Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

for

Phosphanyl-substituted tin half-sandwich complexes

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1. Experimental Details

All manipulations were carried out under an argon inert gas atmosphere (argon 5.0), using either standard Schlenk line techniques or a glovebox. Tin(II) chloride and trimethylsilyltriflate were purchased from abcr and used as received. Platinum(II) chloride and (1,5-cyclooctadiene)palladium(II) chloride were purchased from Carbolution and used as received. Silver tetrakis(perfluoro-*tert*-butoxy)aluminate was synthesized according to a literature procedure.[1] Diphosphanylstannocene, **dippSn**, was prepared as reported before.[2]

NMR-spectra were recorded on Bruker Avance III 300 (solution), Bruker Avance III 400 (solution) and Bruker Ascend 400WB (solid state) spectrometers. ^{1}H and ^{13}C NMR spectra were referenced using the solvent signals[3] and ^{19}F, ^{31}P NMR and ^{119}Sn NMR spectra were referenced using external standards (δ ^{19}F ($CFCl_3$) = 0; δ ^{27}Al (1.1 M $Al(NO_3)_3$ in D_2O) = 0; δ ^{31}P (85% H_3PO_4 in H_2O) = 0; δ ^{119}Sn ($SnMe_4$) = 0).

Elemental analysis were performed with a Elementar vario micro cube.

HRMS measurements were recorded on a Q-TOF Premiere instrument from Waters, Manchester, England, in LIFDI(+) mode, by Linden CMS, Weyhe, Germany.

Single crystal X-ray diffraction analysis were carried out on a Bruker AXS X8 Apex CCD diffractometer and a Bruker D8 Venture diffractometer with a microfocus sealed tube and a Photon II detector operating with graphite monochromated Mo Kα radiation. Data were corrected for absorption effects using the multi-scan method. Structure solution was conducted with direct methods using SHELXT and refinement by full matrix least squares calculations on F^2 using SHELXL2018 in the graphical user interface SHELXLE.[4]

Synthesis of (diisopropylphosphanyl)cyclopentadienyltin(II) chloride 1a

1,1'-bis(diisopropylphosphanylcyclopentadienyl)tin, **dippSn**, (3.24 g; 6.73 mmol) and tin(II) chloride (1.28 g; 6.73 mmol) were mixed and ~100 mL of thf were added. The mixture was stirred overnight. Afterwards the solvent was removed in *vacuo* and the light yellow residue was washed with 250 mL hexane and dried in *vacuo* to obtain **1a** as a colorless solid.

Yield: 4.00 g; 88%.

^{1}H-NMR (400.13 MHz, 298 K, CD_2Cl_2): δ = 6.33 (d, 2H, J_{HH} = 2.3 Hz, CpH), 6.14 (d, 2H, J_{HH} = 2.0 Hz, CpH), 2.35 (sept, 2H, J_{HH} = 6.7 Hz, CH), 1.21 (d, 3H, J_{HH} = 7.1 Hz, CH_3), 1.17 (d, 3H, J_{HH} = 7.1 Hz, CH_3), 1.11 (d, 3H, J_{HH} = 6.9 Hz, CH_3), 1.08 (d, 3H, J_{HH} = 6.8 Hz, CH_3).

^{13}C{^{1}H}-NMR (100.62 MHz, 298 K, CD_2Cl_2): δ = 118.6 (d, J_{CP} = 10 Hz, CpC), 113.7 (d, J_{CP} = 6.3 Hz, CpC), 24.3 (d, J_{CP} = 4.7 Hz, CH), 19.5 (bs, CH_3).

^{13}C{^{1}H}-CP-MAS(13 kHz)-NMR (100.67 MHz, 298 K): δ = 120.6, 115.9, 107.1, 100.0, 24.1, 22.3, 20.8, 18.9, 16.4.

^{31}P{^{1}H}-NMR (161.98 MHz, 298 K, CD_2Cl_2): δ = 3.6.

^{31}P{^{1}H}-CP-MAS(13 kHz)-NMR (162.04 MHz, 298 K): δ = 4.3 ($^{1}J_{PSn}$ = 950 Hz).

^{119}Sn{^{1}H}-CP-MAS(13 kHz)-NMR (149.17 MHz, 298 K). δ = -709.

LIFDI-MS: m/z = 635.00 ($C_{22}H_{36}ClP_2Sn_2^+$), 335.98 ($C_{11}H_{18}ClPSn^+$).

Synthesis of (diisopropylphosphanyl)cyclopentadienyltin(II) triflate 1b

1a (1.00 g; 2.98 mmol) was suspended in 50 mL *o*-difluorobenzene and trimethylsilyltriflate (663 mg; 2.98 mmol) was added. After stirring the mixture at 343 K overnight, the solvent was removed in *vacuo* and the residue was taken up in 20 mL dichloromethane. To this solution, 40 mL hexane was added, and the solution was stored at 253 K overnight yielding colorless crystals of **1b**.

Yield: 400 mg; 30%.

^{1}H-NMR (400.13 MHz, 298 K, CD_2Cl_2): δ = 6.76 (s, 2H, CpH), 6.46-6.43 (m, 2H, CpH), 2.74 (oct, 2H, J_{HH} = 7.1 Hz, CH), 1.31 (d, 3H, J_{HH} = 7.1 Hz, CH_3), 1.28-1.24 (m, 6H, CH_3), 1.22 (d, 3H, J_{HH} = 7.1 Hz, CH_3).

^{13}C{^{1}H}-NMR (75.48 MHz, 298 K, CD_2Cl_2): δ = 120.2 (q, J_{CF} = CF_3), 118.7 (d, J_{CP} = 8.1 Hz, CpC), 112.9 (bs, CpC), 24.8 (d, J_{CP} = 8.9 Hz, CH), 19.3 (s, CH_3), 19.0 (d, J_{CP} = 5.6 Hz, CH_3).

^{19}F{^{1}H}-NMR (282.38 MHz, 298 K, CD_2Cl_2): δ = -78.3.

^{31}P{^{1}H}-NMR (161.98 MHz, 298 K, CD_2Cl_2): δ = 19.8.

^{31}P{^{1}H}-CP-MAS(13 kHz)-NMR (162.04 MHz, 298 K): δ = 19.2 ($^{1}J_{PSn}$ = 1460 Hz).

^{119}Sn{^{1}H}-CP-MAS(13 kHz)-NMR (149.17 MHz, 298 K). δ = -928.

Elemental analysis: calculated for $C_{12}H_{18}F_3O_3PSSn$: C: 32.10%, H: 4.04%, S: 7.14%; found: C: 32.20%, H: 4.17%, S: 6.86%.

Synthesis of palladium complex 2a

(1,5-cyclooctadiene)palladium(II) chloride (213 mg; 0.75 mmol) and **1a** (500 mg; 1.49 mmol) were mixed in 50 mL thf and stirred overnight. The yellow solution was reduced to approximately half of its volume and the same amount of hexane was added. The resulting solution was stored at 253 K to obtain **2a** in the form of red crystals.

Yield: 312 mg; 25%.

^{1}H-NMR (400.13 MHz, 298 K, CD_2Cl_2): δ = 6.70 (s, 2H, CpH), 6.25-5.75 (br, 3H, CpH), 2.77-2.65 (m, 2H, CH), 1.45-1.26 (m, 6H, CH_3), 1.16-1.01 (m, 6H, CH_3).

^{13}C{^{1}H}-NMR (100.62 MHz, 298 K, CD_2Cl_2): δ = 141.1 (s, CpC), 136.6 (s, CpC), 132.5 (bs, CpC), 129.7 (s, CpC), 71.1 (s, CpC), 27.0 (s, CH), 20.3-18.3 (m, CH_3).

^{31}P{^{1}H}-NMR (161.98 MHz, 298 K, CD_2Cl_2): δ = 41.7 ($^{2}J_{PSn}$ = 226 Hz).

^{119}Sn{^{1}H}-NMR (149.21 MHz, 298 K, CD_2Cl_2): δ = 85.3 ($^{2}J_{SnP}$ = 226 Hz).

Elemental analysis: calculated for $C_{22}H_{36}Cl_4P_2PdSn_2$: C: 31.16%, H: 4.28%; found: C: 30.94%, H: 4.25%.

Synthesis of platinum complex 2b

Platinum(II) chloride (198 mg; 0.75 mmol) and **1a** (500 mg; 1.49 mmol) were mixed in 50 mL thf and stirred overnight. The yellow solution was reduced to approximately half of its volume and the same amount of hexane was added. The resulting solution was stored at 253 K to obtain **2b** in the form of yellow crystals.

Yield: 356 mg; 26%.

^{1}H-NMR (400.13 MHz, 298 K, CD_2Cl_2): δ = 7.56-7.11 (br, 1H, CpH), 7.07-6.43 (br, 3H, CpH), 4.84-4.28 (br, 1H, CpH), 2.95-2.86 (m, 2H, CH), 1.33 (q, 6H, *J* = 8.2 Hz, CH_3), 1.08 (br, 6H, CH_3).

^{13}C{^{1}H}-NMR (100.62 MHz, 298 K, CD_2Cl_2): δ = 141.2 (br, CpC), 137.3 (br, CpC), 133.0 (s, J_{CPt} = 59 Hz, CpC), 129.4 (br, CpC), 76.4 (br, CpC), 28.6 (br, CH), 26.1 (br, CH), 19.2 (br, CH_3).

^{31}P{^{1}H}-NMR (161.98 MHz, 298 K, CD_2Cl_2): δ = 32.4 ($^{1}J_{PPt}$ = 2092 Hz, $^{2}J_{PSn}$ = 202 Hz).

^{119}Sn{^{1}H}-NMR (149.21 MHz, 298 K, CD_2Cl_2): δ = 42.8 ($^{2}J_{SnP}$ = 202 Hz).

Elemental analysis: calculated for $C_{22}H_{36}Cl_4P_2PtSn_2$: C: 28.21%, H: 3.87%; found: C: 28.28%, H: 3.54%.

Synthesis of silverchloride complex 3

1a (200 mg; 0.60 mmol) and silver tetrakis(perfluoro-*tert*-butoxy)aluminate (641 mg; 0.60 mmol) were stirred in 30 mL *o*-difluorobenzene at room temperature for two hours. After filtration of the obtained suspension, 30 mL toluene were added to the filtrate and the solution was stored at 253 K overnight affording colorless crystals of **3**.

Yield: 348 mg; 22%.

^{1}H-NMR (400.13 MHz, 298 K, CD_2Cl_2): δ = 7.03 (s, 2H, CpH), 6.75 (s, 2H, CpH), 2.63-2.52 (m, 2H, CH), 1.35-1.20 (m, 12H, CH_3).

^{13}C{^{1}H}-NMR (75.48 MHz, 298 K, CD_2Cl_2): δ = 121.8 (q, J_{CF} = 293 Hz, CF_3), 119.6 (s, CpC), 118.5 (s, CpC), 117.4 (s, CpC), 110.1-109.6 (m, CpC), 24.4-24.1 (m, CH), 20.4-20.1 (m, CH_3).

^{19}F{^{1}H}-NMR (282.38 MHz, 298 K, CD_2Cl_2): δ = -75.6.

^{27}Al{^{1}H}-NMR (78.20 MHz, 298 K, CD_2Cl_2) δ = 34.8.

^{31}P{^{1}H}-NMR (161.98 MHz, 298 K, CD_2Cl_2): δ = 27.9 ($^{1}J_{PAg}$ = 471 Hz (^{107}Ag), $^{1}J_{PAg}$ = 544 Hz (^{109}Ag)).

^{119}Sn{^{1}H}- NMR (149.21 MHz, 298 K). δ = -2122.

Elemental analysis: calculated for $C_{54}H_{36}AgAl_2ClF_{72}O_8P_2Sn_2$: C: 24.22%, H: 1.36%; found: C: 24.80%, H: 1.47%.

2. NMR Spectra

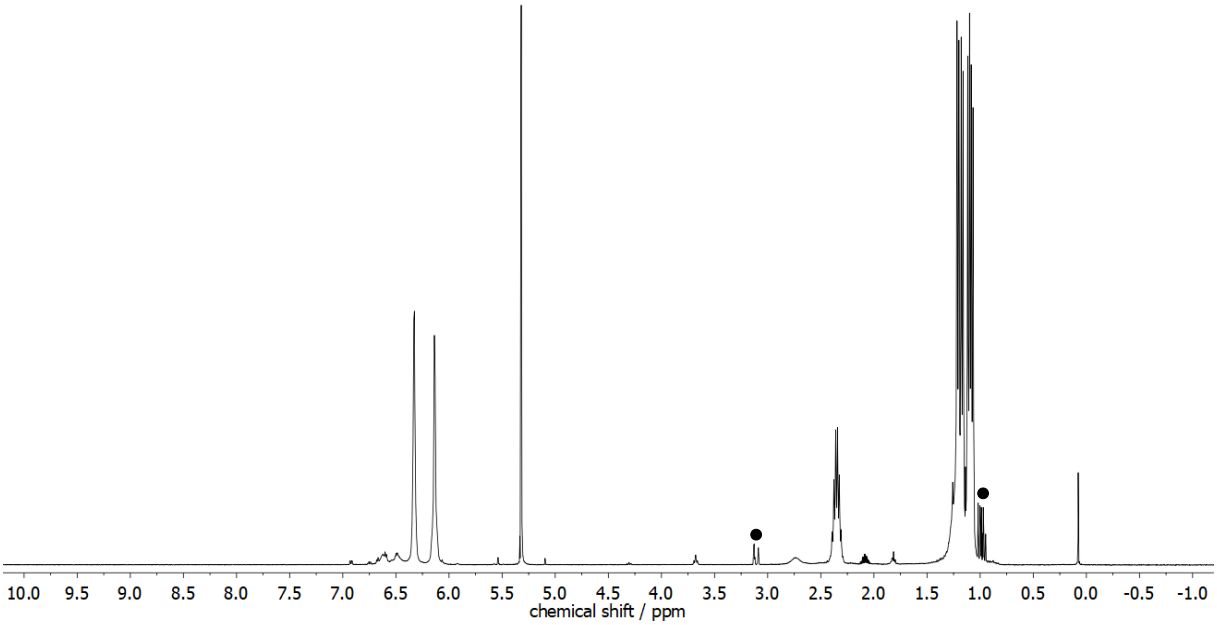


Figure S1: ^{1}H NMR spectrum (CD_2Cl_2) of **1a** (● free ligand).

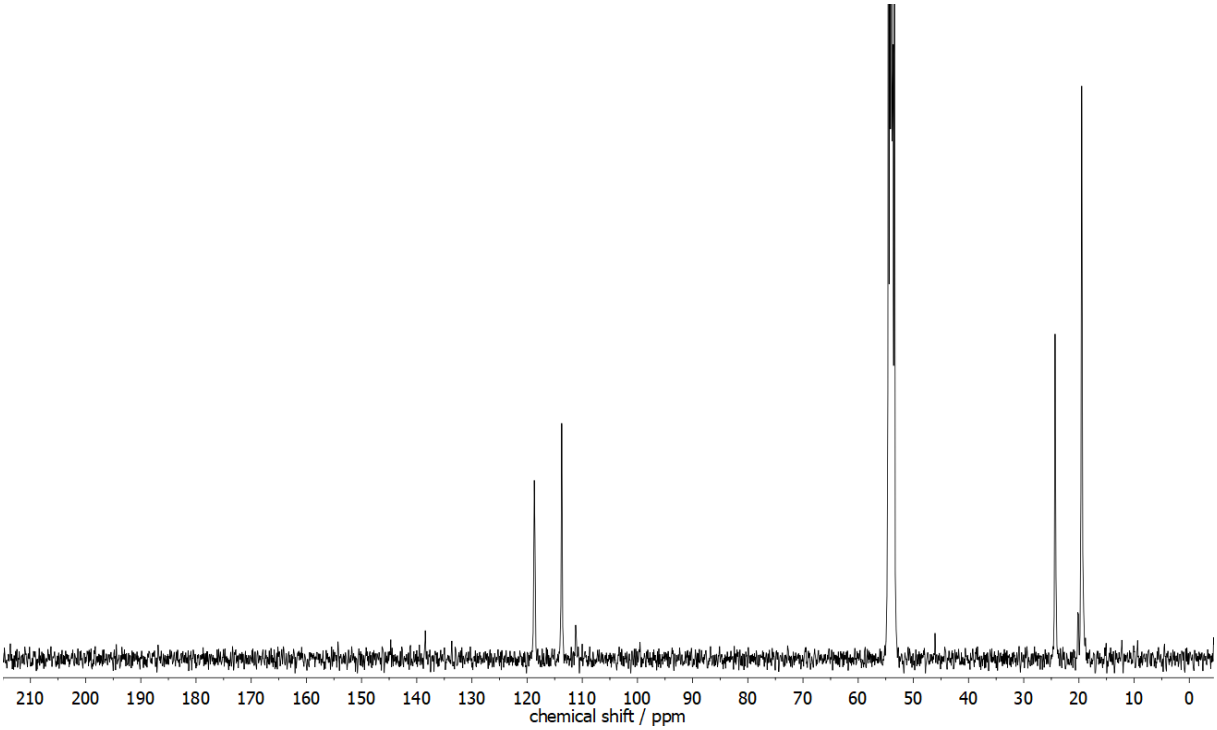


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **1a**.

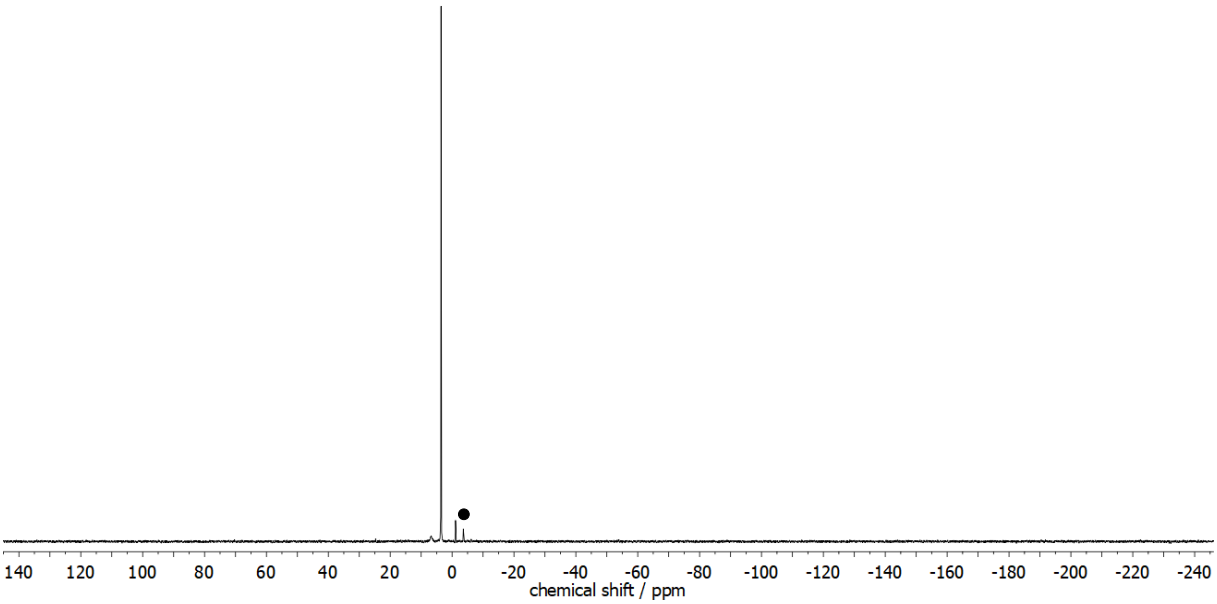


Figure S3: $^{31}P\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **1a** (● free ligand).

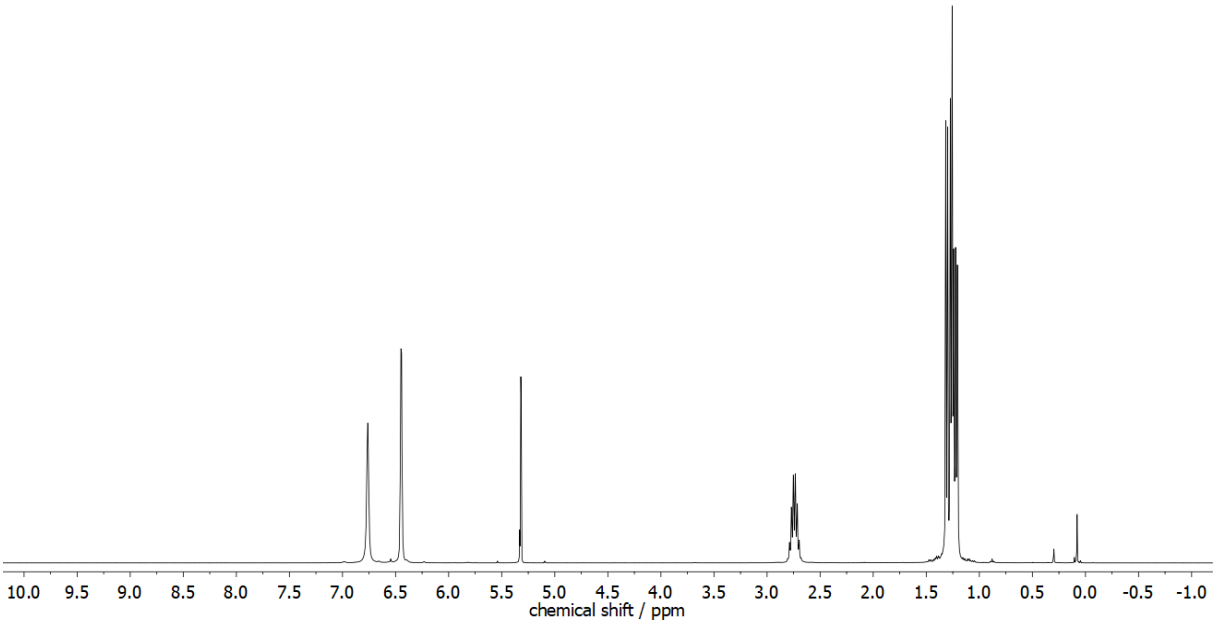


Figure S4: ^{1}H NMR spectrum (CD_2Cl_2) of **1b**.

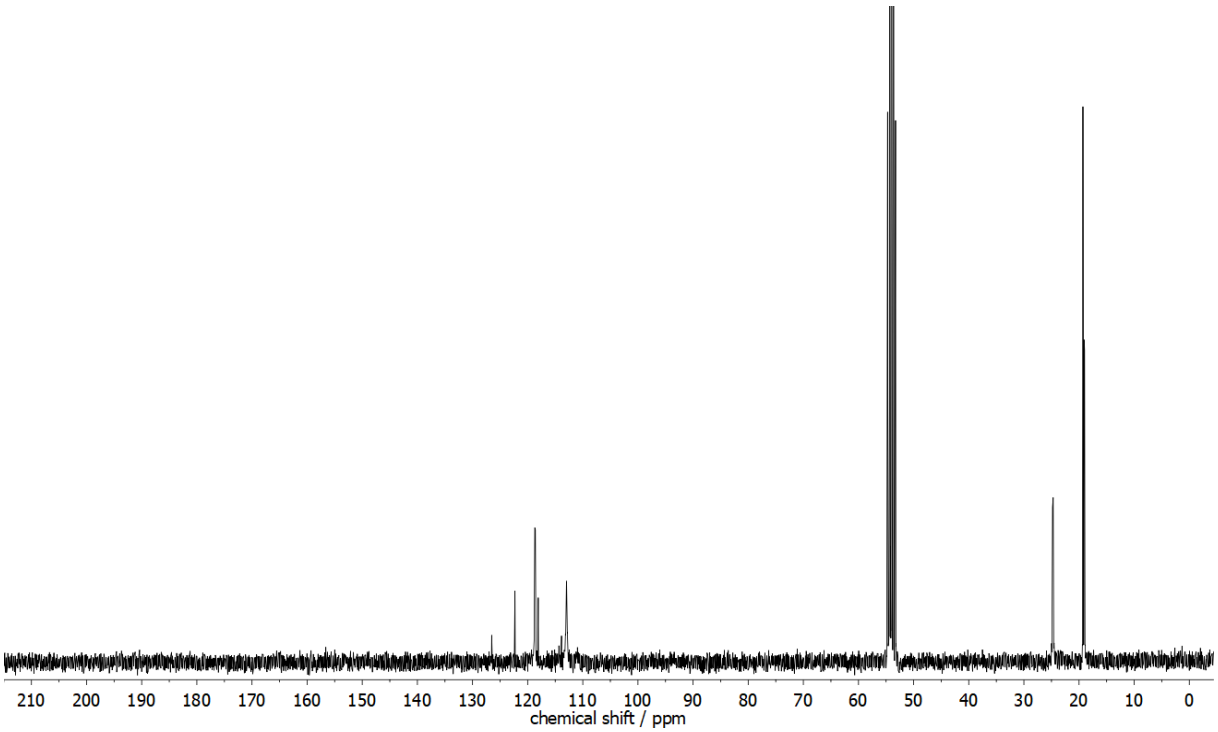


Figure S5: $^{13}C\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **1b**.

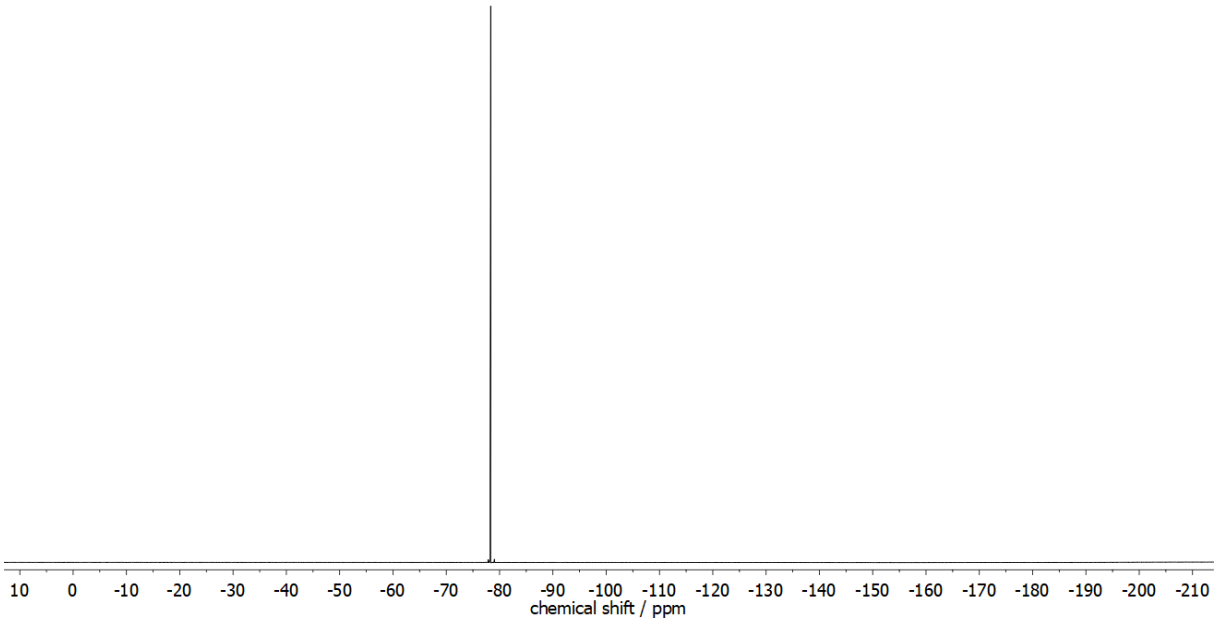


Figure S6: $^{19}F\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **1b**.

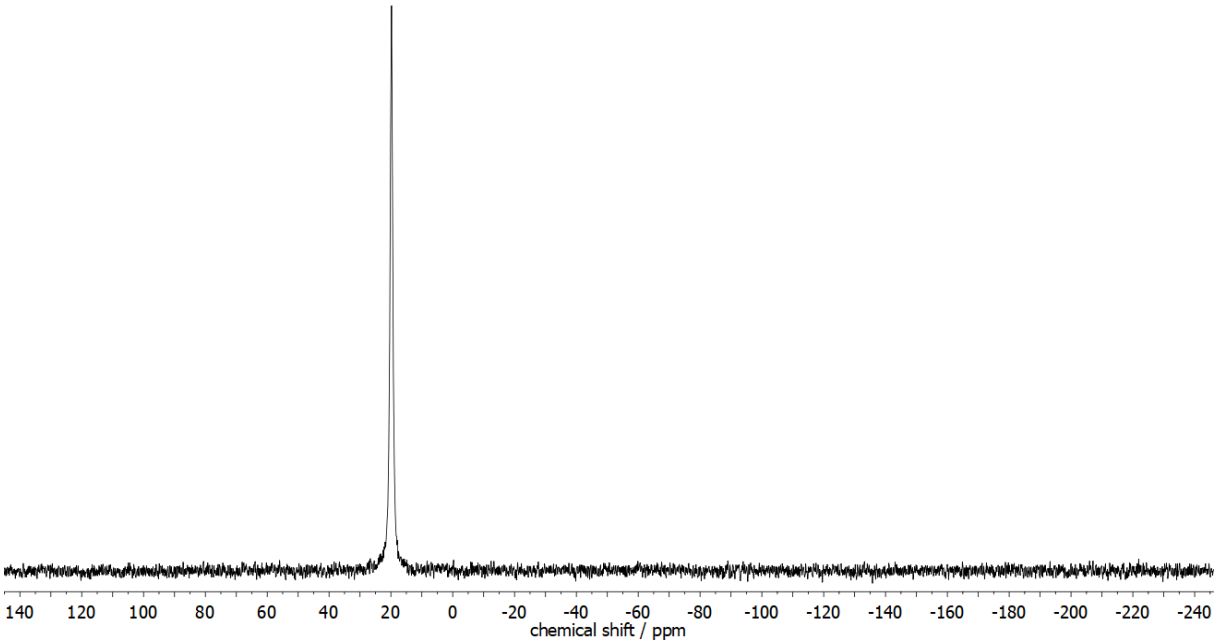


Figure S7: $^{31}P\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **1b**.

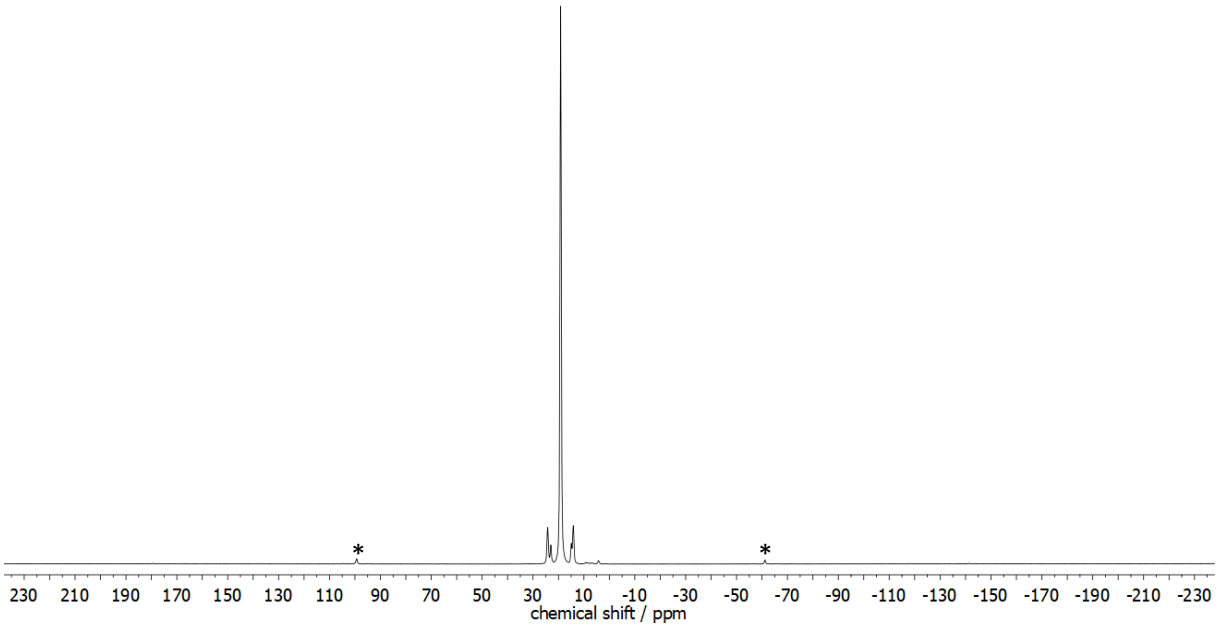


Figure S8: $^{31}P\{^{1}H\}$ CP/MAS NMR spectrum (13 kHz) of **1b** (* = spinning sidebands).

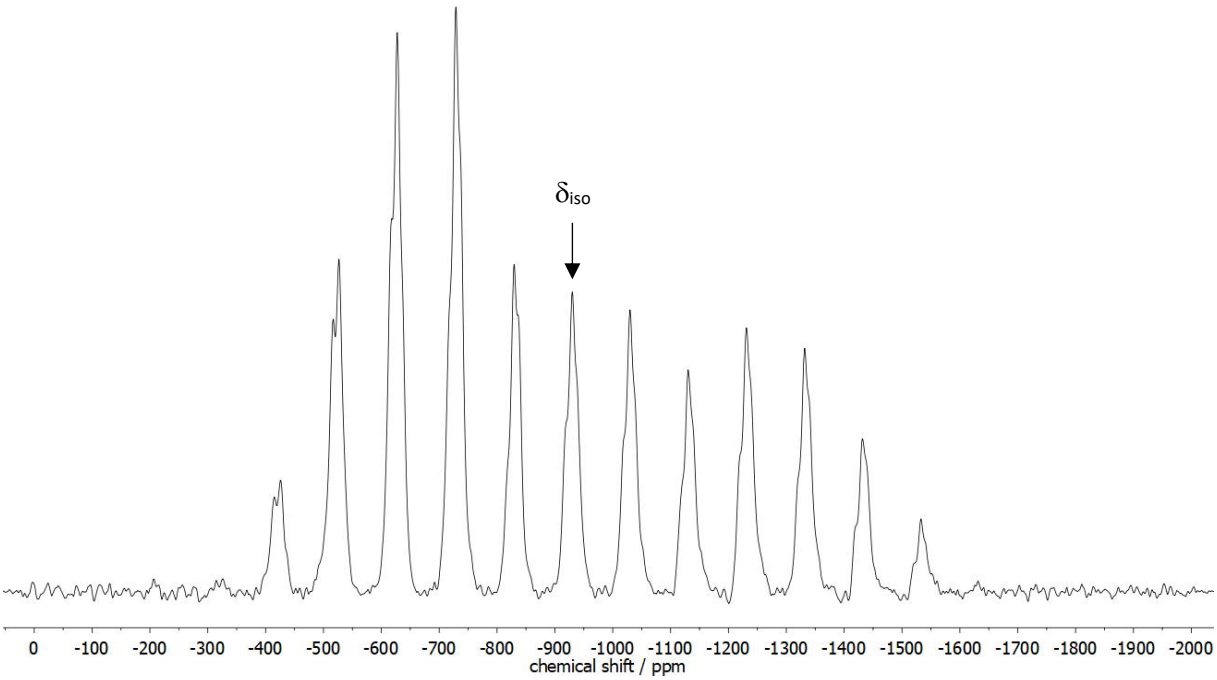


Figure S9: $^{119}Sn\{^{1}H\}$ CP/MAS NMR spectrum (13 kHz) of **1b**.

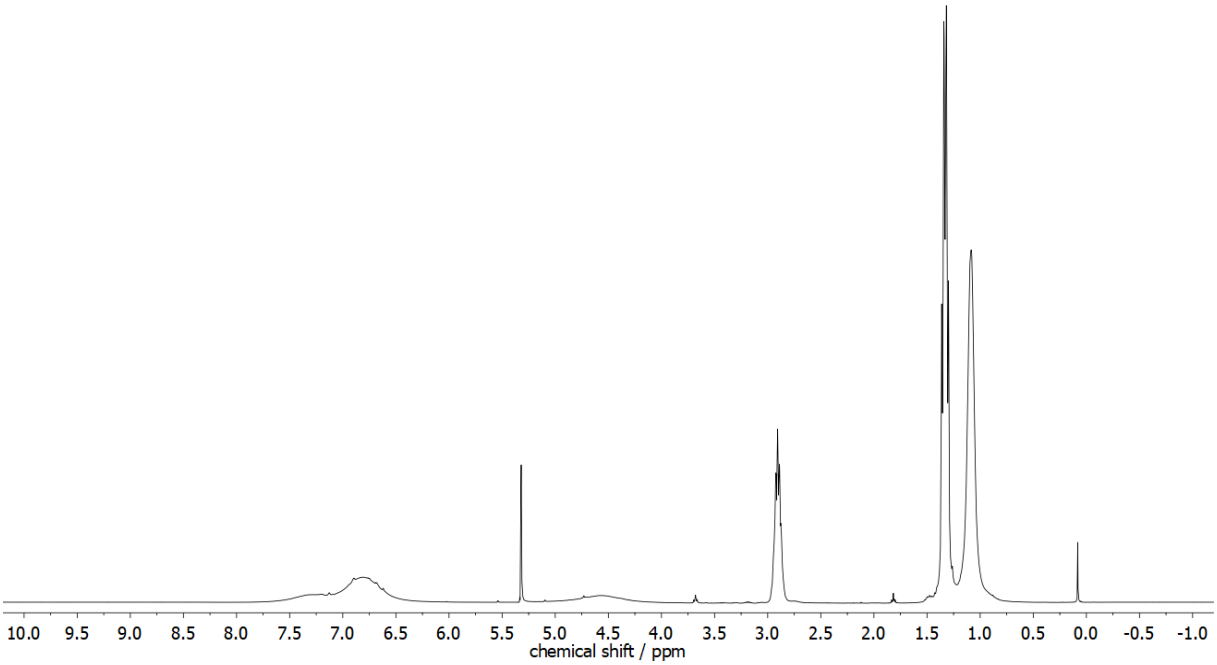


Figure S10: ^{1}H NMR spectrum (CD_2Cl_2) of **2b**. Pt

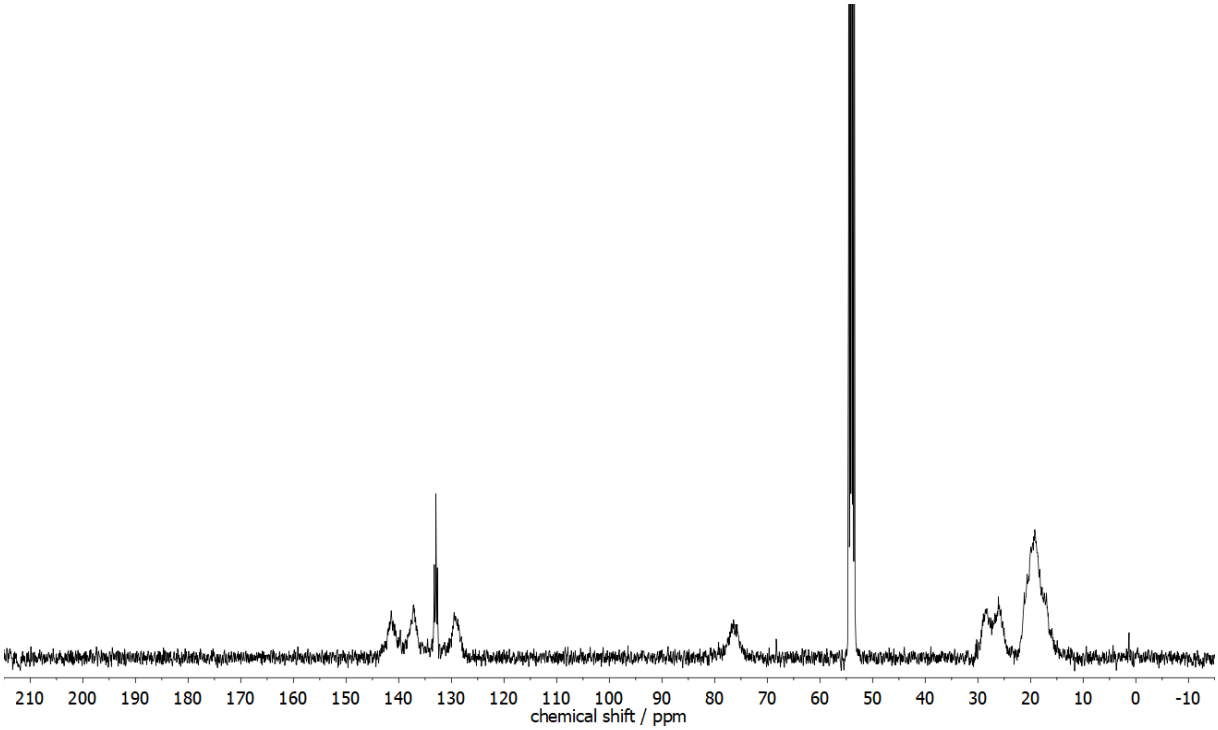


Figure S11: $^{13}C\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **2b**.

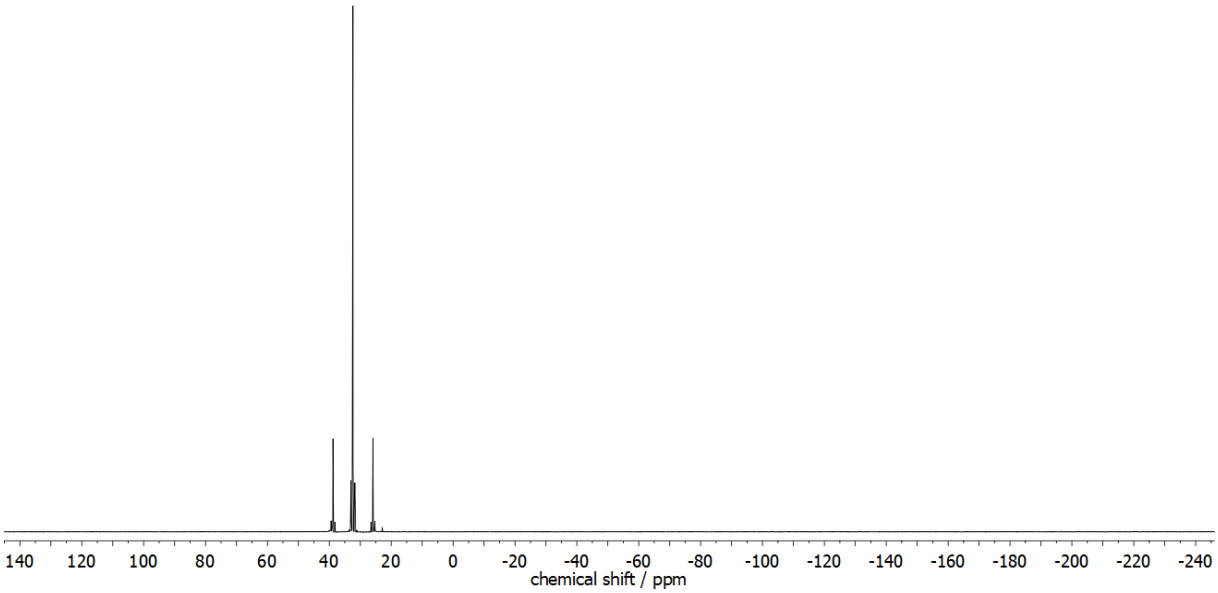


Figure S12: $^{31}P\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **2b**.

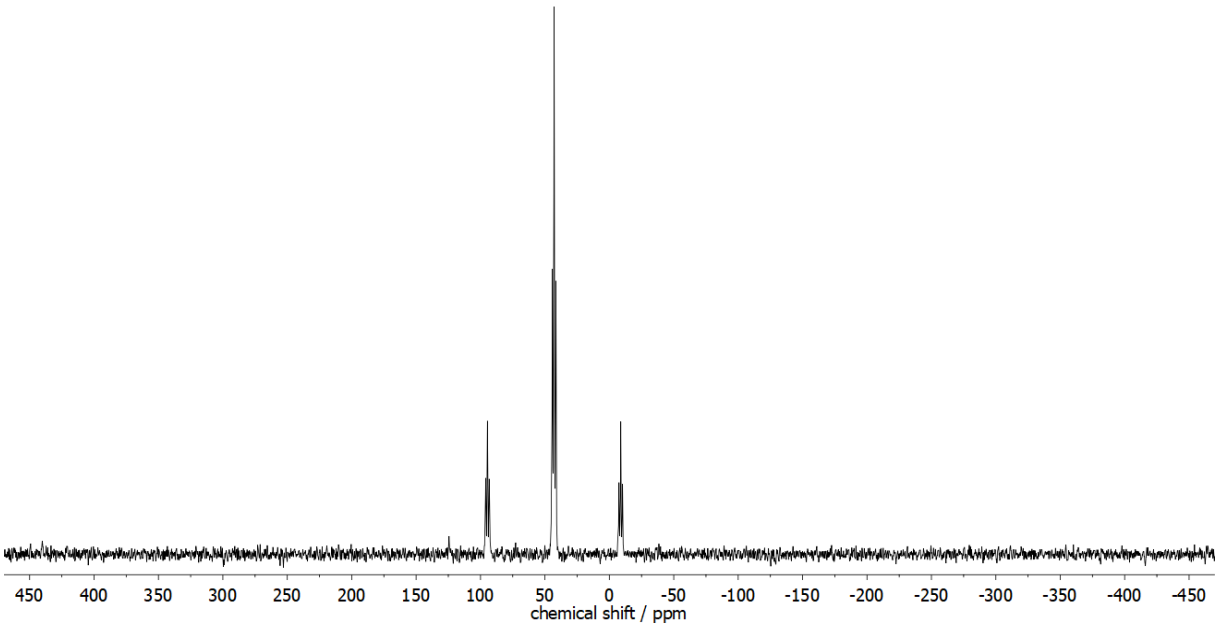


Figure S13: $^{119}Sn\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **2b**. Pt

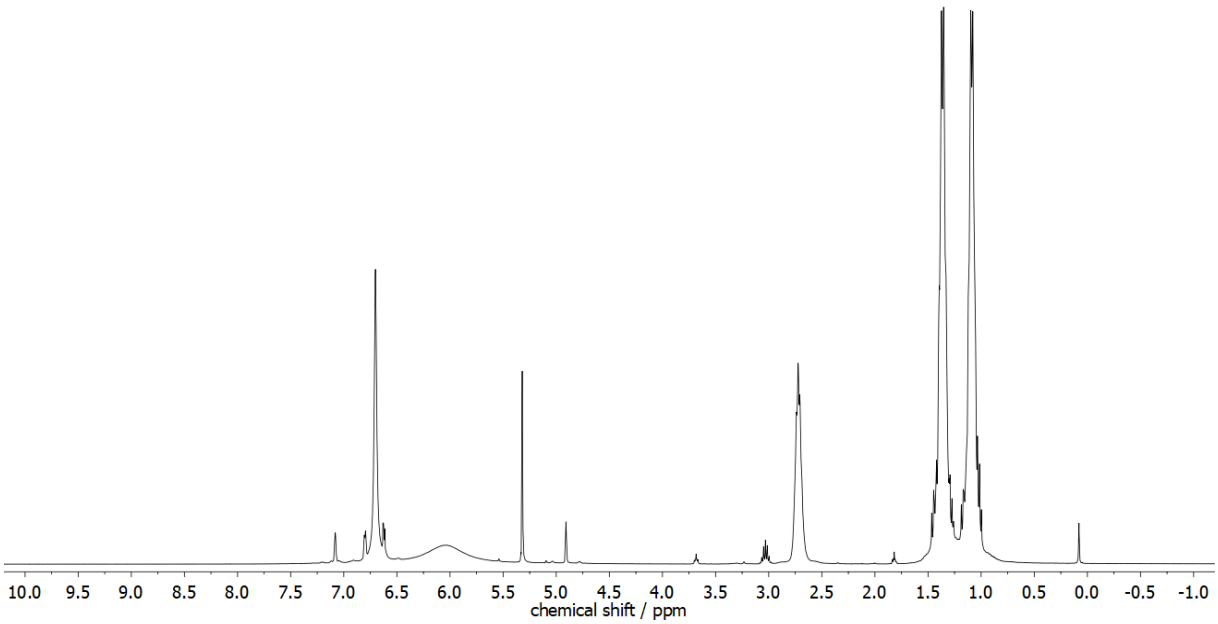


Figure S14: ^{1}H NMR spectrum (CD_2Cl_2) of **2a**.

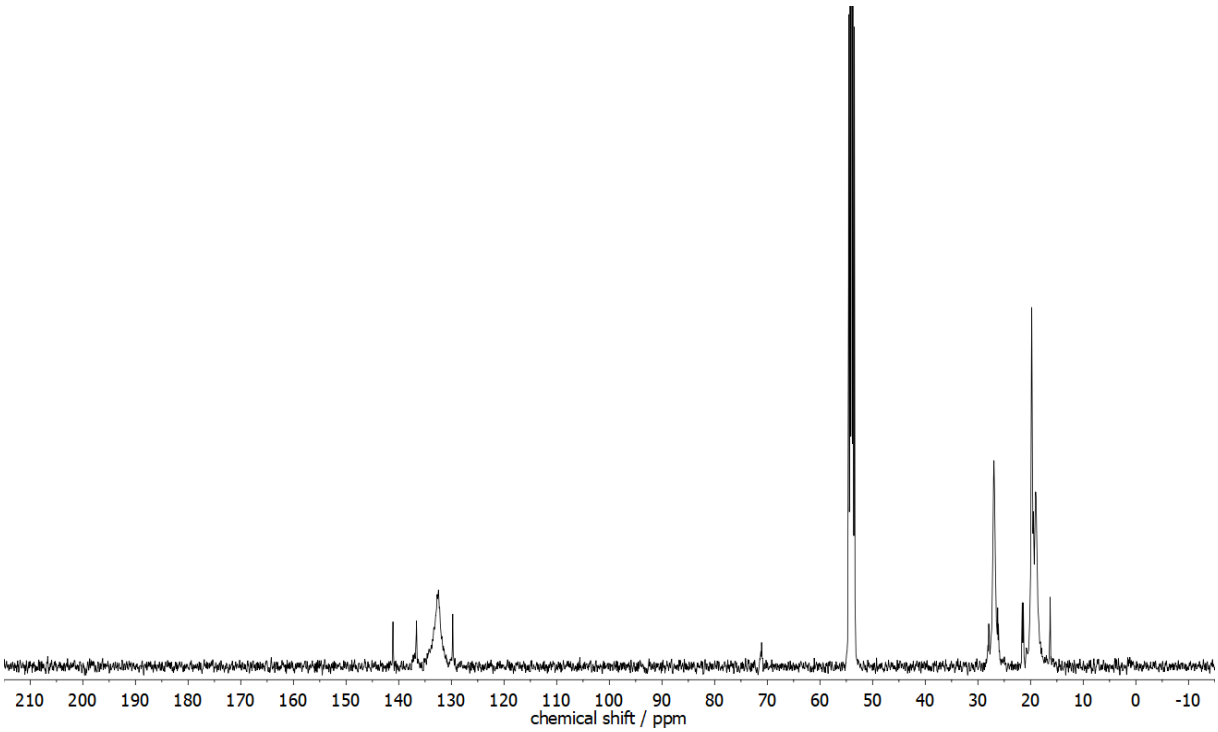


Figure S15: $^{13}C\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **2a**.

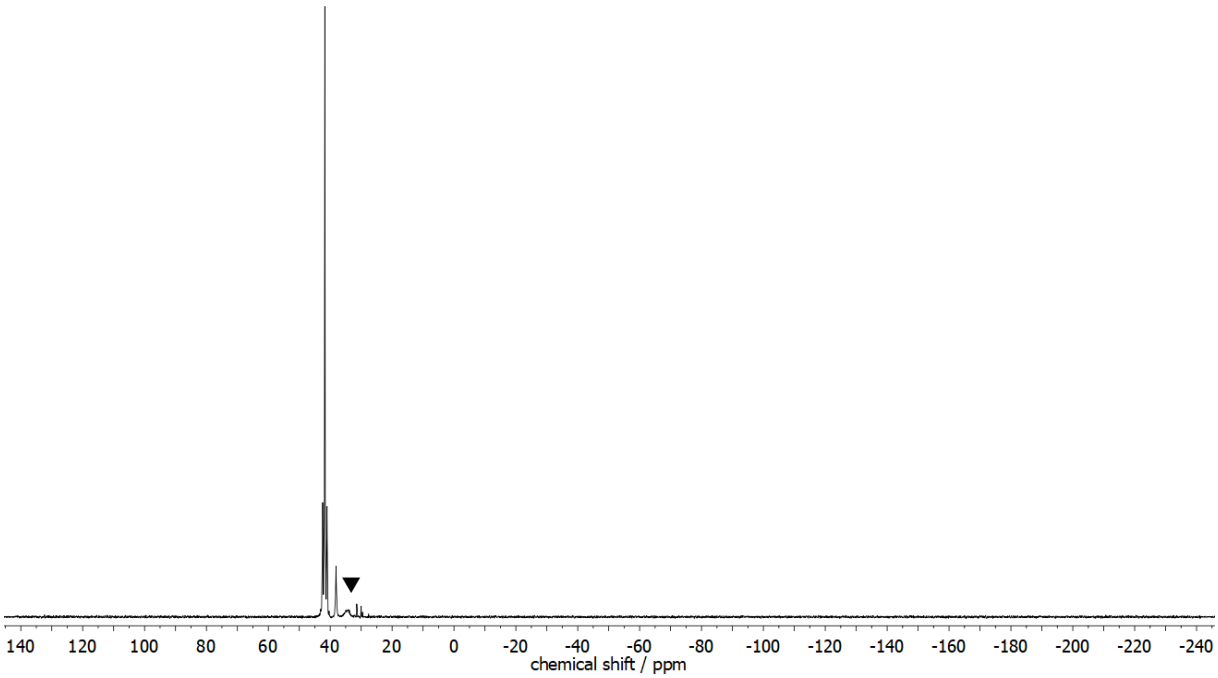


Figure S16: $^{31}P\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **2a** (▼ unidentified byproduct).

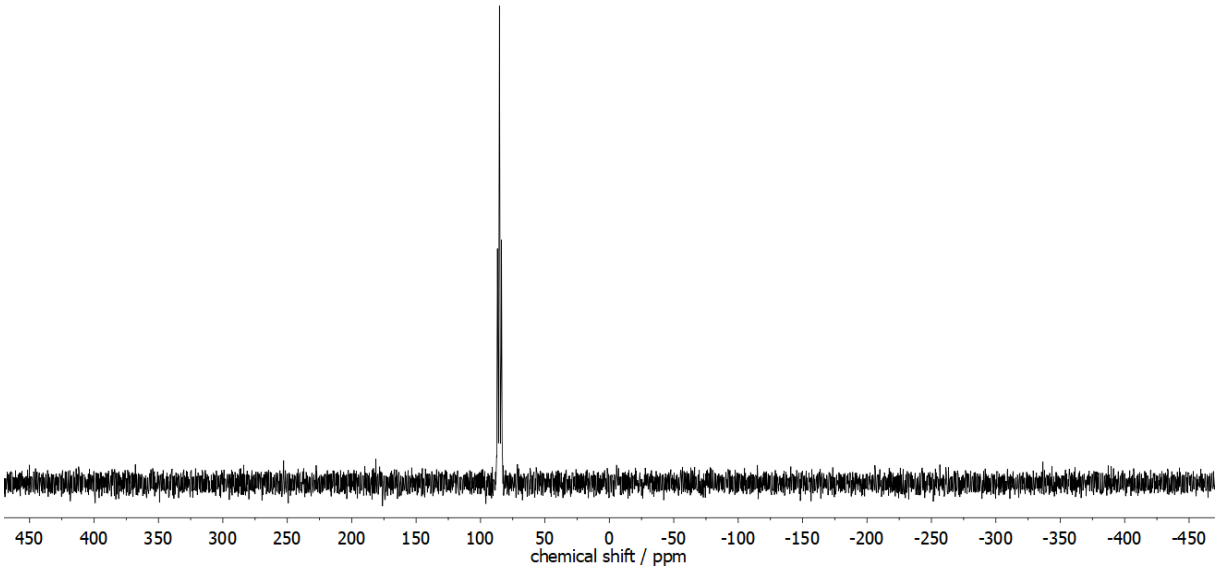


Figure S17: $^{119}Sn\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **2a**.

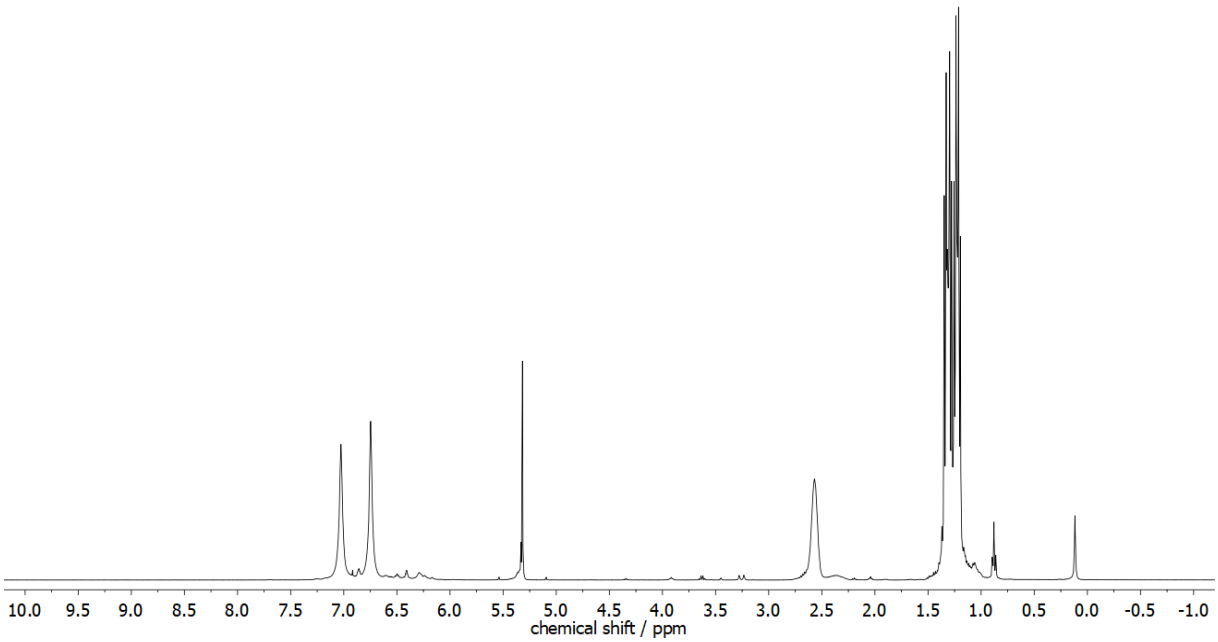


Figure S18: ^{1}H NMR spectrum (CD_2Cl_2) of **3**.

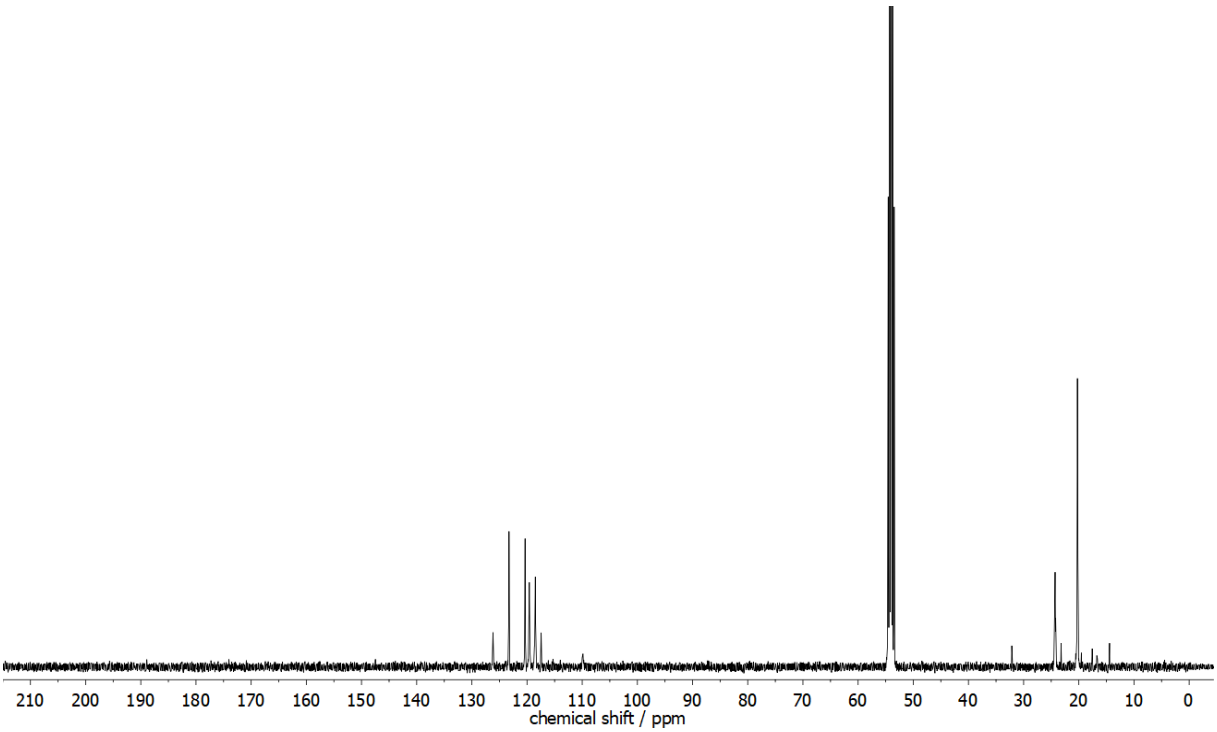


Figure S19: $^{13}C\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **3**.

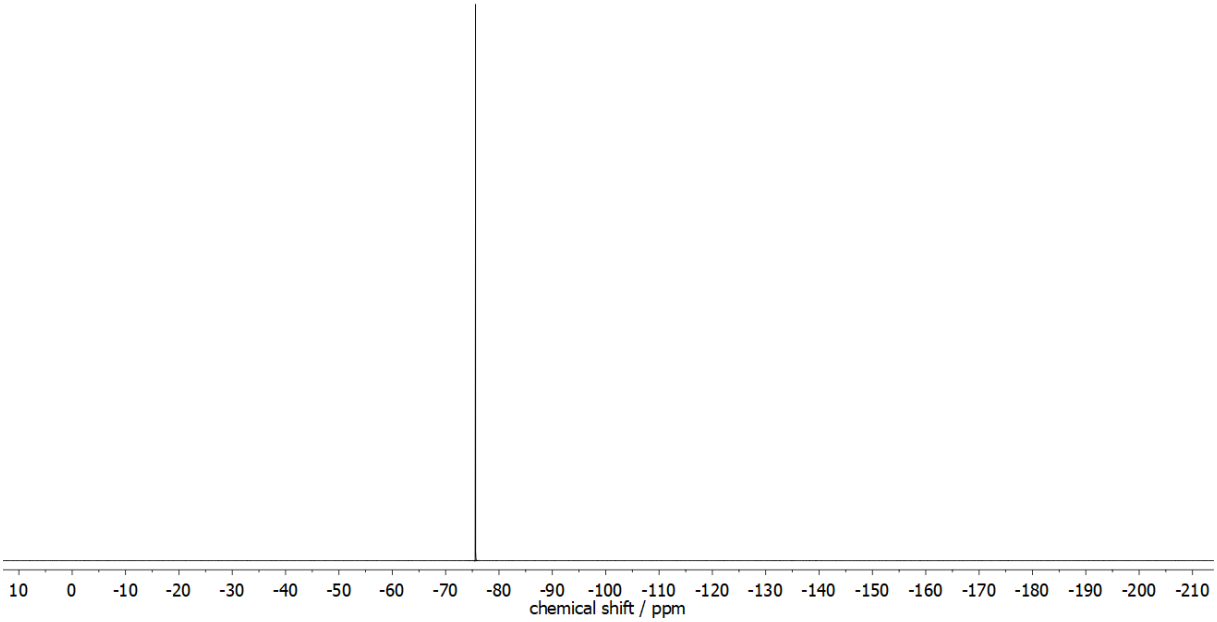


Figure S20: $^{19}F\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **3**.

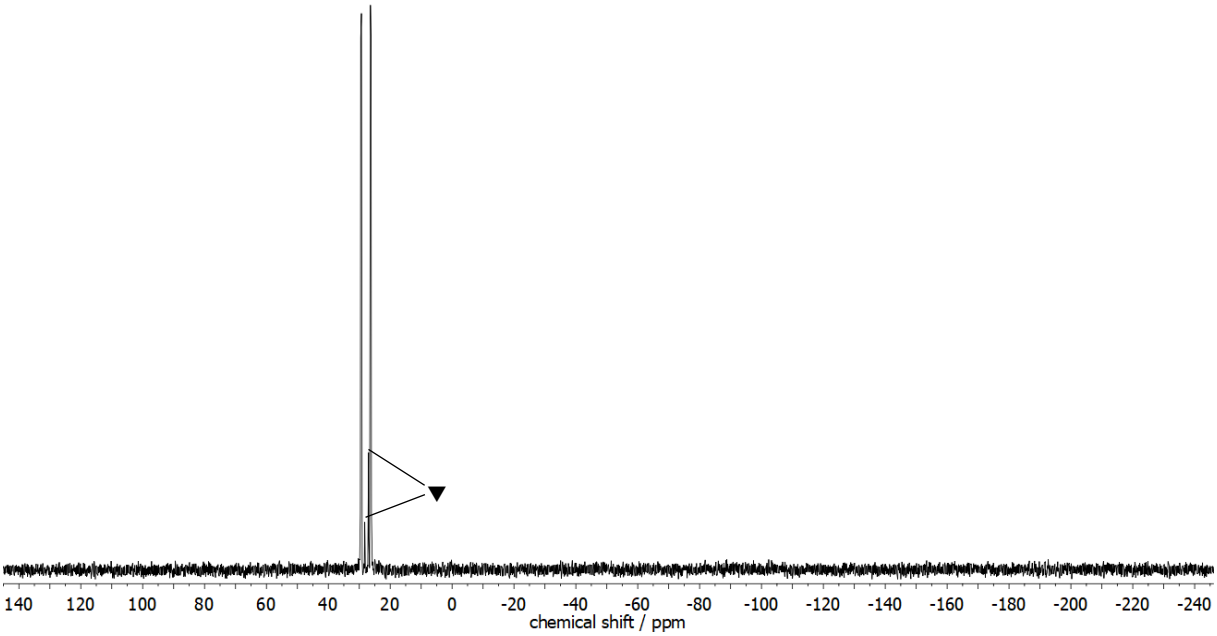


Figure S21: $^{31}P\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **3** (▼unidentified decomposition products).

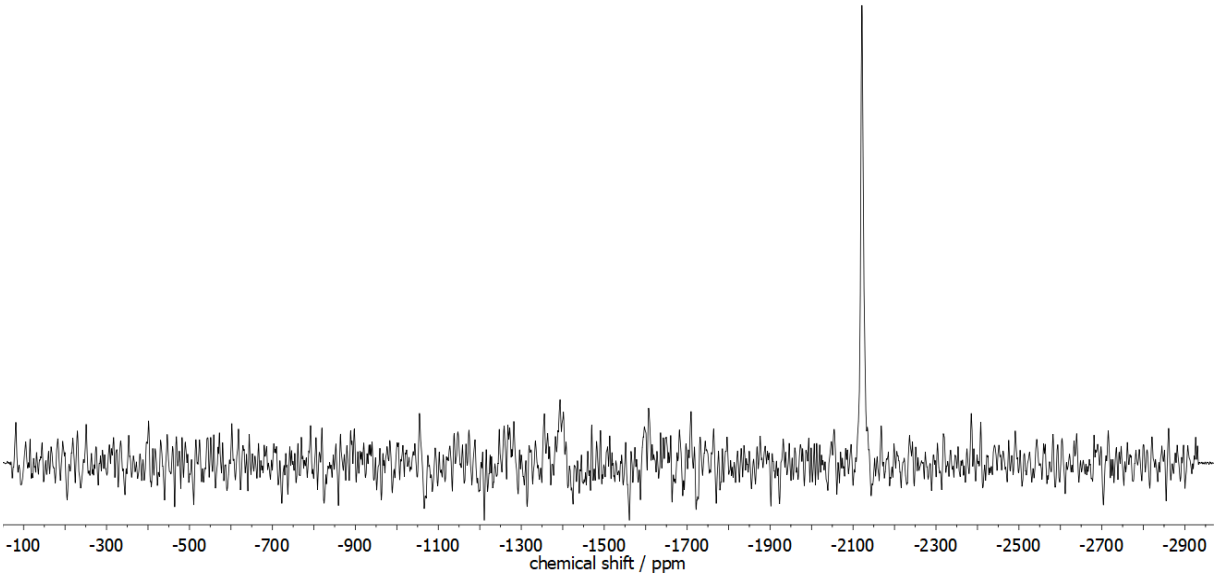


Figure S22: $^{119}Sn\{^{1}H\}$ NMR spectrum (CD_2Cl_2) of **3**.

3. MS Spectra

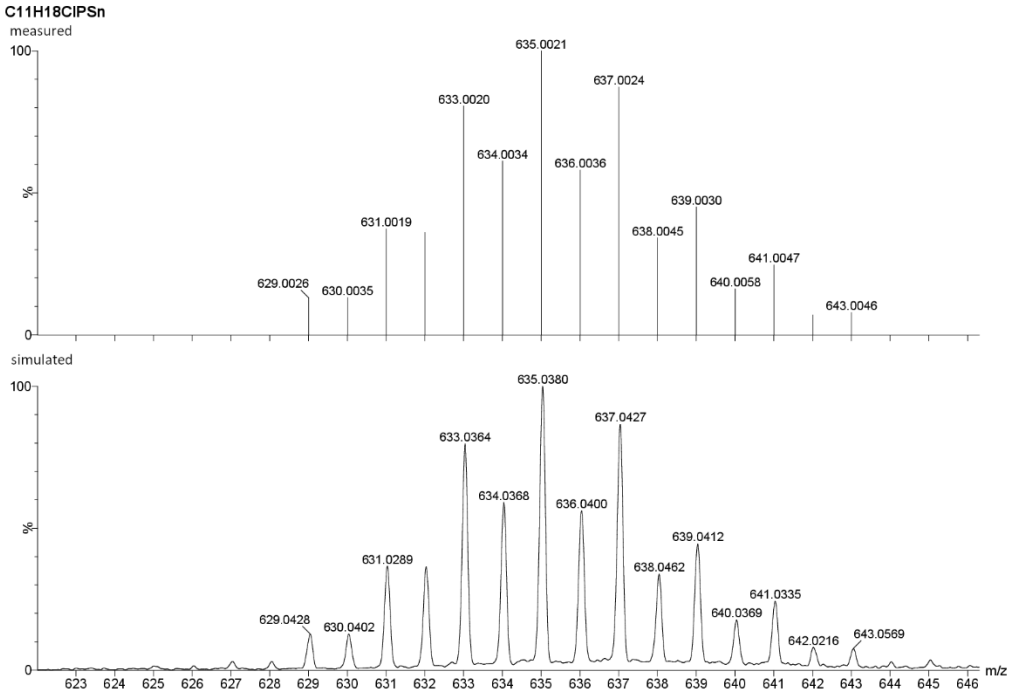


Figure S23: LIFDI mass spectrum of **1a** (635.00 ($C_{22}H_{36}ClP_2Sn_2^+$).

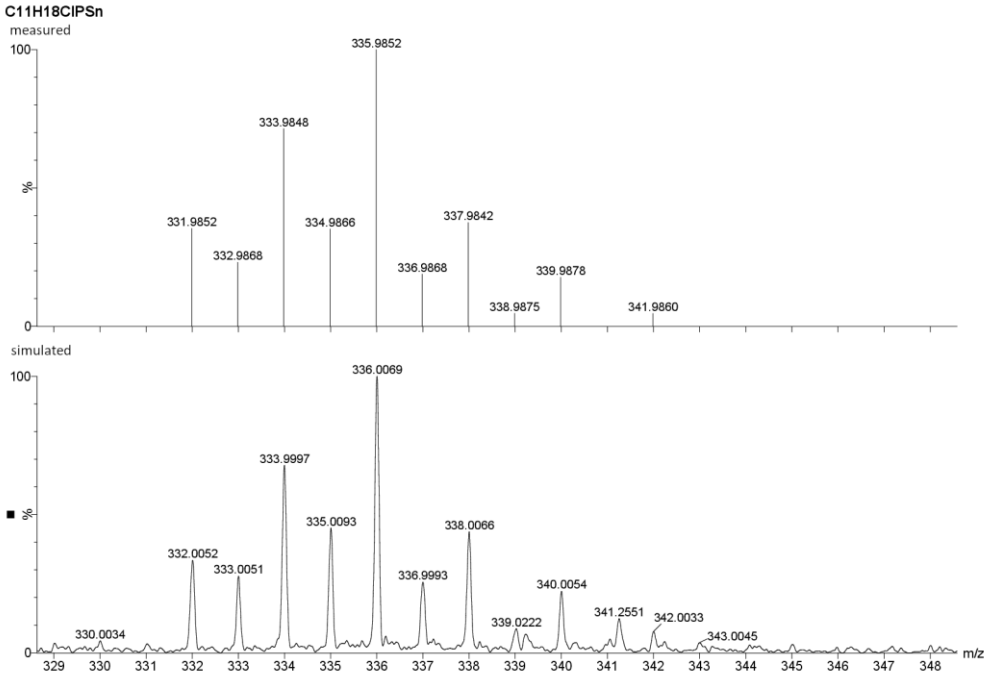


Figure S24: LIFDI mass spectrum of **1a** (335.98 ($C_{11}H_{18}ClPSn^+$).

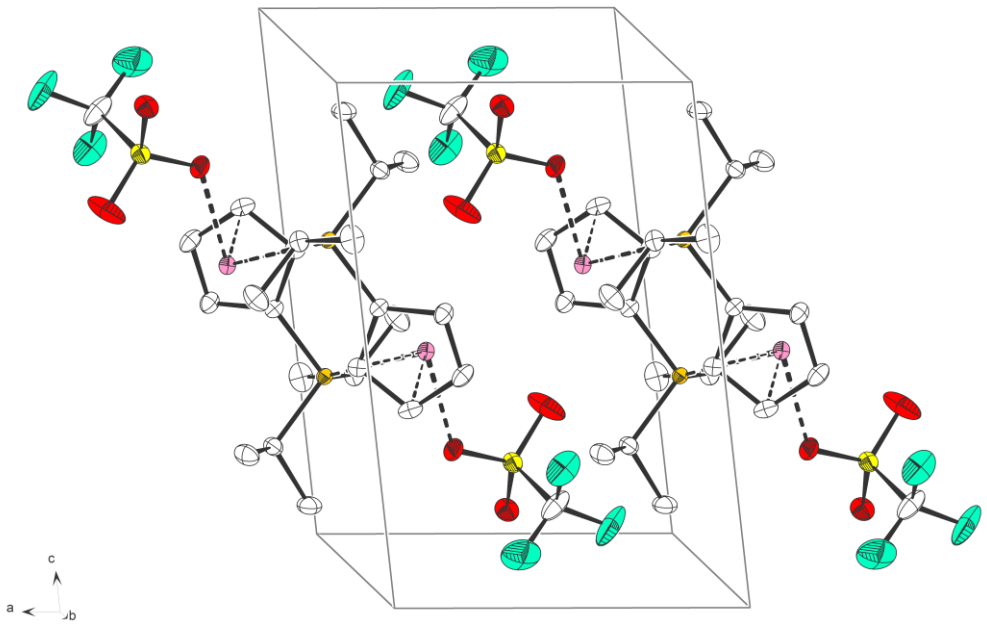
4. XRD Data

Structural details for **1a**

CCDC Deposition Number	2242130	
Empirical formula	$C_{22}H_{36}Cl_2P_2Sn_2$	
Formula weight	670.73	
Temperature	152(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.1679(7) Å	α = 90°
	b = 14.8501(12) Å	β = 108.184(3)°
	c = 11.1754(11) Å	γ = 90°
Volume	1287.8(2) $Å^3$	
Z	2	
Density (calculated)	1.730 mg/m^3	
Absorption coefficient	2.279 mm^{-1}	
F(000)	664	
Crystal size	0.341 x 0.242 x 0.168 mm^3	
Theta range for data collection	2.358 to 27.400°	
Index ranges	-10<=h<=9, -19<=k<=17, -14<=l<=14	
Reflections collected	17249	
Independent reflections	2893 [R(int) = 0.0288]	
Completeness to theta = 25.242°	98.9%	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6442	
Refinement method	full-matrix least-squares on F2	
Data / restraints / parameters	2893 / 0 / 199	
Goodness-of-fit on F2	1.331	
Final R indices [I>2sigma(I)]	R1 = 0.0351, wR2 = 0.0739	
R indices (all data)	R1 = 0.0421, wR2 = 0.0759	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.311 and -0.608 $e.Å^{-3}$	

Structural details for **1b**

CCDC Deposition Number	2242136	
Empirical formula	$C_{26}H_{40}Cl_4F_6O_6P_2S_2Sn_2$	
Formula weight	1067.82	
Temperature	132(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 8.8758(3) Å	α = 74.9070(10)°
	b = 10.4870(3) Å	β = 72.2070(10)°
	c = 12.3520(4) Å	γ = 67.5200(10)°
Volume	998.00(6) Å3	
Z	1	
Density (calculated)	1.777 mg/m^3	
Absorption coefficient	1.768 mm^{-1}	
F(000)	528	
Crystal size	0.439 x 0.285 x 0.176 mm^3	
Theta range for data collection	1.755 to 27.905°	
Index ranges	-11<=h<=11, -10<=k<=13, -16<=l<=16	
Reflections collected	15330	
Independent reflections	4781 [R(int) = 0.0132]	
Completeness to theta = 25.242°	100.0%	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6141	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	4781 / 169 / 270	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0159, wR2 = 0.0373	
R indices (all data)	R1 = 0.0171, wR2 = 0.0378	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.919 and -1.056 e.Å^{-3}	



Structural details for **2a**

CCDC Deposition Number	2242132	
Empirical formula	$C_{30}H_{52}Cl_4O_2P_2PdSn_2$	
Formula weight	992.23	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	*C*2/c	
Unit cell dimensions	a = 18.1277(7) Å	α = 90°
	b = 11.2789(7) Å	β = 101.435(2)°
	c = 19.2577(9) Å	γ = 90°
Volume	3859.3(3) $Å^3$	
Z	4	
Density (calculated)	1.708 mg/m^3	
Absorption coefficient	2.130 mm^{-1}	
F(000)	1968	
Crystal size	0.289 x 0.256 x 0.090 mm^3	
Theta range for data collection	2.139 to 36.361°	
Index ranges	-30<=h<=30, -18<=k<=18, -32<=l<=32	
Reflections collected	155905	
Independent reflections	9372 [R(int) = 0.0285]	
Completeness to theta = 25.242°	99.8%	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.7471 and 0.6397	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	9372 / 6 / 268	
Goodness-of-fit on F^2	1.148	
Final R indices [I>2sigma(I)]	R1 = 0.0172, wR2 = 0.0433	
R indices (all data)	R1 = 0.0178, wR2 = 0.0436	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.788 and -0.777 e.$Å^{-3}$	

Structural details for **2b**

CCDC Deposition Number	2242131	
Empirical formula	$C_{30}H_{52}Cl_4O_2P_2PtSn_2$	
Formula weight	1080.92	
Temperature	222(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	*C*2/c	
Unit cell dimensions	a = 18.1877(9) Å	α = 90°
	b = 11.4015(9) Å	β = 101.731(2)°
	c = 19.3541(10) Å	γ = 90°
Volume	3929.6(4) Å^3	
Z	4	
Density (calculated)	1.827 mg/m^3	
Absorption coefficient	5.191 mm^{-1}	
F(000)	2096	
Crystal size	0.184 x 0.161 x 0.033 mm^3	
Theta range for data collection	2.121 to 27.959°	
Index ranges	-23<=h<=23, -15<=k<=14, -25<=l<=25	
Reflections collected	28954	
Independent reflections	4723 [R(int) = 0.0486]	
Completeness to theta = 25.242°	100.0%	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6159	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	4723 / 18 / 224	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0261, wR2 = 0.0507	
R indices (all data)	R1 = 0.0379, wR2 = 0.0552	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.469 and -0.827 e.Å^{-3}	

Structural details for **3[Al(OC(CF$_3$)$_3$)$_4$]$_2$**

CCDC Deposition Number	2242137	
Empirical formula	$C_{68}H_{52}AgAl_2ClF_{72}O_8P_2Sn_2$	
Formula weight	2861.69	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 14.6726(5) Å	α = 90°
	b = 30.0339(11) Å	β = 94.9170(10)°
	c = 22.3253(6) Å	γ = 90°
Volume	9802.0(6) Å^3	
Z	4	
Density (calculated)	1.939 Mg/m^3	
Absorption coefficient	0.968 mm^{-1}	
F(000)	5568	
Crystal size	0.315 x 0.232 x 0.093 mm^3	
Theta range for data collection	1.944 to 27.102°	
Index ranges	-18<=h<=18, -33<=k<=38, -28<=l<=28	
Reflections collected	194671	
Independent reflections	21626 [R(int) = 0.0411]	
Completeness to theta = 25.242°	100.0%	
Absorption correction	semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6871	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	21626 / 10019 / 2177	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0637, wR2 = 0.1769	
R indices (all data)	R1 = 0.0782, wR2 = 0.1927	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.512 and -1.074 e.Å^{-3}	

Please note:

One of the Al(OC(CF$_3$)$_3$)$_4$ anions and an incorporated toluene molecule are severely disordered, requiring a large number of restraints and resulting in a slightly elevated wR2.

5. Computational Details

All calculations were performed using the Gaussian 16, Revision C.01 package of programs.[5] Geometry optimizations have been carried out at the B3LYP-D3/def2-TZVP level of theory.[6] The optimized structures were confirmed to be a minimum on the potential energy surface by subsequent frequency analysis (all positive eigenvalues).

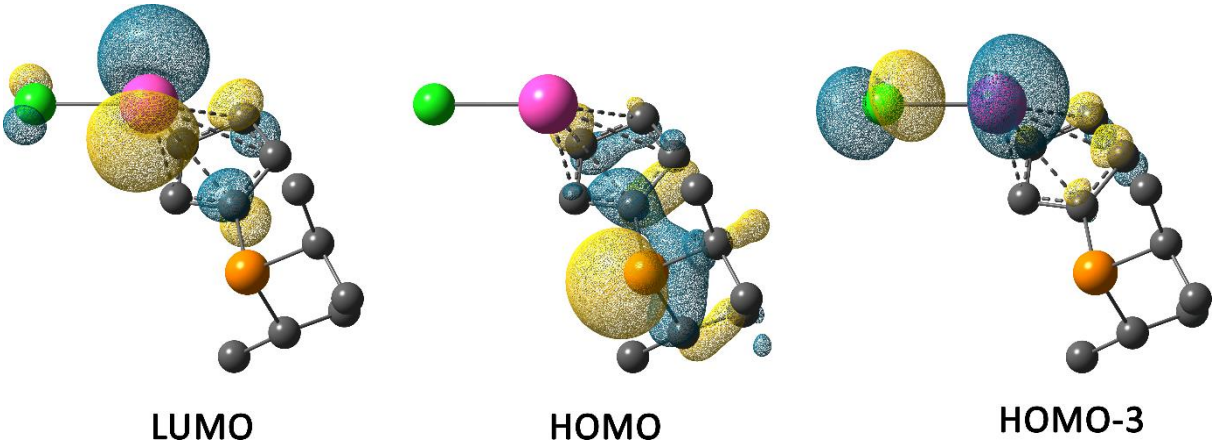


Figure S25: Kohn-Sham molecular orbital contours of **1a** (calculated at B3LYP-D3/def2-TZVPP//B3LYP-D3/def2-SVP; isodensity = 0.05 a.u.).

optimized geometry of **1a**

Sn	2.01584400	-1.70201100	0.67930800
P	2.54108400	0.96714100	-0.09749100
Cl	4.26998400	-2.26718000	-0.16889200
C	0.84328500	-2.60140000	-1.32763300
H	3.46992300	0.28883000	2.66578700
H	-0.03797100	-0.57546200	-1.64327300
H	0.03795300	0.57546300	1.64326100
H	1.63814900	-2.63224300	-2.05900600
C	1.13949200	1.98975400	0.33981400
C	3.97240200	1.55782100	0.94752900
C	3.00334800	1.41864000	-1.84434400
C	0.32178000	-3.73107500	-0.61185500
C	-0.10289900	-1.54202900	-1.17331700
C	3.66324900	1.33753000	2.43248900
Sn	-2.01584800	1.70200600	-0.67932400
C	0.10288600	1.54202900	1.17330300
C	0.86509000	3.35100400	0.00310700
C	4.36721500	3.01354700	0.68557000
H	4.79682100	0.89712900	0.66424400
C	4.36697800	0.84381100	-2.24301300
C	1.91911800	0.98804200	-2.83534500
H	3.05744600	2.51147200	-1.85347300
C	-0.86509100	-3.35100500	-0.00311600
H	0.79297200	-4.70016200	-0.54774800
C	-1.13949700	-1.98975600	-0.33982100
H	4.51607400	1.65297700	3.03741800
H	2.79431200	1.92057900	2.74376900
P	-2.54108100	-0.96714100	0.09750100
Cl	-4.26999100	2.26718700	0.16885900
C	-0.84329600	2.60140300	1.32761300
H	-3.46996200	-0.28885900	-2.66577200
H	-1.63816200	2.63224900	2.05898400
C	-0.32178700	3.73107500	0.61183400
H	1.46375600	3.97153100	-0.64627100
H	5.22251600	3.28090800	1.31121300
H	3.54774200	3.68993500	0.93477000
H	4.65322600	3.18951900	-0.35138400
H	4.36867800	-0.24505500	-2.18840300
H	4.59595700	1.13524900	-3.27078700
H	5.17586300	1.20747400	-1.60984600
H	0.94104300	1.39405300	-2.57510600
H	2.17286400	1.34819200	-3.83490000
H	1.84521400	-0.09968400	-2.88726200
H	-1.46375100	-3.97153300	0.64626800
C	-3.97242000	-1.55782500	-0.94748900
C	-3.00330600	-1.41862800	1.84436600
C	-3.66329000	-1.33755500	-2.43245700
H	-0.79297800	4.70016200	0.54772100
C	-4.36723900	-3.01354500	-0.68550400
H	-4.79683000	-0.89712500	-0.66419800
C	-4.36693500	-0.84381400	2.24305800
C	-1.91905800	-0.98800600	2.83533800
H	-3.05739100	-2.51146100	1.85350600
H	-4.51612600	-1.65300600	-3.03736700
H	-2.79436000	-1.92061200	-2.74374300
H	-5.22255000	-3.28090800	-1.31113200
H	-3.54777400	-3.68994200	-0.93470500
H	-4.65323800	-3.18950000	0.35145600
H	-4.36864900	0.24505200	2.18844500
H	-4.59589200	-1.13525200	3.27083700
H	-5.17582800	-1.20748900	1.60990700
H	-0.94098400	-1.39400700	2.57507800
H	-2.17277500	-1.34815000	3.83490300
H	-1.84516600	0.09972100	2.88724100

optimized geometry of

1a-monomer

Sn	2.07666000	0.55912600	0.14557700
Cl	3.84273600	-0.40327700	-1.25550300
C	1.26154000	-1.61101500	1.07353300
H	0.57944200	-1.77064600	-1.06784800
H	2.08504400	-2.32425500	1.11510000
C	0.68771400	-0.90179400	2.17269800
C	0.46596800	-1.31349400	-0.08397200
C	-0.44744400	-0.20387000	1.71042300
H	1.06431400	-0.90932000	3.19618800
C	-0.60873900	-0.44375100	0.32100300
P	-1.91402600	0.11432900	-0.84945000
H	-2.33187700	-2.44912200	-2.21299500
H	-1.07333800	0.44787700	2.31858400
C	-3.20556400	-1.25607000	-0.58505600
C	-2.67078800	1.56927000	0.08642600
C	-2.67838100	-2.57183600	-1.17424000
C	-3.69876200	-1.44897800	0.85129300
H	-4.05077300	-0.92090700	-1.21283100
C	-4.01299800	1.96406000	-0.54583100
C	-1.69785200	2.75647500	0.08662300
H	-2.85386800	1.26583300	1.13093600
H	-3.47014800	-3.33968300	-1.16931000
H	-1.83634100	-2.96335900	-0.57992700
H	-4.44213500	-2.26362700	0.89563500
H	-2.86712600	-1.71982100	1.52169700
H	-4.18019700	-0.54602600	1.25700600
H	-3.89396800	2.20982600	-1.61481900
H	-4.42370700	2.85661400	-0.04458700
H	-4.76768200	1.16679000	-0.46506200
H	-0.74558900	2.51010500	0.58023900
H	-2.13784100	3.61460300	0.62254700
H	-1.47147200	3.08561300	-0.94150400

optimized geometry of

1a-Cl-bridged dimer

Sn	-1.95714200	0.67955900	0.22294900
Cl	0.35499900	0.39982300	1.69288500
C	-2.73488500	-1.49808900	0.97673400
H	-3.50499200	-1.76027700	-1.12260100
H	-1.89827500	-2.19495300	1.02229800
C	-3.27008000	-0.74261400	2.07431400
C	-3.61716300	-1.30198200	-0.13955500
C	-4.44937000	-0.10681500	1.63108100
H	-2.83889200	-0.68876500	3.07422800
C	-4.67914600	-0.44387000	0.26521900
P	-6.04752900	0.02800400	-0.86840800
H	-6.55463300	-2.62198400	-2.02742700
H	-5.06547400	0.55932700	2.23402800
C	-7.32246200	-1.31521400	-0.43501100
C	-6.76248300	1.54757000	-0.00268300
C	-6.82672500	-2.66940300	-0.96067400
C	-7.72998300	-1.40733900	1.03788000
H	-8.20431300	-1.02410700	-1.03367000
C	-8.14016700	1.89140400	-0.58644200
C	-5.80017600	2.73486200	-0.14337200
H	-6.88605600	1.32252700	1.07011700
H	-7.60880400	-3.43848100	-0.84351100
H	-5.94057700	-3.01107600	-0.40047800
H	-8.47033600	-2.21320100	1.18276400
H	-6.86013300	-1.63629500	1.67464400
H	-8.18515600	-0.47615600	1.40890600
H	-8.08236400	2.05449200	-1.67616800
H	-8.52753500	2.81926700	-0.13274000
H	-8.88455000	1.10155100	-0.40284700
H	-4.82145200	2.52896400	0.31574700
H	-6.21684500	3.62957300	0.34988700
H	-5.63024300	2.98610800	-1.20381500
P	6.04752300	-0.02800700	0.86840500
H	6.55462500	2.62198700	2.02741300
H	3.50499200	1.76028200	1.12260500
C	4.67914000	0.44387500	-0.26522000
C	7.32246000	1.31520700	0.43500700
C	6.76247000	-1.54757300	0.00267400
C	6.82672200	2.66939900	0.96066100
Sn	1.95715000	-0.67955600	-0.22294500
C	3.61716100	1.30199000	0.13955800
C	4.44936200	0.10682400	-1.63108200
C	7.72999000	1.40732300	-1.03788200
H	8.20430700	1.02410100	1.03367300
C	8.14016400	-1.89139900	0.58641500
C	5.80016900	-2.73486800	0.14338100
H	6.88602700	-1.32253300	-1.07012700
H	7.60880300	3.43847600	0.84349700
H	5.94057800	3.01107000	0.40045800
Cl	-0.35499500	-0.39983100	-1.69287800
C	2.73487900	1.49809600	-0.97672700
H	1.89826600	2.19495700	-1.02228700
C	3.27007200	0.74262500	-2.07431100
H	5.06546300	-0.55931800	-2.23403100
H	8.47034500	2.21318300	-1.18276600
H	6.86014300	1.63627700	-1.67465100
H	8.18516300	0.47613700	-1.40889900
H	8.08237600	-2.05448400	1.67614300
H	8.52752900	-2.81926200	0.13271100
H	8.88454000	-1.10154400	0.40280800
H	4.82143800	-2.52897600	-0.31572500
H	6.21683400	-3.62957900	-0.34988000
H	5.63025100	-2.98611200	1.20382700
H	2.83888100	0.68877800	-3.07422400

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