.296414000	2.072514000
H	-2.691648000	0.890555000	1.639696000
C	2.546032000	4.559847000	-0.483603000
H	2.666066000	5.633014000	-0.372778000
C	-5.011220000	-2.277227000	0.024551000
H	-5.662712000	-3.092509000	-0.244476000
C	-1.259955000	4.018857000	-0.610431000
C	1.190771000	2.640312000	-0.770951000
C	-2.546082000	4.559815000	-0.483580000
H	-2.666121000	5.632979000	-0.372721000
C	3.746637000	-2.392125000	-2.149424000
H	2.926194000	-1.785296000	-2.543936000
C	4.965800000	-1.517026000	1.149440000
H	5.569346000	-1.551930000	2.041729000
C	-4.970909000	-2.220163000	-3.041584000
H	-4.731334000	-2.562900000	-4.051485000
H	-5.273435000	-1.170676000	-3.098144000
H	-5.820890000	-2.810946000	-2.685065000
C	3.499820000	0.296420000	2.072542000
H	2.691692000	0.890568000	1.639749000
C	2.960812000	-0.526451000	3.240274000
H	2.201967000	-1.240475000	2.907225000
H	2.504372000	0.142450000	3.974575000
H	3.761625000	-1.081234000	3.739641000
C	-4.632529000	1.230271000	2.483557000
H	-5.000262000	1.808349000	1.634010000
H	-4.260086000	1.931400000	3.234758000
H	-5.468522000	0.682330000	2.929796000
C	3.283123000	-3.837411000	-2.014058000
H	4.073507000	-4.477196000	-1.607597000
H	3.016704000	-4.224580000	-3.001155000
H	2.406566000	-3.904694000	-1.364179000
C	4.970957000	-2.220054000	-3.041593000
H	5.273492000	-1.170568000	-3.098115000
H	4.731390000	-2.562755000	-4.051508000
H	5.820930000	-2.810856000	-2.685087000
C	-0.000035000	4.888372000	-0.612763000
C	-0.000086000	5.789316000	0.638675000
H	-0.879198000	6.438955000	0.655163000
H	0.878891000	6.439134000	0.655118000
H	-0.000002000	5.186568000	1.551203000
C	-2.960729000	-0.526462000	3.240228000
H	-3.761527000	-1.081246000	3.739614000
H	-2.504267000	0.142434000	3.974520000
H	-2.201895000	-1.240486000	2.907153000

C	5.011253000	-2.277187000	0.024520000
H	5.662763000	-3.092444000	-0.244537000
C	-0.000034000	5.758670000	-1.888211000
H	0.000003000	5.132900000	-2.785070000
H	0.885788000	6.400526000	-1.917393000
H	-0.885893000	6.400475000	-1.917430000
C	4.632604000	1.230261000	2.483556000
H	5.468600000	0.682305000	2.929771000
H	4.260191000	1.931394000	3.234769000
H	5.000323000	1.808335000	1.634001000
C	-3.283085000	-3.837492000	-2.013982000
H	-2.406533000	-3.904755000	-1.364095000
H	-3.016656000	-4.224687000	-3.001066000
H	-4.073470000	-4.477268000	-1.607511000

Cartesian coordinates and energies (E_h) of **6 FcP_2CuCl**, scrf=(cpcm,solvent=thf)

E(RB3PW91) = -6437.87831401
Sum of electronic and zero-point Energies= -6436.809092
Sum of electronic and thermal Energies= -6436.739003
Sum of electronic and thermal Enthalpies= -6436.738059
Sum of electronic and thermal Free Energies= -6436.917479

Fe	-0.040950000	-2.949767000	-0.032790000
P	-1.656335000	-0.112582000	-0.864702000
P	1.656664000	0.093396000	-0.423895000
Cl	-0.799016000	0.930557000	2.962355000
Cu	-0.176273000	0.664823000	0.799547000
N	-3.586518000	1.819630000	-0.949952000
N	-4.487250000	0.042537000	-0.115030000
N	3.683725000	1.660975000	0.691057000
N	4.491369000	-0.230098000	0.036147000
C	-3.311445000	0.531331000	-0.593358000
C	-4.921802000	2.137796000	-0.700380000
C	-5.493788000	1.019812000	-0.181649000
C	3.322122000	0.457067000	0.171507000
C	5.067172000	1.733201000	0.878533000
C	5.575741000	0.542021000	0.467246000
C	-2.639058000	2.664774000	-1.605777000
C	-1.798954000	3.482658000	-0.844951000
C	-0.861140000	4.260976000	-1.531730000
C	-0.750793000	4.230294000	-2.921475000
C	-1.621935000	3.406040000	-3.646393000
C	-2.572847000	2.612515000	-3.008550000
C	-1.883969000	3.538691000	0.653439000

C	0.299507000	5.043400000	-3.630268000
C	-3.488418000	1.700496000	-3.776649000
C	-4.715791000	-1.274568000	0.389869000
C	-4.682337000	-1.477216000	1.773571000
C	-4.921563000	-2.770016000	2.242129000
C	-5.171371000	-3.832403000	1.369408000
C	-5.208291000	-3.579831000	-0.005033000
C	-4.986818000	-2.302510000	-0.519131000
C	-4.339234000	-0.348694000	2.702936000
C	-5.348039000	-5.232254000	1.893351000
C	-5.006951000	-2.023058000	-1.994991000
C	2.800762000	2.699189000	1.126702000
C	2.535266000	3.772395000	0.269372000
C	1.792757000	4.837051000	0.783351000
C	1.295782000	4.825413000	2.090759000
C	1.565626000	3.719329000	2.902196000
C	2.331093000	2.646988000	2.444812000
C	3.019633000	3.757590000	-1.153496000
C	0.449956000	5.961736000	2.598700000
C	2.632904000	1.453587000	3.301694000
C	4.655238000	-1.517095000	-0.566743000
C	4.727149000	-1.589891000	-1.964583000
C	4.903566000	-2.847832000	-2.539873000
C	5.014220000	-4.002735000	-1.758827000
C	4.967556000	-3.878063000	-0.369387000
C	4.789775000	-2.641519000	0.253963000
C	4.607051000	-0.348219000	-2.803059000
C	5.136749000	-5.357464000	-2.403070000
C	4.750935000	-2.533594000	1.752806000
C	-1.756104000	-1.854006000	-0.335821000
C	-1.697275000	-2.982590000	-1.219754000
C	-1.623933000	-4.168989000	-0.436526000
C	-1.624443000	-3.786524000	0.938477000
C	-1.687836000	-2.367325000	1.001268000
C	1.624216000	-1.725691000	-0.187056000
C	1.625943000	-2.739063000	-1.199683000
C	1.610574000	-4.014684000	-0.569570000
C	1.577663000	-3.807862000	0.841992000
C	1.566594000	-2.402909000	1.076701000
C	-5.457470000	3.492026000	-0.990757000
C	-6.888317000	0.723619000	0.235941000
C	5.710505000	2.940855000	1.456613000
C	6.970121000	0.034608000	0.399024000
H	-0.196694000	4.896449000	-0.955505000
H	-1.553562000	3.379053000	-4.731705000

H	-2.419786000	2.683696000	1.068152000
H	-2.390286000	4.455396000	0.979253000
H	-0.882705000	3.534439000	1.093355000
H	0.668303000	5.858244000	-3.001152000
H	-0.086118000	5.473625000	-4.559780000
H	1.159035000	4.416226000	-3.894688000
H	-4.541603000	1.901350000	-3.552170000
H	-3.297517000	0.655689000	-3.503941000
H	-3.340666000	1.809166000	-4.853451000
H	-4.889394000	-2.954978000	3.313506000
H	-5.405237000	-4.398189000	-0.693820000
H	-4.390526000	-0.669627000	3.746025000
H	-5.011100000	0.506988000	2.576570000
H	-3.323046000	0.015621000	2.510714000
H	-5.728096000	-5.235333000	2.918974000
H	-4.386023000	-5.759290000	1.897714000
H	-6.034365000	-5.813001000	1.269785000
H	-5.698099000	-1.208806000	-2.239200000
H	-5.303027000	-2.908990000	-2.561274000
H	-4.013246000	-1.712597000	-2.337935000
H	1.603618000	5.700290000	0.149331000
H	1.172852000	3.688556000	3.914925000
H	2.808142000	4.706150000	-1.651515000
H	2.519727000	2.959829000	-1.715323000
H	4.096115000	3.566435000	-1.216844000
H	-0.612575000	5.753735000	2.424747000
H	0.687440000	6.899715000	2.088617000
H	0.580909000	6.110313000	3.674411000
H	2.267075000	1.595999000	4.319796000
H	3.707591000	1.242503000	3.337825000
H	2.129148000	0.575599000	2.881196000
H	4.952891000	-2.928579000	-3.623554000
H	5.052980000	-4.768153000	0.249644000
H	5.307379000	0.427016000	-2.472226000
H	3.598697000	0.075120000	-2.717378000
H	4.805292000	-0.563612000	-3.855566000
H	4.144097000	-5.800680000	-2.549601000
H	5.713021000	-6.048817000	-1.781200000
H	5.615428000	-5.296243000	-3.384737000
H	4.310194000	-3.432581000	2.189724000
H	4.161776000	-1.674099000	2.079715000
H	5.760520000	-2.423242000	2.166702000
H	-1.693135000	-2.927594000	-2.300969000
H	-1.546148000	-5.180464000	-0.814674000
H	-1.548962000	-4.458755000	1.783524000

H	-1.664112000	-1.751638000	1.890981000
H	1.653241000	-2.553341000	-2.264921000
H	1.599758000	-4.973141000	-1.072285000
H	1.530769000	-4.581490000	1.597768000
H	1.510603000	-1.908234000	2.037717000
H	-4.942093000	4.252507000	-0.393972000
H	-6.522712000	3.538758000	-0.759030000
H	-5.322334000	3.756691000	-2.044871000
H	-6.946616000	0.439838000	1.291785000
H	-7.302922000	-0.106469000	-0.346503000
H	-7.521106000	1.599383000	0.082256000
H	5.340342000	3.139331000	2.468125000
H	5.501722000	3.830406000	0.853343000
H	6.791983000	2.805461000	1.507867000
H	7.119633000	-0.824957000	1.059934000
H	7.670347000	0.817301000	0.695272000
H	7.221356000	-0.285982000	-0.617350000

Cartesian coordinates and energies (E_h) of **7 [bisNHCPSnCl]$^+$**

E(RB3PW91) = -8517.17593642
Sum of electronic and zero-point Energies= -8516.300440
Sum of electronic and thermal Energies= -8516.246005
Sum of electronic and thermal Enthalpies= -8516.245061
Sum of electronic and thermal Free Energies= -8516.391575

Sn	1.639310000	-0.233926000	-0.041352000
Cl	2.156191000	-0.490787000	-2.439511000
N	0.026343000	-3.417248000	0.317178000
N	-2.085641000	-2.965358000	-0.003329000
N	-0.654659000	3.586461000	0.183159000
N	1.517556000	3.350562000	0.244666000
N	-0.461388000	-1.162337000	-0.319148000
N	0.293796000	1.470314000	-0.556135000
C	-0.831327000	-2.398903000	-0.024715000
C	-0.685066000	-4.593708000	0.537378000
C	-1.985944000	-4.318901000	0.340194000
C	0.357679000	2.704608000	-0.090531000
C	-0.113798000	4.776872000	0.679050000
C	1.225036000	4.625799000	0.722196000
C	-1.471820000	-0.211974000	-0.800993000
C	-0.791878000	1.003207000	-1.415388000
C	1.446565000	-3.325624000	0.433861000
C	2.230027000	-3.513894000	-0.714766000
C	3.614293000	-3.391846000	-0.572809000

C	4.207026000	-3.132945000	0.666475000
C	3.389138000	-3.020743000	1.797988000
C	2.001743000	-3.105715000	1.706362000
C	1.585851000	-3.832361000	-2.032994000
C	5.694337000	-2.941089000	0.780195000
C	1.111149000	-2.913458000	2.901738000
C	-3.376609000	-2.351291000	-0.120815000
C	-4.089714000	-2.517973000	-1.316168000
C	-5.391124000	-2.021601000	-1.365947000
C	-5.982873000	-1.391392000	-0.265337000
C	-5.225921000	-1.226343000	0.896904000
C	-3.917925000	-1.706356000	0.996062000
C	-3.460064000	-3.209717000	-2.493837000
C	-7.418863000	-0.947042000	-0.336345000
C	-3.107015000	-1.552185000	2.252690000
C	-2.040053000	3.245457000	0.301686000
C	-2.436506000	2.427526000	1.367679000
C	-3.794361000	2.116444000	1.473382000
C	-4.734067000	2.612623000	0.568185000
C	-4.292728000	3.432459000	-0.476320000
C	-2.948649000	3.765500000	-0.630968000
C	-1.433299000	1.903499000	2.358365000
C	-6.196542000	2.294246000	0.703674000
C	-2.475020000	4.636618000	-1.761805000
C	2.830189000	2.802722000	0.087603000
C	3.532234000	2.404779000	1.236211000
C	4.792440000	1.832711000	1.057190000
C	5.337744000	1.641703000	-0.215670000
C	4.610857000	2.071919000	-1.330410000
C	3.357788000	2.671132000	-1.207368000
C	2.918962000	2.539091000	2.602663000
C	6.679038000	0.985418000	-0.398510000
C	2.578378000	3.112502000	-2.411708000
H	-0.175064000	-5.504478000	0.805910000
H	-2.869852000	-4.931268000	0.412438000
H	-0.750477000	5.601425000	0.955226000
H	2.010782000	5.300735000	1.019899000
H	-2.126786000	0.118968000	0.013577000
H	-2.109780000	-0.666070000	-1.566139000
H	-0.350582000	0.726138000	-2.380535000
H	-1.544519000	1.772991000	-1.598139000
H	4.240011000	-3.493988000	-1.455028000
H	3.843530000	-2.836287000	2.768197000
H	2.326646000	-3.858913000	-2.833331000
H	0.843062000	-3.075074000	-2.299813000

H	1.078791000	-4.803150000	-1.992075000
H	6.231344000	-3.461426000	-0.017143000
H	6.074874000	-3.299145000	1.740989000
H	5.941588000	-1.875728000	0.703900000
H	0.467097000	-2.035367000	2.766810000
H	1.698001000	-2.764458000	3.810329000
H	0.449718000	-3.772063000	3.057627000
H	-5.966399000	-2.144972000	-2.280568000
H	-5.671949000	-0.737152000	1.758959000
H	-2.494154000	-2.761037000	-2.751987000
H	-4.105672000	-3.157603000	-3.372844000
H	-3.265720000	-4.266476000	-2.280346000
H	-7.717549000	-0.386945000	0.552562000
H	-8.083945000	-1.813508000	-0.422115000
H	-7.600047000	-0.318081000	-1.214396000
H	-2.750031000	-2.522023000	2.615929000
H	-3.693582000	-1.087096000	3.048012000
H	-2.220004000	-0.931982000	2.079592000
H	-4.124821000	1.483883000	2.292967000
H	-5.016656000	3.823580000	-1.187308000
H	-1.930381000	1.480536000	3.233830000
H	-0.757603000	2.695312000	2.699195000
H	-0.810072000	1.120260000	1.909792000
H	-6.397225000	1.674239000	1.580358000
H	-6.560465000	1.759356000	-0.178606000
H	-6.789516000	3.210097000	0.796927000
H	-2.129155000	5.611364000	-1.400503000
H	-3.275410000	4.814264000	-2.482938000
H	-1.631320000	4.180146000	-2.290838000
H	5.348930000	1.505248000	1.931642000
H	5.023882000	1.927546000	-2.325062000
H	3.542649000	2.058661000	3.359191000
H	1.927912000	2.070754000	2.633600000
H	2.786466000	3.586767000	2.893124000
H	6.594060000	0.104610000	-1.043822000
H	7.110568000	0.670316000	0.555038000
H	7.388580000	1.668556000	-0.877761000
H	3.228168000	3.206410000	-3.283824000
H	2.084292000	4.074274000	-2.241350000
H	1.809168000	2.370140000	-2.650609000

Cartesian coordinates and energies (E_h) of **7 [bisNHCPSnCl]**$^+$, scrf=(cpcm,solvent=thf)

E(RB3PW91) = -8517.22414533
Sum of electronic and zero-point Energies= -8516.349355

Sum of electronic and thermal Energies= -8516.294895
Sum of electronic and thermal Enthalpies= -8516.293950
Sum of electronic and thermal Free Energies= -8516.439528

Sn	1.630189000	-0.261235000	-0.230046000
Cl	1.921026000	-0.590036000	-2.716381000
N	0.020311000	-3.379404000	0.380540000
N	-2.087803000	-2.960724000	0.008215000
N	-0.596832000	3.547542000	0.268598000
N	1.572265000	3.292169000	0.217769000
N	-0.475376000	-1.151474000	-0.343729000
N	0.296582000	1.463180000	-0.620148000
C	-0.840775000	-2.383257000	-0.011765000
C	-0.683037000	-4.555919000	0.630979000
C	-1.982406000	-4.300101000	0.401194000
C	0.391187000	2.673927000	-0.093408000
C	-0.021432000	4.710110000	0.792458000
C	1.315988000	4.547204000	0.767444000
C	-1.502045000	-0.197210000	-0.787545000
C	-0.850911000	1.028805000	-1.412551000
C	1.422217000	-3.237401000	0.603703000
C	2.307683000	-3.523392000	-0.446027000
C	3.672339000	-3.331101000	-0.206641000
C	4.147129000	-2.902597000	1.036780000
C	3.230829000	-2.693197000	2.075958000
C	1.859497000	-2.848003000	1.882487000
C	1.789923000	-4.016292000	-1.766870000
C	5.611309000	-2.640895000	1.259919000
C	0.864087000	-2.554285000	2.969478000
C	-3.377409000	-2.360505000	-0.175168000
C	-4.022570000	-2.521969000	-1.408980000
C	-5.307877000	-1.998292000	-1.537979000
C	-5.946156000	-1.343460000	-0.477573000
C	-5.262278000	-1.201185000	0.732349000
C	-3.973220000	-1.710832000	0.910566000
C	-3.332015000	-3.223115000	-2.545725000
C	-7.347897000	-0.823087000	-0.650881000
C	-3.235810000	-1.570905000	2.212995000
C	-1.982920000	3.222399000	0.426384000
C	-2.353913000	2.372691000	1.476630000
C	-3.713594000	2.083613000	1.625080000
C	-4.677336000	2.629599000	0.774769000
C	-4.260421000	3.480032000	-0.255945000
C	-2.916424000	3.794351000	-0.449853000
C	-1.324550000	1.791959000	2.406861000

C	-6.139010000	2.325073000	0.952131000
C	-2.468566000	4.699566000	-1.563812000
C	2.866477000	2.721462000	0.008325000
C	3.595451000	2.278471000	1.124281000
C	4.832014000	1.674085000	0.891025000
C	5.328582000	1.490361000	-0.403213000
C	4.580360000	1.969423000	-1.483888000
C	3.348896000	2.602028000	-1.305571000
C	3.036454000	2.396612000	2.515113000
C	6.626784000	0.767196000	-0.638893000
C	2.546036000	3.097029000	-2.473793000
H	-0.170584000	-5.449951000	0.946130000
H	-2.860902000	-4.919751000	0.476047000
H	-0.635862000	5.526709000	1.134256000
H	2.120078000	5.201004000	1.062548000
H	-2.128415000	0.119595000	0.053947000
H	-2.161703000	-0.641893000	-1.537648000
H	-0.482102000	0.777789000	-2.413699000
H	-1.605344000	1.808937000	-1.525747000
H	4.376853000	-3.518065000	-1.012772000
H	3.593909000	-2.375858000	3.050329000
H	2.595769000	-4.090262000	-2.499255000
H	1.030073000	-3.340204000	-2.169419000
H	1.328737000	-5.003999000	-1.656727000
H	6.223040000	-3.037481000	0.445995000
H	5.955853000	-3.083516000	2.199675000
H	5.795780000	-1.562445000	1.322534000
H	0.254761000	-1.679904000	2.709753000
H	1.366234000	-2.344558000	3.915929000
H	0.173206000	-3.389961000	3.119359000
H	-5.829294000	-2.110255000	-2.485705000
H	-5.746723000	-0.696872000	1.563976000
H	-2.373478000	-2.746843000	-2.782008000
H	-3.949092000	-3.212773000	-3.446474000
H	-3.110412000	-4.265927000	-2.294605000
H	-7.744067000	-0.408546000	0.279181000
H	-8.021352000	-1.621570000	-0.979907000
H	-7.385068000	-0.039635000	-1.416236000
H	-2.887258000	-2.542442000	2.578724000
H	-3.869711000	-1.122369000	2.980487000
H	-2.347140000	-0.939673000	2.099964000
H	-4.025020000	1.429009000	2.434590000
H	-5.002730000	3.909654000	-0.924408000
H	-1.796389000	1.346771000	3.285059000
H	-0.617987000	2.556092000	2.747582000

H	-0.737865000	1.011172000	1.908046000
H	-6.323828000	1.731909000	1.850838000
H	-6.523830000	1.766725000	0.093454000
H	-6.725210000	3.246866000	1.026647000
H	-2.076133000	5.645797000	-1.175631000
H	-3.296379000	4.929417000	-2.237706000
H	-1.664150000	4.241061000	-2.149169000
H	5.407561000	1.313795000	1.740031000
H	4.962694000	1.845795000	-2.493897000
H	3.680752000	1.889244000	3.236018000
H	2.039104000	1.946245000	2.576173000
H	2.934312000	3.440701000	2.828204000
H	6.434891000	-0.261536000	-0.965218000
H	7.233454000	0.719793000	0.269196000
H	7.216429000	1.251155000	-1.423241000
H	3.169814000	3.184859000	-3.365735000
H	2.094045000	4.071517000	-2.265350000
H	1.735731000	2.394058000	-2.696996000

Cartesian coordinates and energies (E_h) of **7 [bisNHCPSnCl]$^+$**, scrf=(cpcm,solvent=acetonitrile)

E(RB3PW91) = -8517.23072269
Sum of electronic and zero-point Energies= -8516.355989
Sum of electronic and thermal Energies= -8516.301543
Sum of electronic and thermal Enthalpies= -8516.300599
Sum of electronic and thermal Free Energies= -8516.446010

Sn	1.627936000	-0.262062000	-0.250304000
Cl	1.900047000	-0.588671000	-2.753828000
N	0.027381000	-3.372570000	0.404666000
N	-2.081935000	-2.960272000	0.035739000
N	-0.602145000	3.540030000	0.278007000
N	1.566806000	3.287496000	0.223369000
N	-0.471955000	-1.155047000	-0.349666000
N	0.292858000	1.461592000	-0.624460000
C	-0.835744000	-2.382876000	0.001805000
C	-0.674162000	-4.545643000	0.676004000
C	-1.974599000	-4.293456000	0.448345000
C	0.386195000	2.669889000	-0.089919000
C	-0.027512000	4.700393000	0.807669000
C	1.309951000	4.539310000	0.780526000
C	-1.503763000	-0.201626000	-0.784320000
C	-0.859544000	1.027529000	-1.409977000
C	1.430229000	-3.226774000	0.618301000
C	2.309451000	-3.523830000	-0.433443000

C	3.675566000	-3.328085000	-0.205002000
C	4.157494000	-2.884110000	1.030318000
C	3.247234000	-2.662207000	2.072316000
C	1.874769000	-2.821315000	1.889603000
C	1.782736000	-4.030343000	-1.745698000
C	5.623286000	-2.622994000	1.243800000
C	0.885788000	-2.517754000	2.979664000
C	-3.371828000	-2.366430000	-0.165537000
C	-4.000598000	-2.534071000	-1.406857000
C	-5.284013000	-2.010777000	-1.555461000
C	-5.935902000	-1.350875000	-0.506438000
C	-5.269330000	-1.205719000	0.712852000
C	-3.982619000	-1.714387000	0.910336000
C	-3.294346000	-3.240150000	-2.530817000
C	-7.332620000	-0.824914000	-0.702381000
C	-3.262891000	-1.570127000	2.222058000
C	-1.988751000	3.215264000	0.433423000
C	-2.361272000	2.364122000	1.481916000
C	-3.721418000	2.075930000	1.628650000
C	-4.683850000	2.623920000	0.778029000
C	-4.265372000	3.476138000	-0.250672000
C	-2.920891000	3.790049000	-0.442416000
C	-1.332912000	1.781526000	2.411975000
C	-6.145849000	2.319200000	0.953244000
C	-2.471071000	4.697714000	-1.553517000
C	2.861307000	2.718368000	0.012974000
C	3.588895000	2.269103000	1.127378000
C	4.827085000	1.668323000	0.892338000
C	5.326743000	1.494375000	-0.402056000
C	4.579672000	1.979350000	-1.481119000
C	3.346501000	2.608263000	-1.300722000
C	3.028653000	2.378971000	2.518342000
C	6.627438000	0.775994000	-0.639201000
C	2.544720000	3.111437000	-2.466322000
H	-0.160090000	-5.434452000	1.002960000
H	-2.852563000	-4.912153000	0.535944000
H	-0.642541000	5.514234000	1.154827000
H	2.113474000	5.192096000	1.079293000
H	-2.124876000	0.111022000	0.062506000
H	-2.167179000	-0.645076000	-1.531571000
H	-0.497957000	0.780872000	-2.414779000
H	-1.616186000	1.806315000	-1.515651000
H	4.375602000	-3.525441000	-1.012638000
H	3.615926000	-2.332106000	3.040295000
H	2.586672000	-4.129178000	-2.477431000

H	1.032130000	-3.349332000	-2.157734000
H	1.305914000	-5.008489000	-1.619306000
H	6.226548000	-2.991578000	0.410656000
H	5.980123000	-3.094347000	2.164991000
H	5.805202000	-1.546737000	1.339841000
H	0.268241000	-1.651704000	2.712219000
H	1.393936000	-2.290717000	3.918828000
H	0.201990000	-3.355982000	3.146682000
H	-5.792565000	-2.126274000	-2.509735000
H	-5.764970000	-0.698444000	1.535973000
H	-2.337602000	-2.758190000	-2.763037000
H	-3.903343000	-3.242894000	-3.437119000
H	-3.066596000	-4.278546000	-2.267292000
H	-7.748952000	-0.426030000	0.225772000
H	-7.999889000	-1.615234000	-1.062101000
H	-7.349952000	-0.027052000	-1.453521000
H	-2.921100000	-2.540621000	2.596651000
H	-3.906302000	-1.116888000	2.978718000
H	-2.371349000	-0.941454000	2.118556000
H	-4.034211000	1.420564000	2.436949000
H	-5.006647000	3.907466000	-0.919187000
H	-1.805710000	1.330642000	3.286663000
H	-0.629277000	2.545840000	2.758196000
H	-0.742853000	1.004677000	1.911178000
H	-6.331980000	1.727900000	1.852898000
H	-6.528866000	1.758711000	0.095102000
H	-6.732610000	3.240948000	1.024058000
H	-2.076847000	5.641757000	-1.161895000
H	-3.298445000	4.930964000	-2.226795000
H	-1.667321000	4.239375000	-2.139899000
H	5.401795000	1.304028000	1.740186000
H	4.965526000	1.865345000	-2.491037000
H	3.674087000	1.870025000	3.237073000
H	2.032510000	1.926033000	2.577321000
H	2.923637000	3.421487000	2.835471000
H	6.439468000	-0.256186000	-0.956888000
H	7.238153000	0.737547000	0.266588000
H	7.210887000	1.257363000	-1.429732000
H	3.166908000	3.195700000	-3.359792000
H	2.101383000	4.089206000	-2.254747000
H	1.726841000	2.416646000	-2.687758000

Cartesian coordinates and energies (E_h) of **7 [bisNHCPSnCl]$^+$[SnCl$_3$]$^-$**, scrf=(cpcm,solvent=THF)

E(RB3PW91) = -15919.1377496

Sum of electronic and zero-point Energies= -15918.259496

Sum of electronic and thermal Energies= -15918.196501
Sum of electronic and thermal Enthalpies= -15918.195557
Sum of electronic and thermal Free Energies= -15918.365376

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symmetry c1

Sn	2.143647000	-1.288530000	-0.133685000
Sn	-7.013528000	-1.122220000	-0.189017000
Cl	2.144622000	-1.767816000	-2.611516000
Cl	-5.086696000	-2.142609000	-1.428290000
Cl	-6.064478000	1.204462000	-0.273957000
Cl	-6.029821000	-1.607411000	2.079895000
N	-1.289656000	-1.506085000	0.673106000
N	-1.980763000	0.548731000	0.454402000
N	4.222230000	2.647509000	0.236016000
N	5.142597000	0.667046000	0.289709000
N	0.284806000	0.009178000	-0.310607000
N	2.920367000	0.749234000	-0.564460000
C	-0.904537000	-0.268987000	0.221802000
C	-2.588743000	-1.451560000	1.179659000
C	-3.014703000	-0.185478000	1.045761000
C	3.996373000	1.329739000	-0.059638000
C	5.511108000	2.793646000	0.759857000
C	6.074103000	1.570341000	0.798980000
C	0.560336000	1.386856000	-0.740696000
C	1.939804000	1.468905000	-1.374682000
C	-0.537538000	-2.712284000	0.563317000
C	-0.472588000	-3.348449000	-0.688391000
C	0.295912000	-4.510419000	-0.778769000
C	0.948255000	-5.050597000	0.335355000
C	0.800960000	-4.420011000	1.575857000
C	0.065476000	-3.242575000	1.715487000
C	-1.198777000	-2.774843000	-1.870419000
C	1.807893000	-6.277006000	0.188996000
C	-0.039347000	-2.526345000	3.032359000
C	-2.201139000	1.910059000	0.062651000
C	-2.677236000	2.160589000	-1.231636000
C	-2.947272000	3.485192000	-1.572556000
C	-2.778804000	4.530194000	-0.656270000
C	-2.318408000	4.229870000	0.628356000
C	-2.025520000	2.918906000	1.013102000
C	-2.879197000	1.028743000	-2.198018000
C	-3.098492000	5.945191000	-1.059507000
C	-1.542855000	2.585482000	2.396682000
C	3.222211000	3.668026000	0.334888000

C	2.303501000	3.601551000	1.390489000
C	1.343064000	4.613139000	1.475689000
C	1.298253000	5.663578000	0.556174000
C	2.246051000	5.696528000	-0.472974000
C	3.222038000	4.709489000	-0.603734000
C	2.351158000	2.478318000	2.389888000
C	0.248702000	6.735992000	0.651887000
C	4.230924000	4.737069000	-1.718426000
C	5.349900000	-0.738939000	0.138518000
C	5.340841000	-1.546693000	1.287750000
C	5.499409000	-2.921570000	1.112797000
C	5.645058000	-3.489087000	-0.157752000
C	5.665467000	-2.645313000	-1.272675000
C	5.534814000	-1.260351000	-1.151370000
C	5.106508000	-0.951848000	2.648645000
C	5.805687000	-4.976399000	-0.320334000
C	5.546067000	-0.360649000	-2.353233000
H	-3.088018000	-2.332068000	1.546692000
H	-3.963450000	0.275640000	1.260755000
H	5.881299000	3.761296000	1.056244000
H	7.050390000	1.243087000	1.116749000
H	0.509998000	2.078996000	0.108189000
H	-0.166025000	1.728698000	-1.482822000
H	1.916862000	0.993251000	-2.362131000
H	2.199905000	2.517977000	-1.520982000
H	0.385046000	-5.005658000	-1.742235000
H	1.291417000	-4.840569000	2.450138000
H	-1.146552000	-3.451150000	-2.725798000
H	-0.750629000	-1.821491000	-2.170119000
H	-2.250971000	-2.586793000	-1.632028000
H	1.334128000	-7.020441000	-0.459262000
H	2.014496000	-6.743419000	1.155739000
H	2.769501000	-6.015211000	-0.267091000
H	0.326235000	-1.496319000	2.944764000
H	0.547660000	-3.033034000	3.801202000
H	-1.076929000	-2.464964000	3.376511000
H	-3.314243000	3.706257000	-2.572110000
H	-2.193040000	5.030332000	1.352620000
H	-1.938658000	0.504163000	-2.405736000
H	-3.280377000	1.390241000	-3.147147000
H	-3.575877000	0.290112000	-1.788304000
H	-3.065941000	6.626341000	-0.205173000
H	-4.095621000	6.009347000	-1.507200000
H	-2.387355000	6.310117000	-1.809900000
H	-2.225430000	1.890875000	2.897479000

H	-1.459197000	3.483072000	3.013101000
H	-0.563338000	2.096191000	2.366372000
H	0.622374000	4.584477000	2.287762000
H	2.222648000	6.511546000	-1.192453000
H	1.734708000	2.704060000	3.262372000
H	3.374499000	2.292048000	2.732244000
H	1.983946000	1.542665000	1.950822000
H	-0.236542000	6.740149000	1.631162000
H	-0.528432000	6.576621000	-0.102515000
H	0.676332000	7.727576000	0.474951000
H	5.244480000	4.900065000	-1.336159000
H	4.006236000	5.534503000	-2.429696000
H	4.248139000	3.785781000	-2.261553000
H	5.479785000	-3.567819000	1.986815000
H	5.782543000	-3.073902000	-2.264691000
H	5.011592000	-1.734595000	3.403969000
H	4.187826000	-0.354108000	2.661078000
H	5.922701000	-0.286810000	2.949399000
H	5.373908000	-5.322669000	-1.263567000
H	5.328899000	-5.521981000	0.498567000
H	6.866942000	-5.252480000	-0.325477000
H	5.936707000	-0.883773000	-3.228489000
H	6.154961000	0.531803000	-2.177839000
H	4.527482000	-0.030457000	-2.584785000

Cartesian coordinates and energies (E_h) of **7** **[bisNHCPSnCl]$^+$[SnCl$_3$]$^-$**, scrf=(cpcm,solvent=acetonitrile)

E(RB3PW91) = -15919.1440922
Sum of electronic and zero-point Energies= -15918.266011
Sum of electronic and thermal Energies= -15918.202953
Sum of electronic and thermal Enthalpies= -15918.202009
Sum of electronic and thermal Free Energies= -15918.371804

Sn	2.147036000	-1.286603000	-0.170027000
Sn	-7.042523000	-1.133884000	-0.205267000
Cl	2.090147000	-1.727697000	-2.667404000
Cl	-5.113826000	-2.165192000	-1.437817000
Cl	-6.082949000	1.190229000	-0.297771000
Cl	-6.057908000	-1.606856000	2.068877000
N	-1.280518000	-1.499557000	0.698999000
N	-1.988131000	0.545938000	0.449046000
N	4.218267000	2.636313000	0.259908000
N	5.140316000	0.656807000	0.275677000
N	0.282791000	0.014792000	-0.304993000

N	2.916878000	0.751758000	-0.574322000
C	-0.903349000	-0.265737000	0.231113000
C	-2.582053000	-1.449351000	1.198739000
C	-3.018287000	-0.188775000	1.045506000
C	3.994004000	1.325014000	-0.059644000
C	5.507591000	2.774366000	0.784726000
C	6.071828000	1.551127000	0.800963000
C	0.556477000	1.395478000	-0.729285000
C	1.933445000	1.484673000	-1.368267000
C	-0.512139000	-2.698028000	0.624663000
C	-0.453316000	-3.379059000	-0.602687000
C	0.332858000	-4.532011000	-0.660901000
C	1.010710000	-5.017482000	0.463107000
C	0.869434000	-4.342807000	1.681533000
C	0.116321000	-3.173403000	1.787418000
C	-1.204333000	-2.859416000	-1.794592000
C	1.898108000	-6.227656000	0.354417000
C	0.018945000	-2.406759000	3.076133000
C	-2.210015000	1.905300000	0.052116000
C	-2.675699000	2.151746000	-1.246624000
C	-2.936224000	3.475981000	-1.596808000
C	-2.766318000	4.525106000	-0.685089000
C	-2.319827000	4.228376000	0.605447000
C	-2.037175000	2.917847000	0.999457000
C	-2.871656000	1.015749000	-2.209823000
C	-3.062571000	5.941557000	-1.100479000
C	-1.564116000	2.589860000	2.387623000
C	3.220248000	3.658122000	0.367151000
C	2.299238000	3.583211000	1.420066000
C	1.341576000	4.596989000	1.513635000
C	1.301311000	5.656580000	0.604444000
C	2.251013000	5.697070000	-0.422851000
C	3.225061000	4.709078000	-0.561062000
C	2.341378000	2.449734000	2.408066000
C	0.256411000	6.732815000	0.710451000
C	4.237304000	4.745831000	-1.672369000
C	5.347450000	-0.746494000	0.101162000
C	5.343991000	-1.572505000	1.236790000
C	5.508846000	-2.944506000	1.039166000
C	5.655849000	-3.490564000	-0.239853000
C	5.667844000	-2.628548000	-1.341940000
C	5.530218000	-1.246938000	-1.198216000
C	5.113611000	-1.001774000	2.608618000
C	5.826948000	-4.973235000	-0.432079000
C	5.535248000	-0.327472000	-2.385285000

H	-3.071540000	-2.328910000	1.581048000
H	-3.970874000	0.268000000	1.252154000
H	5.877324000	3.736695000	1.098414000
H	7.048318000	1.218947000	1.112825000
H	0.508324000	2.081304000	0.124572000
H	-0.172067000	1.741447000	-1.467001000
H	1.905234000	1.025661000	-2.363273000
H	2.193956000	2.535460000	-1.499841000
H	0.415543000	-5.063470000	-1.605534000
H	1.379655000	-4.721935000	2.563439000
H	-1.142485000	-3.559051000	-2.630454000
H	-0.784584000	-1.903548000	-2.125879000
H	-2.258917000	-2.690536000	-1.552111000
H	1.512538000	-6.943481000	-0.377070000
H	2.004863000	-6.736794000	1.316012000
H	2.900952000	-5.932202000	0.024873000
H	0.390782000	-1.383260000	2.947676000
H	0.605650000	-2.886248000	3.862293000
H	-1.017545000	-2.326146000	3.419459000
H	-3.291586000	3.694434000	-2.601168000
H	-2.193950000	5.031929000	1.326042000
H	-1.929630000	0.489856000	-2.407484000
H	-3.264065000	1.373823000	-3.164004000
H	-3.572009000	0.279512000	-1.801889000
H	-3.065624000	6.621390000	-0.244537000
H	-4.036796000	6.011256000	-1.595035000
H	-2.314630000	6.303842000	-1.815595000
H	-2.247800000	1.894291000	2.885521000
H	-1.487560000	3.489523000	3.001660000
H	-0.582836000	2.103725000	2.366288000
H	0.620419000	4.563085000	2.325056000
H	2.231320000	6.519301000	-1.134170000
H	1.721540000	2.667368000	3.280219000
H	3.363001000	2.259062000	2.752835000
H	1.975111000	1.518598000	1.958678000
H	-0.243322000	6.716352000	1.682243000
H	-0.509946000	6.598505000	-0.059828000
H	0.693180000	7.725507000	0.564363000
H	5.249362000	4.905782000	-1.284974000
H	4.014672000	5.549232000	-2.377504000
H	4.256595000	3.799060000	-2.223227000
H	5.496099000	-3.604137000	1.903171000
H	5.788347000	-3.041153000	-2.340479000
H	5.011034000	-1.798333000	3.348328000
H	4.201171000	-0.395187000	2.632935000

H	5.936455000	-0.350953000	2.922032000
H	5.273147000	-5.325745000	-1.307377000
H	5.485357000	-5.534009000	0.441865000
H	6.882180000	-5.222829000	-0.594276000
H	5.923006000	-0.835580000	-3.270663000
H	6.144040000	0.562478000	-2.197659000
H	4.515754000	0.007329000	-2.606449000

Cartesian coordinates and energies (E_h) of **bisNHCP**

E(RB3PW91) = -2035.97364634
Sum of electronic and zero-point Energies= -2035.102159
Sum of electronic and thermal Energies= -2035.051581
Sum of electronic and thermal Enthalpies= -2035.050637
Sum of electronic and thermal Free Energies= -2035.187156

N	-0.440370000	2.425757000	-1.160744000
N	1.532529000	2.202887000	-0.178681000
N	0.440436000	-2.426131000	-1.160353000
N	-1.532507000	-2.202484000	-0.178563000
N	-0.507197000	1.401035000	0.959591000
N	0.507372000	-1.401500000	0.960016000
C	0.163170000	1.938764000	0.008436000
C	0.526524000	2.956292000	-2.015879000
C	1.725063000	2.823971000	-1.420629000
C	-0.163064000	-1.938926000	0.008731000
C	-0.526559000	-2.956109000	-2.015712000
C	-1.725126000	-2.823375000	-1.420606000
C	0.134173000	0.755885000	2.083142000
C	-0.134037000	-0.756018000	2.083361000
C	-1.840181000	2.500207000	-1.412417000
C	-2.392979000	1.705005000	-2.428591000
C	-3.749230000	1.844493000	-2.723102000
C	-4.570651000	2.720024000	-2.010619000
C	-3.996630000	3.476732000	-0.988581000
C	-2.637408000	3.393013000	-0.679389000
C	-1.564256000	0.659808000	-3.115651000
C	-6.044231000	2.805978000	-2.307154000
C	-2.049265000	4.220642000	0.422949000
C	2.524351000	2.312322000	0.848490000
C	3.530121000	1.338708000	0.933217000
C	4.507681000	1.488234000	1.918051000
C	4.501683000	2.565955000	2.806792000
C	3.489153000	3.520392000	2.687286000
C	2.495241000	3.416572000	1.712871000

C	3.497452000	0.151014000	0.025146000
C	5.544249000	2.678022000	3.887726000
C	1.397572000	4.435454000	1.606969000
C	1.840225000	-2.500603000	-1.412093000
C	2.637429000	-3.393552000	-0.679302000
C	3.996662000	-3.477270000	-0.988636000
C	4.570612000	-2.720411000	-2.010551000
C	3.749184000	-1.844579000	-2.722739000
C	2.393011000	-1.705091000	-2.428083000
C	2.049343000	-4.221300000	0.422977000
C	6.044075000	-2.806364000	-2.307687000
C	1.564214000	-0.659597000	-3.114594000
C	-2.524351000	-2.311992000	0.848580000
C	-2.495232000	-3.416255000	1.712940000
C	-3.489164000	-3.520103000	2.687335000
C	-4.501725000	-2.565700000	2.806819000
C	-4.507732000	-1.487968000	1.918088000
C	-3.530141000	-1.338395000	0.933294000
C	-1.397552000	-4.435124000	1.607023000
C	-5.544326000	-2.677804000	3.887717000
C	-3.497486000	-0.150702000	0.025214000
H	0.253594000	3.372113000	-2.972455000
H	2.713936000	3.104041000	-1.746747000
H	-0.253660000	-3.371930000	-2.972297000
H	-2.714062000	-3.103049000	-1.746869000
H	-0.285825000	1.165777000	3.013573000
H	1.217894000	0.906154000	2.132946000
H	0.285936000	-1.165652000	3.013912000
H	-1.217761000	-0.906277000	2.133165000
H	-4.181159000	1.227974000	-3.508922000
H	-4.620045000	4.163147000	-0.419118000
H	-0.692992000	1.083058000	-3.624287000
H	-2.154775000	0.109005000	-3.852255000
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H	-6.594186000	2.017808000	-1.778021000
H	-6.247102000	2.681558000	-3.375461000
H	-6.463680000	3.765841000	-1.991571000
H	-1.773641000	3.566707000	1.257959000
H	-2.755504000	4.976650000	0.775269000
H	-1.135345000	4.723899000	0.093385000
H	5.288976000	0.735071000	1.996601000
H	3.472227000	4.369999000	3.367053000
H	2.596757000	-0.445329000	0.223490000
H	4.369939000	-0.491990000	0.161886000
H	3.457636000	0.448531000	-1.026003000

H	5.707898000	3.718750000	4.183297000
H	6.503453000	2.261725000	3.564902000
H	5.236036000	2.127595000	4.785175000
H	0.443761000	4.003532000	1.927800000
H	1.264223000	4.768691000	0.572181000
H	1.604586000	5.309913000	2.228972000
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H	4.181133000	-1.227812000	-3.508360000
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H	2.755645000	-4.977259000	0.775279000
H	6.593081000	-2.012315000	-1.786430000
H	6.245627000	-2.691280000	-3.377320000
H	6.465608000	-3.762539000	-1.983874000
H	0.693622000	-1.082799000	-3.624446000
H	2.154985000	-0.107562000	-3.850069000
H	1.187281000	0.056704000	-2.377065000
H	-3.472226000	-4.369714000	3.367098000
H	-5.289062000	-0.734839000	1.996618000
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H	-1.264148000	-4.768266000	0.572210000
H	-1.604609000	-5.309642000	2.228930000
H	-5.707799000	-3.718519000	4.183431000
H	-6.503591000	-2.261734000	3.564780000
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H	-3.458086000	-0.448201000	-1.025959000
H	-2.596593000	0.445437000	0.223261000
H	-4.369799000	0.492476000	0.162240000

Cartesian coordinates and energies (E_h) of **bisNHCPS**, scrf=(cpcm,solvent=THF)

E(RB3PW91) = -2035.98526287
Sum of electronic and zero-point Energies= -2035.115023
Sum of electronic and thermal Energies= -2035.064248
Sum of electronic and thermal Enthalpies= -2035.063304
Sum of electronic and thermal Free Energies= -2035.200665

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N	-1.523745000	-2.254350000	-0.179315000
N	-0.447197000	2.469348000	-1.159033000
N	1.523717000	2.254331000	-0.179240000
N	0.507126000	-1.416315000	0.948574000
N	-0.507217000	1.416123000	0.948536000
C	-0.158672000	-1.977600000	0.002983000

C	-0.514669000	-3.014502000	-2.011573000
C	-1.714232000	-2.886929000	-1.417651000
C	0.158643000	1.977490000	0.003028000
C	0.514636000	3.014563000	-2.011458000
C	1.714199000	2.886950000	-1.417555000
C	-0.146552000	-0.753920000	2.055785000
C	0.146270000	0.753668000	2.055833000
C	1.848731000	-2.530339000	-1.407769000
C	2.403108000	-1.709697000	-2.402278000
C	3.763642000	-1.834042000	-2.687493000
C	4.584838000	-2.720689000	-1.987254000
C	4.006362000	-3.508871000	-0.989945000
C	2.643340000	-3.439637000	-0.691930000
C	1.570248000	-0.662779000	-3.082014000
C	6.061915000	-2.789357000	-2.270997000
C	2.044870000	-4.303899000	0.377857000
C	-2.518320000	-2.347895000	0.845731000
C	-3.548057000	-1.396159000	0.885794000
C	-4.529910000	-1.527883000	1.869673000
C	-4.505195000	-2.569672000	2.801782000
C	-3.469548000	-3.504794000	2.725405000
C	-2.471380000	-3.417713000	1.752274000
C	-3.541401000	-0.247176000	-0.073431000
C	-5.553606000	-2.664405000	3.878777000
C	-1.356260000	-4.420941000	1.688006000
C	-1.848748000	2.530308000	-1.407727000
C	-2.643365000	3.439500000	-0.691757000
C	-4.006383000	3.508784000	-0.989767000
C	-4.584851000	2.720766000	-1.987211000
C	-3.763645000	1.834248000	-2.687599000
C	-2.403112000	1.709851000	-2.402393000
C	-2.044908000	4.303594000	0.378174000
C	-6.061928000	2.789474000	-2.270942000
C	-1.570249000	0.663077000	-3.082348000
C	2.518327000	2.347883000	0.845779000
C	2.471503000	3.417788000	1.752229000
C	3.469727000	3.504898000	2.725298000
C	4.505322000	2.569720000	2.801703000
C	4.529941000	1.527864000	1.869669000
C	3.548036000	1.396116000	0.885844000
C	1.356439000	4.421076000	1.687943000
C	5.553786000	2.664475000	3.878644000
C	3.541273000	0.247052000	-0.073282000
H	-0.239526000	-3.433799000	-2.966139000
H	-2.700657000	-3.177237000	-1.742494000

H	0.239492000	3.433913000	-2.966001000
H	2.700622000	3.177278000	-1.742385000
H	0.241774000	-1.166309000	2.999838000
H	-1.234224000	-0.883866000	2.081878000
H	-0.242200000	1.166024000	2.999845000
H	1.233929000	0.883592000	2.082120000
H	4.198349000	-1.197952000	-3.455720000
H	4.628791000	-4.207580000	-0.434541000
H	0.699198000	-1.088120000	-3.588933000
H	2.157292000	-0.107467000	-3.817603000
H	1.193924000	0.051759000	-2.342089000
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H	-2.157203000	0.108145000	-3.818297000
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H	5.330859000	0.792530000	1.911930000
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H	1.215270000	4.790342000	0.666744000
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H	5.265087000	2.072175000	4.755606000
H	3.504312000	0.586998000	-1.111913000
H	2.649940000	-0.372194000	0.088611000
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Cartesian coordinates and energies (E_h) of **bisNHCPS**, scrf=(cpcm,solvent=acetonitrile)

E(RB3PW91) = -2035.98706972
Sum of electronic and zero-point Energies= -2035.116981
Sum of electronic and thermal Energies= -2035.066189
Sum of electronic and thermal Enthalpies= -2035.065245
Sum of electronic and thermal Free Energies= -2035.202783

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N	-1.523927000	-2.262134000	-0.179507000
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N	0.505995000	-1.418972000	0.946278000
C	0.159405000	1.984617000	0.001895000
C	0.514525000	3.025282000	-2.010528000
C	1.714253000	2.897351000	-1.417094000
C	-0.159457000	-1.984237000	0.001870000
C	-0.514653000	-3.025052000	-2.010465000
C	-1.714367000	-2.897007000	-1.417027000
C	0.149186000	0.753471000	2.050613000
C	-0.149131000	-0.753137000	2.050605000
C	-1.848535000	2.536983000	-1.406847000
C	-2.403521000	1.711765000	-2.397156000
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C	-4.585542000	2.722977000	-1.982880000
C	-4.005961000	3.516880000	-0.990472000
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C	-1.570460000	0.664033000	-3.075429000
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C	2.519021000	2.352788000	0.845124000
C	3.552752000	1.404977000	0.877400000
C	4.535539000	1.533781000	1.860901000
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C	3.468280000	3.500573000	2.731596000
C	2.469289000	3.416432000	1.758881000
C	3.550711000	0.262595000	-0.090120000

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C	-3.468022000	-3.500324000	2.731761000
C	-4.507729000	-2.568944000	2.800590000
C	-4.535514000	-1.533609000	1.861170000
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H	5.693301000	3.691183000	4.218379000

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H	4.200694000	-1.195125000	-3.445051000
H	1.139134000	-4.823190000	0.005552000
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