Electronic Supplementary Information

for

Bi- and Tridentate Stannylphosphines and their Coordination to Low-Valent Platinum

J. Jacobo Salazar-Díaz,[a] Miguel A. Muñoz-Hernández,[a,b] Ernesto Rufino-Felipe,[a] Marcos Flores-Alamo,[c] Alejandro Ramírez-Solís[d] and Virginia Montiel-Palma[a,b,]*

[a] Centro de Investigaciones Químicas-IICBA, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Col. Chamilpa, Cuernavaca, Morelos 62209, Mexico

[b] Department of Chemistry, Mississippi State University, Box 9573, Mississippi State, Mississippi 39762, United States

[c] Centro de Investigación en Ciencias-IICBA, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Col. Chamilpa, Cuernavaca, Morelos 62209, Mexico

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1. Spectroscopic characterization of compound **1**

1.1 NMR spectroscopy

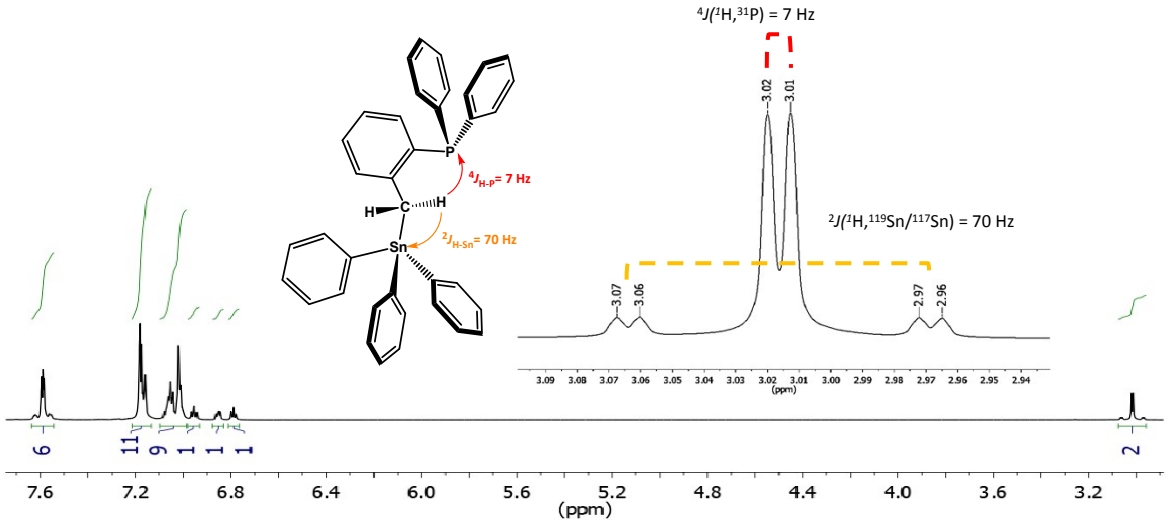


Figure S1. ^{1}H NMR spectrum of compound **1** (700 MHz, C_6D_6, 298 K).

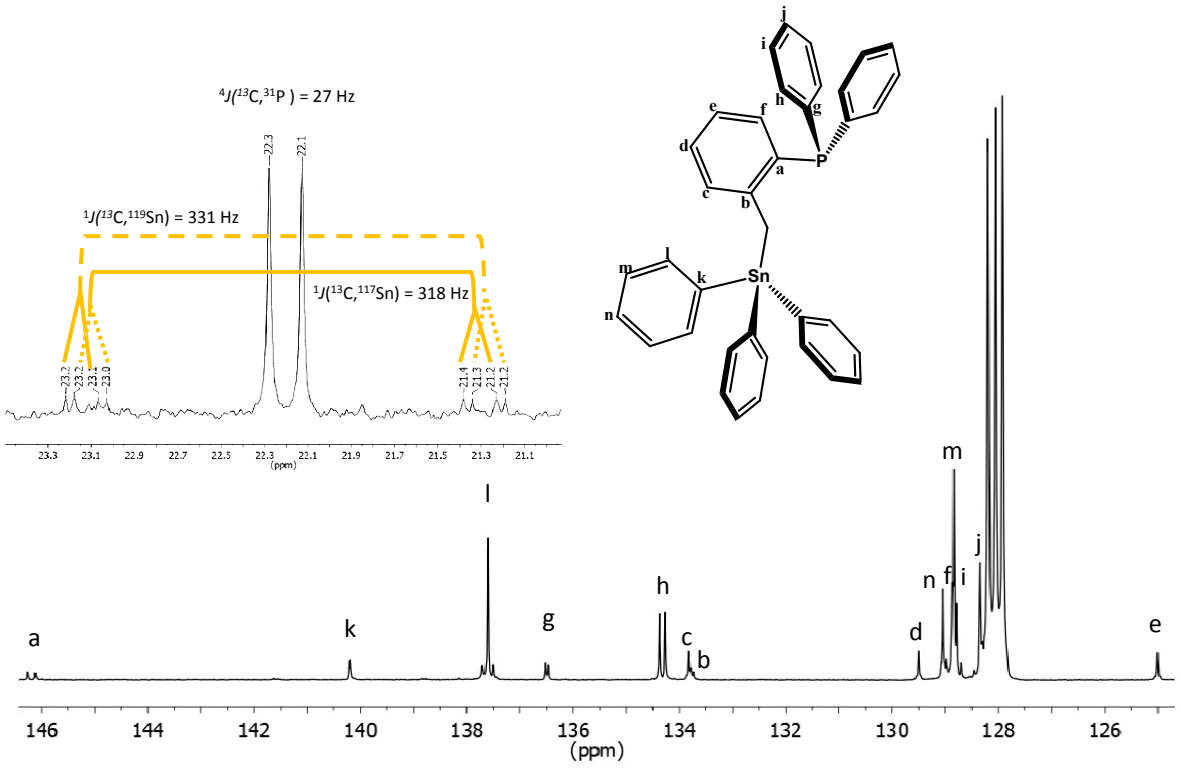


Figure S2. $^{13}C\{^1H\}$ NMR spectrum of compound **1** (176.04 MHz, C_6D_6, 298 K).

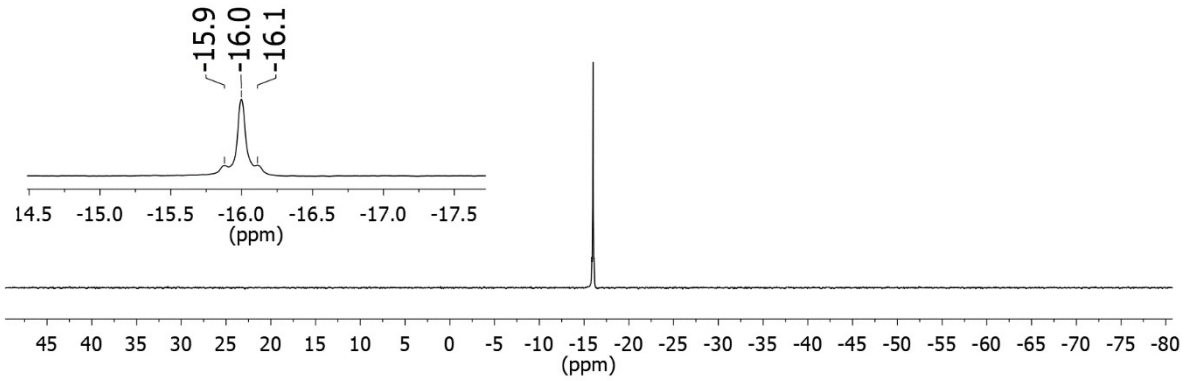


Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of compound **1** (161.97 MHz, C_6D_6, 298 K).

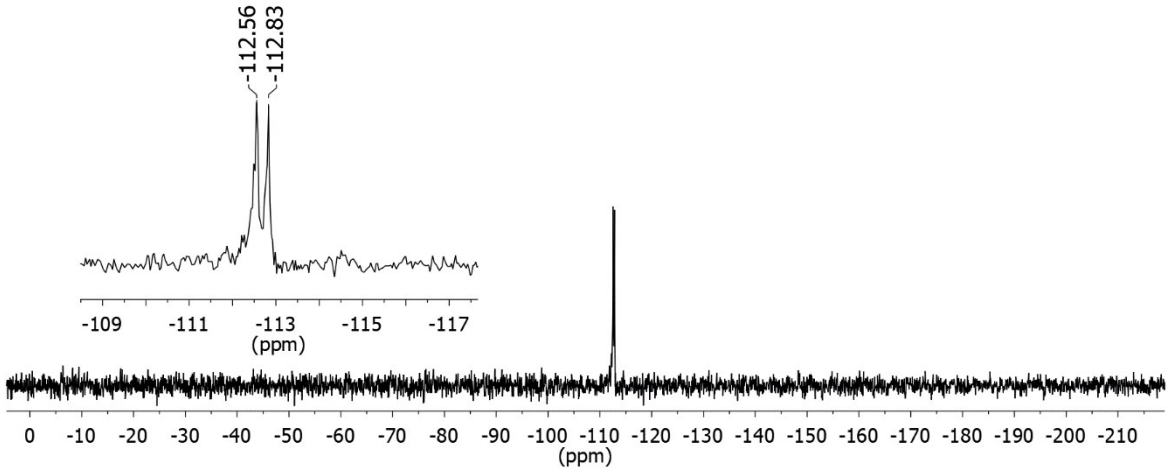


Figure S4. $^{119}Sn\{^{1}H\}$ NMR spectrum of compound **1** (149.21 MHz, C_6D_6, 298 K).

1.2 FT-IR spectroscopy

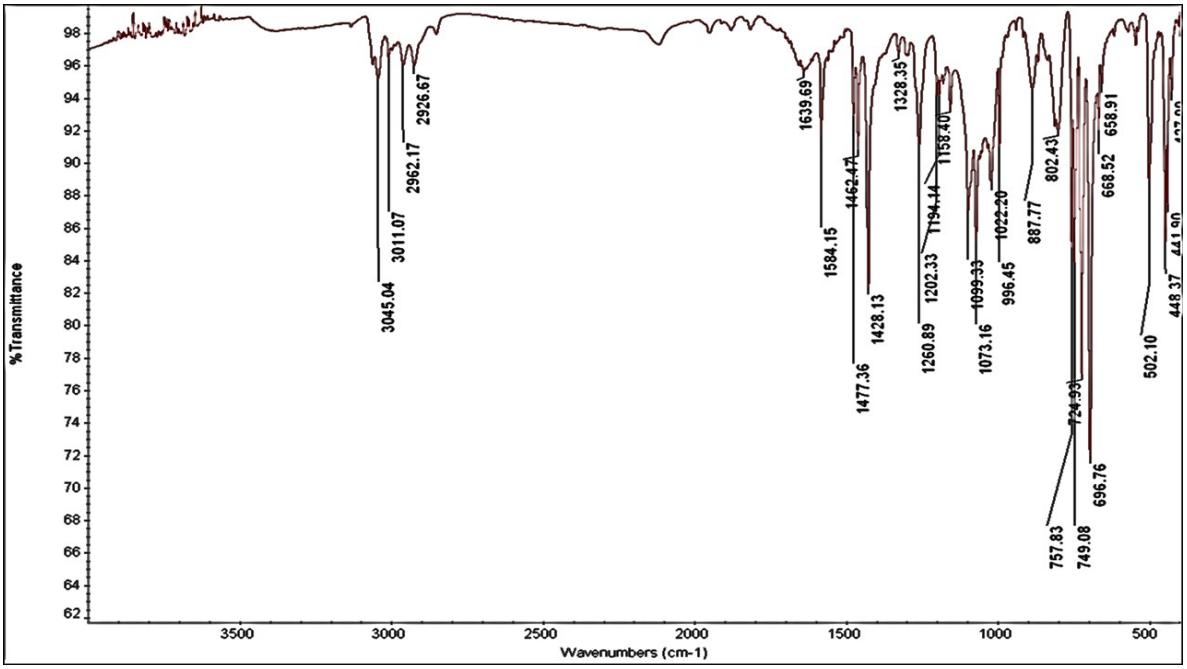


Figure S5. FT- IR spectrum of compound **1** as KBr pellet.

2. Spectroscopic characterization of compound **2**

2.1 NMR spectroscopy

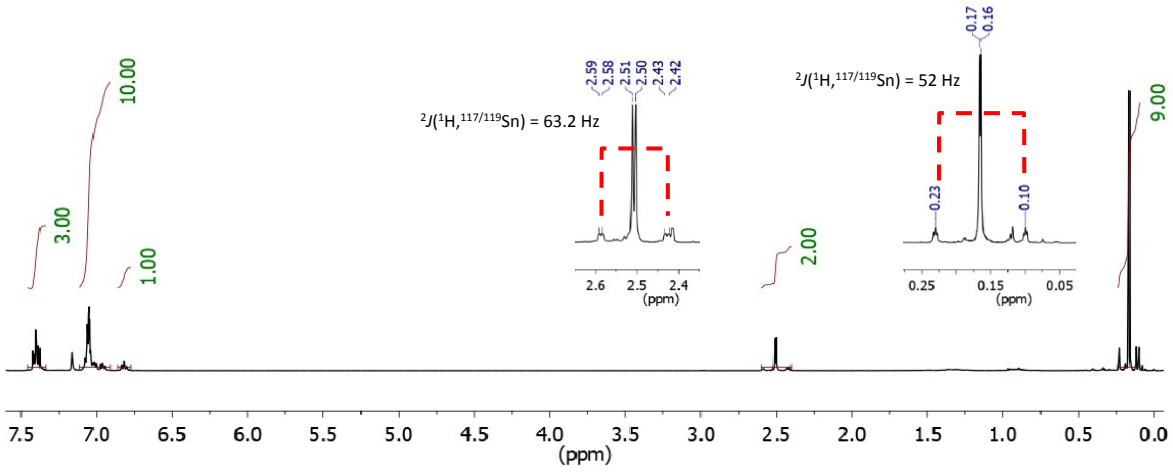


Figure S6. ^1H NMR spectrum (400 MHz, C_6D_6, 298 K) of compound **2**

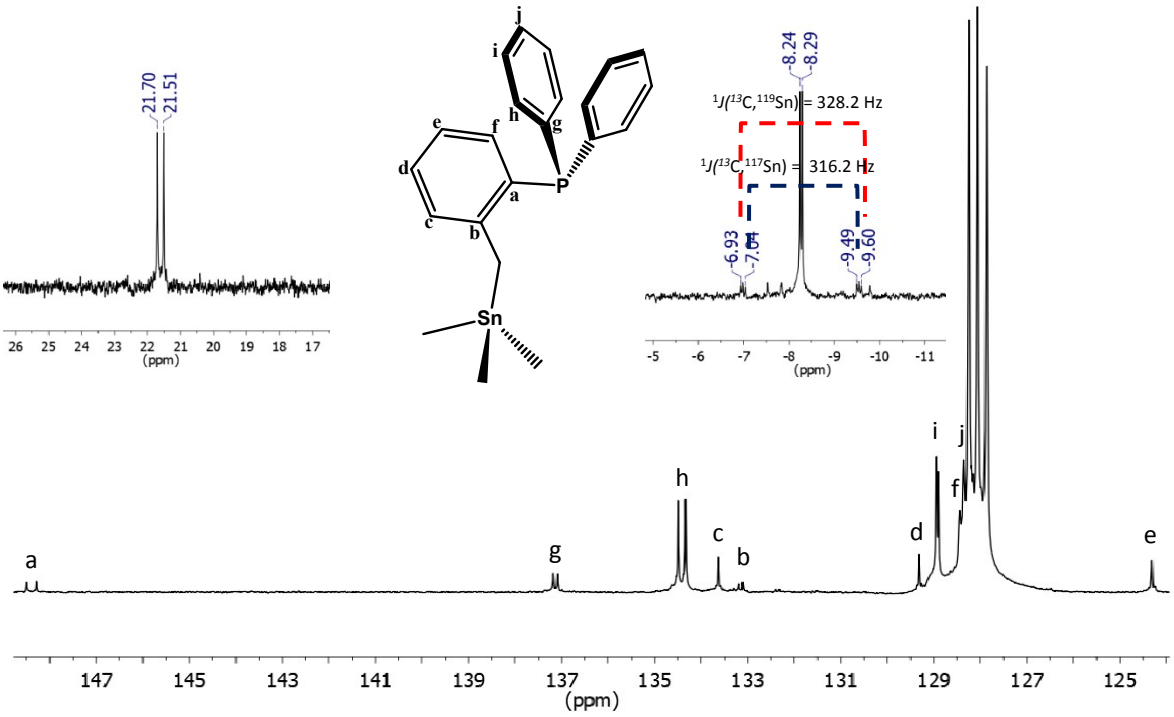


Figure S7. $^{13}C\{^1H\}$ NMR spectrum of compound **2** (125.75 MHz, C_6D_6, 298 K).

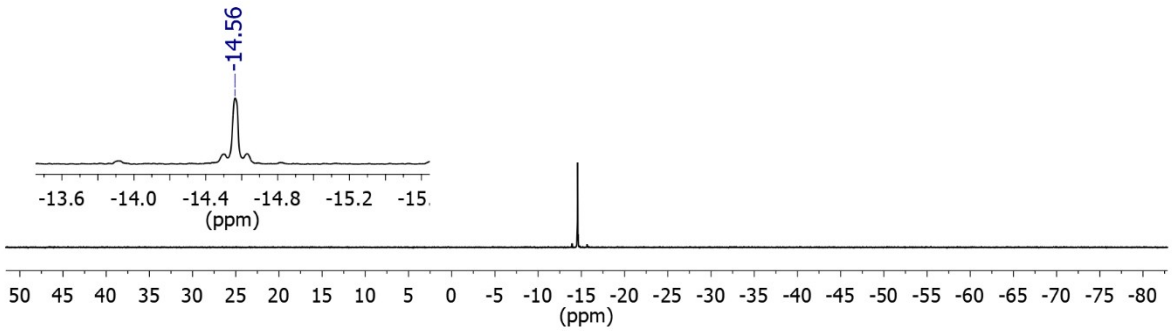


Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum of compound **2** (161.97 MHz, C_6D_6, 298 K).

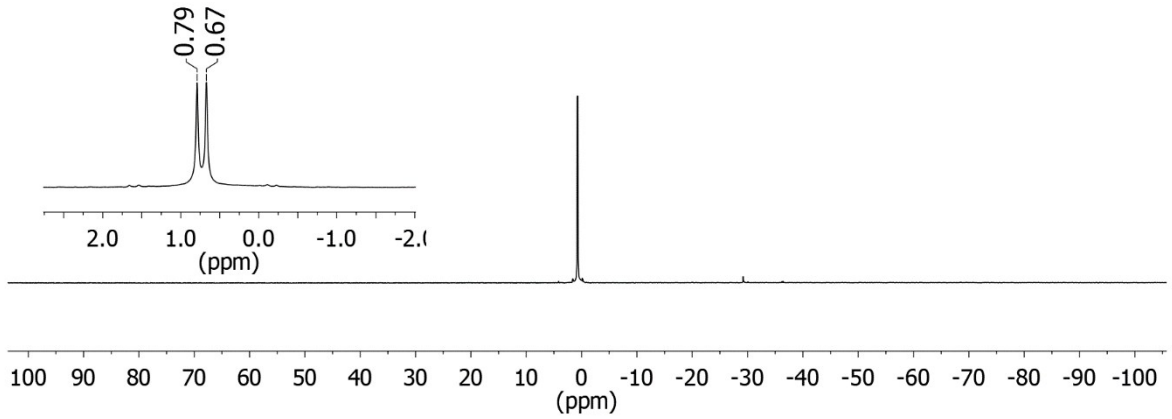


Figure S9. $^{119}Sn\{^{1}H\}$ NMR spectrum of compound **2** (186.50 MHz, C_6D_6, 298 K).

2.2 FT-IR spectroscopy

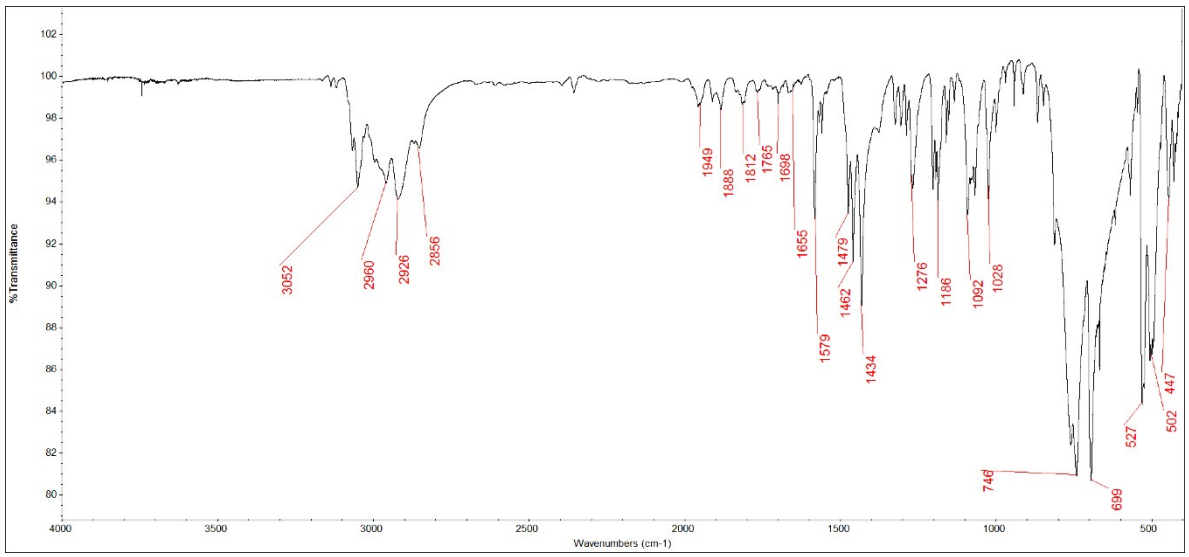


Figure S10. FT- IR spectrum of compound **2** as KBr pellet.

3. Spectroscopic characterization of compound **3**

3.1 NMR spectroscopy

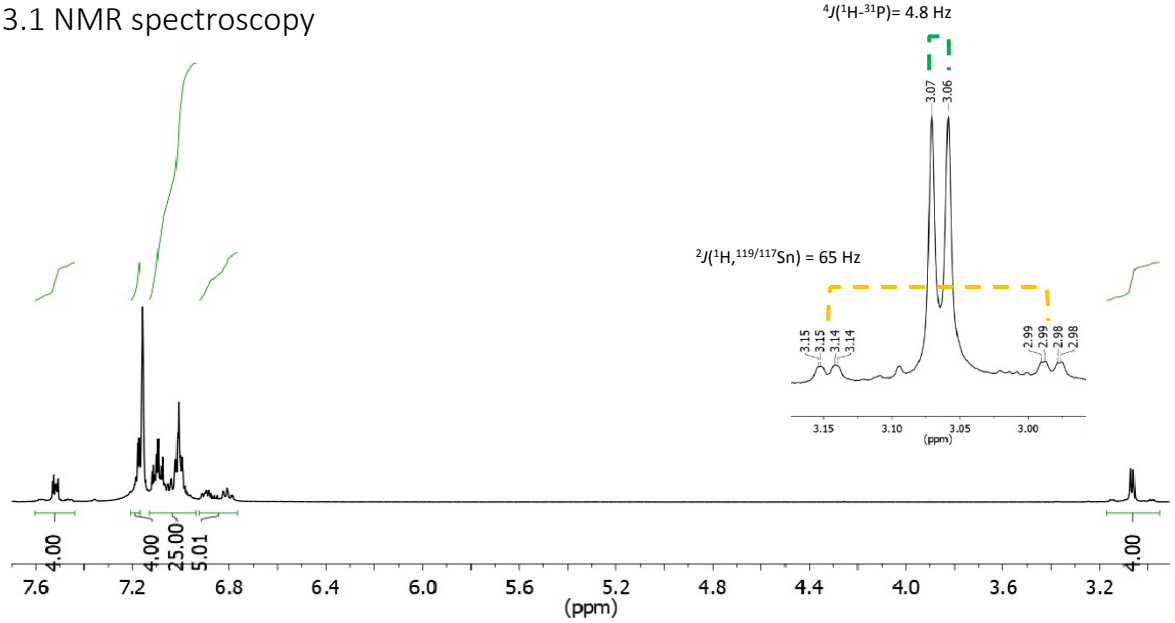


Figure S11. ^1H NMR spectrum (400 MHz, C_6D_6, 298 K) of compound **3**.

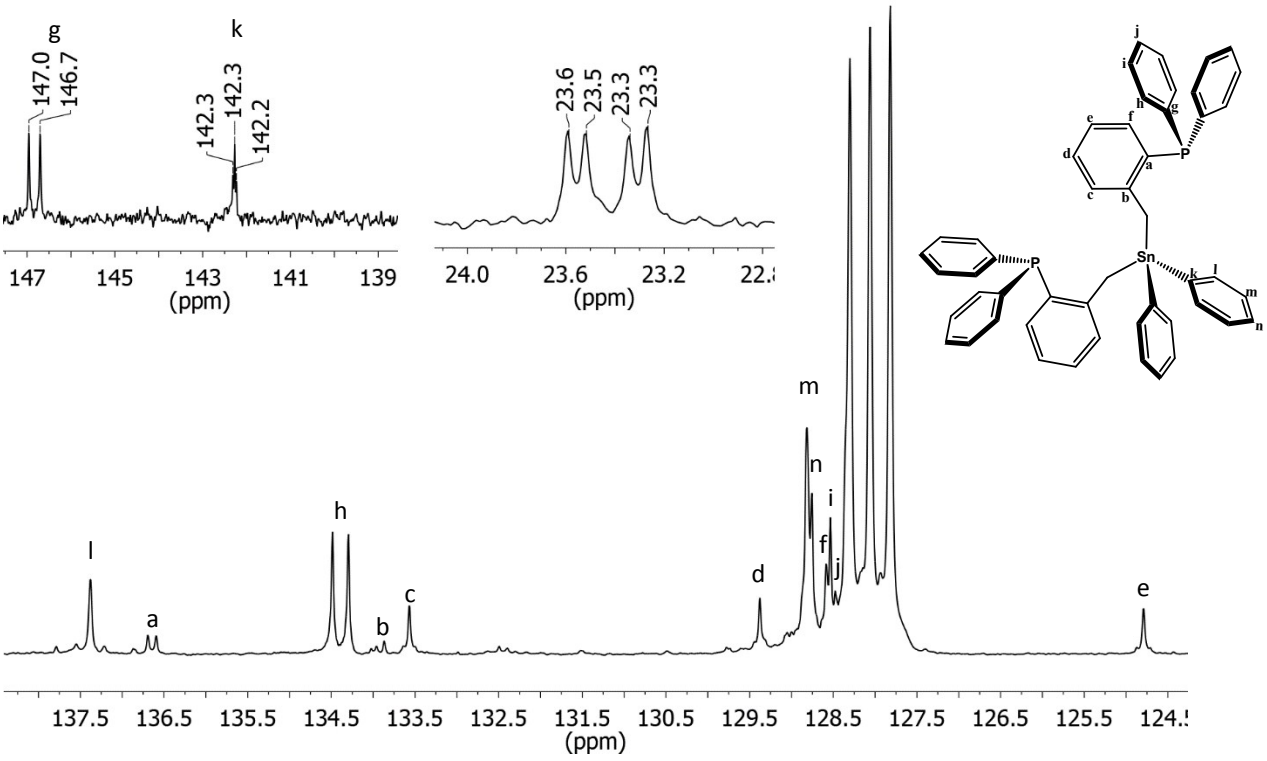


Figure S12. $^{13}C\{^1H\}$ NMR spectrum of compound **3** (100.65 MHz, C_6D_6, 298 K).

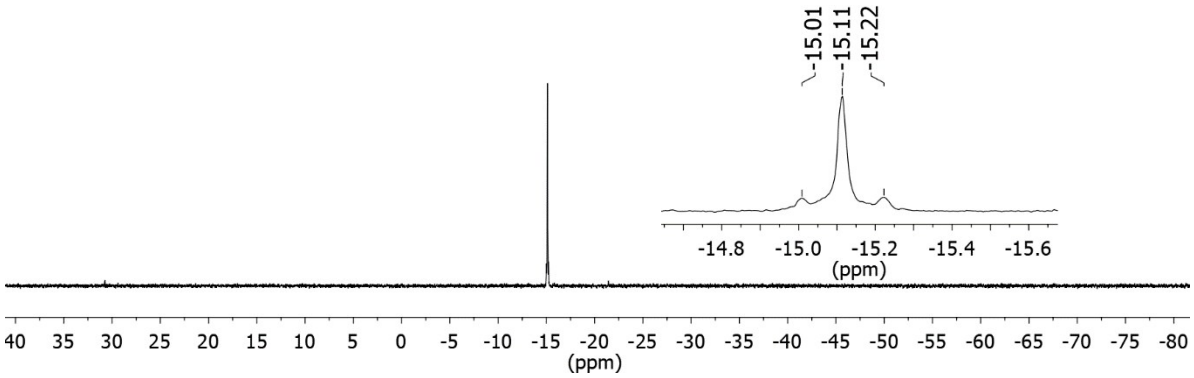


Figure S13. $^{31}P\{^{1}H\}$ NMR spectrum of compound **3** (161.97 MHz, C_6D_6, 298 K).

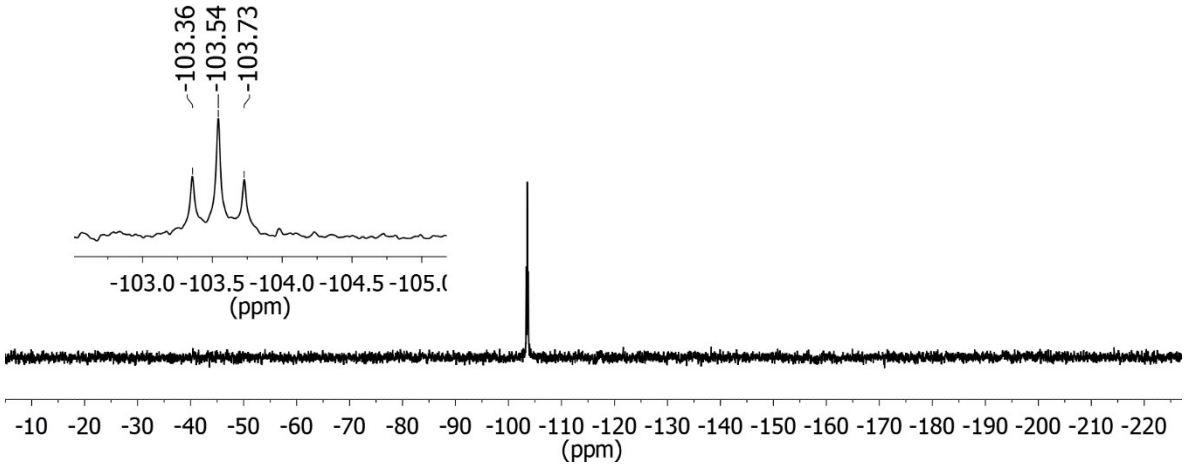


Figure S14. $^{119}Sn\{^{1}H\}$ NMR spectrum of compound **3** (149.21 MHz, C_6D_6, 298 K).

3.2 FT-IR spectroscopy

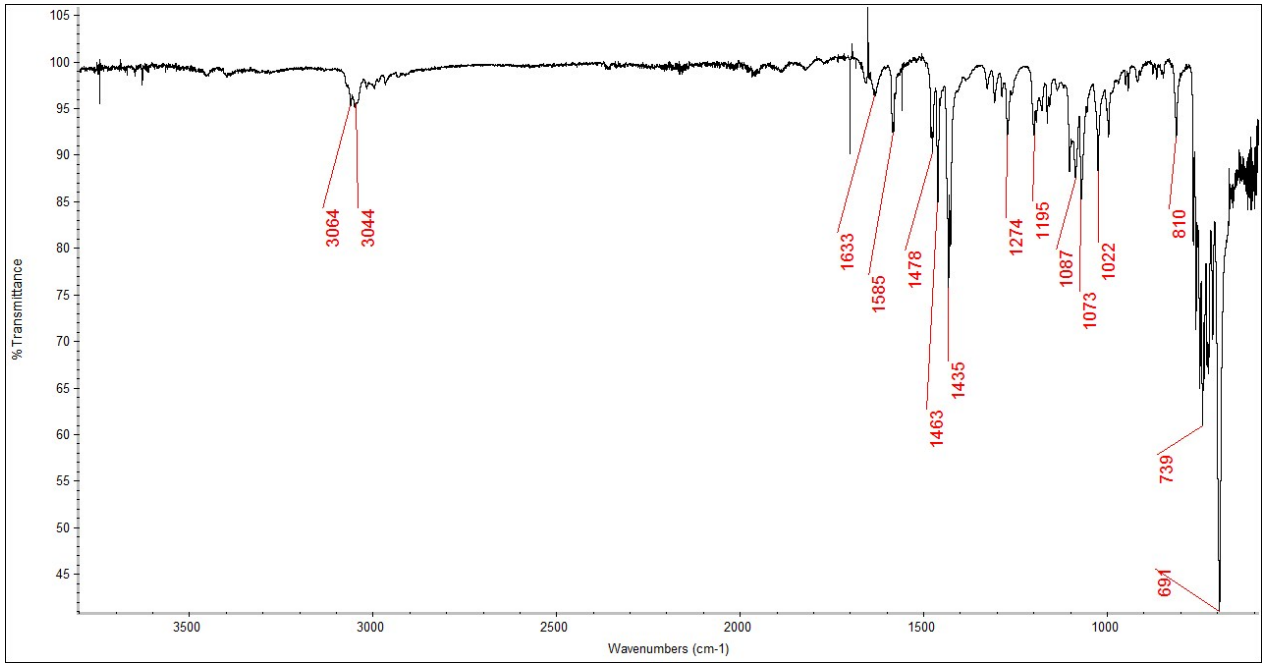


Figure S15. FT- IR spectrum of compound **3** as KBr pellet.

4. Spectroscopic characterization of compound **4**

4.1 NMR spectroscopy

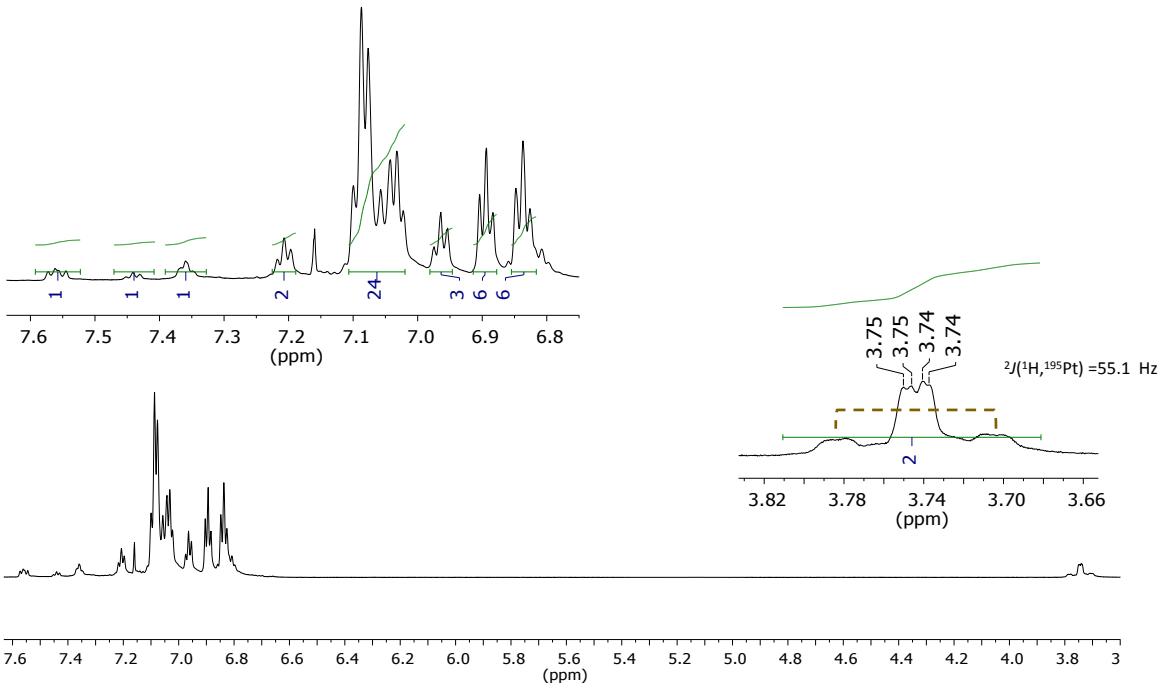


Figure S16. ^1H NMR spectrum (700 MHz, $CDCl_3$) of compound **4** at room temperature.

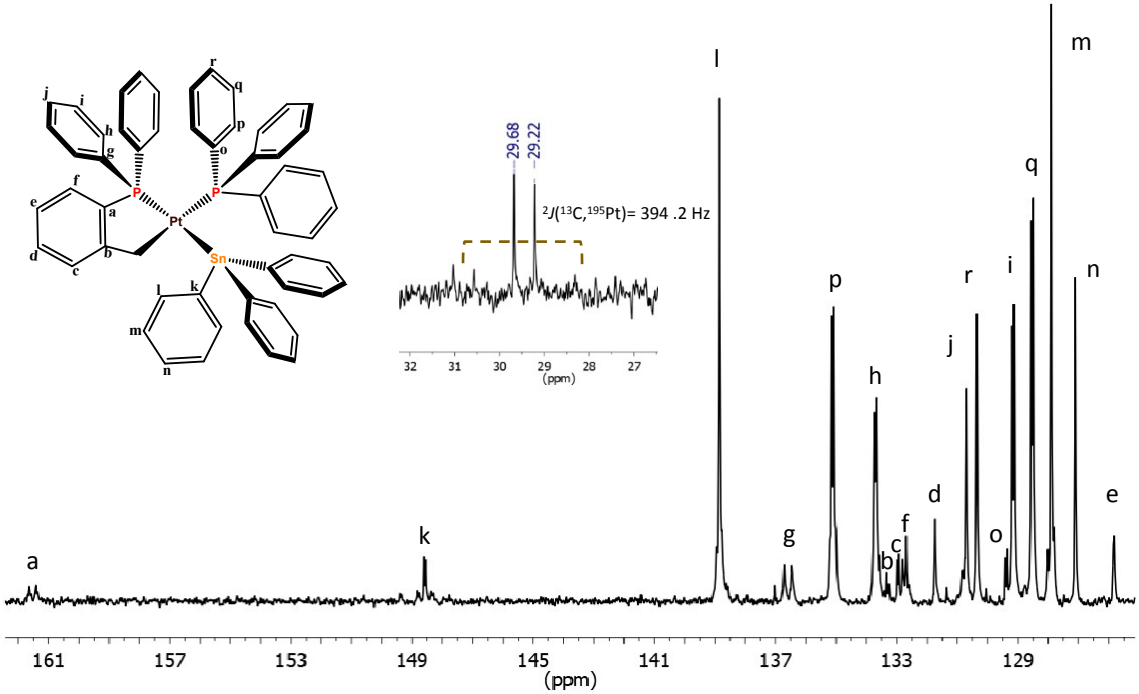


Figure S17. $^{13}C\{^1H\}$ NMR spectrum of compound **4** (176.04 MHz, $CDCl_3$, 298 K).

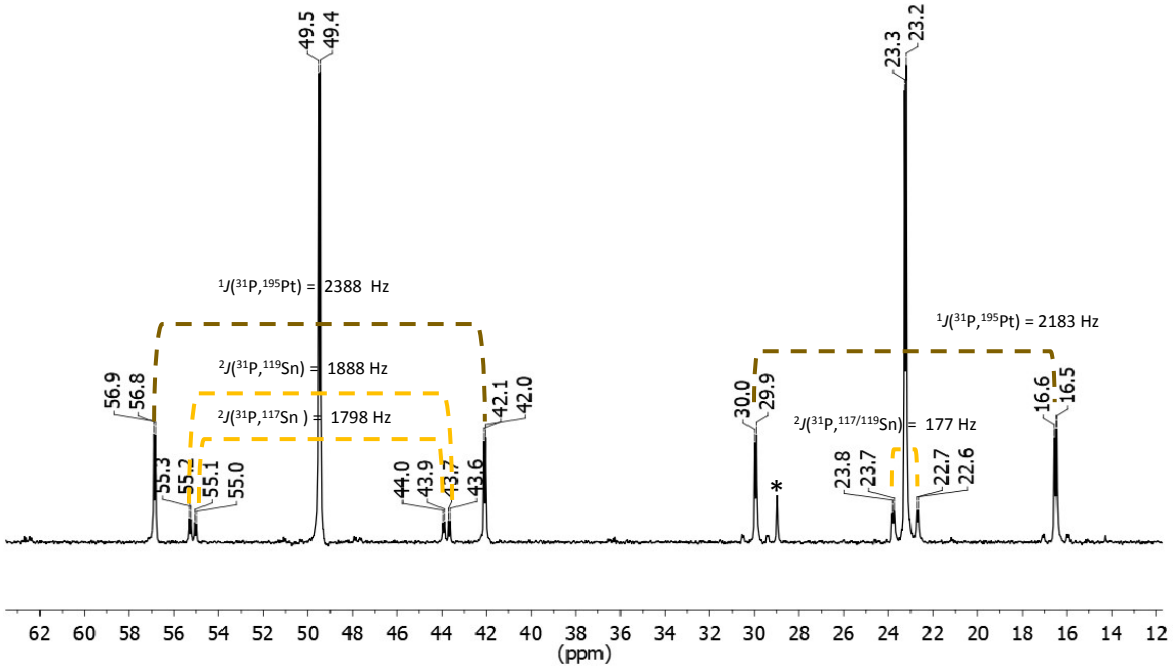


Figure S18. $^{31}P\{^1H\}$ NMR spectrum of compound **4** (161.97 MHz, C_6D_6, 298 K). * denotes $OPPh_3$ as impurity

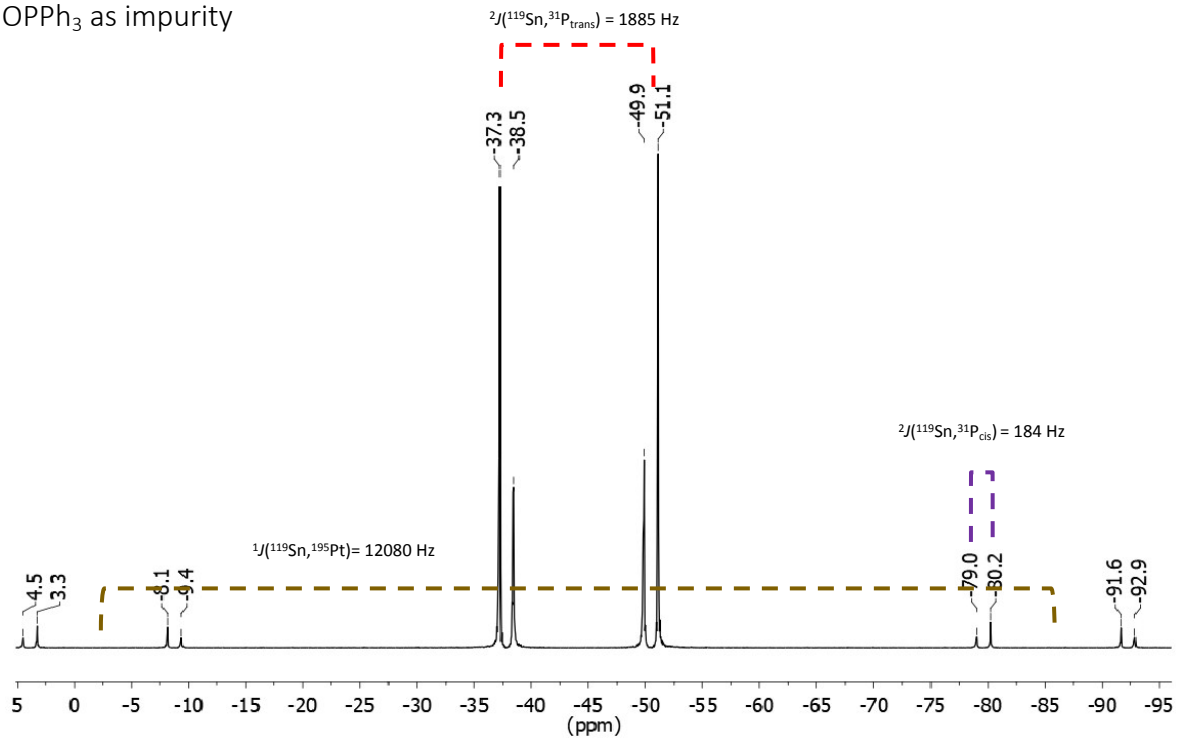


Figure S19. $^{119}Sn\{^1H\}$ NMR spectrum for **4** (149.21 MHz, C_6D_6, 298 K).

4.2 FT-IR spectroscopy

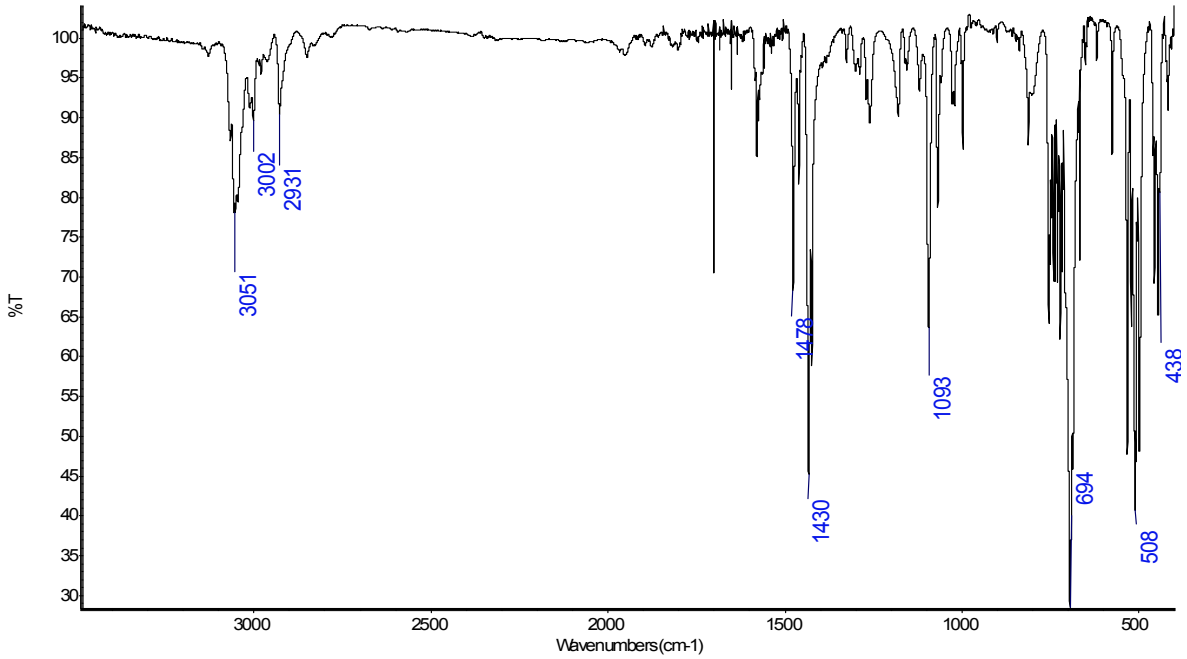


Figure S20. FT- IR spectrum for **4** as KBr pellet.

5. Spectroscopic characterization of complex **5**

5.1 NMR spectroscopy

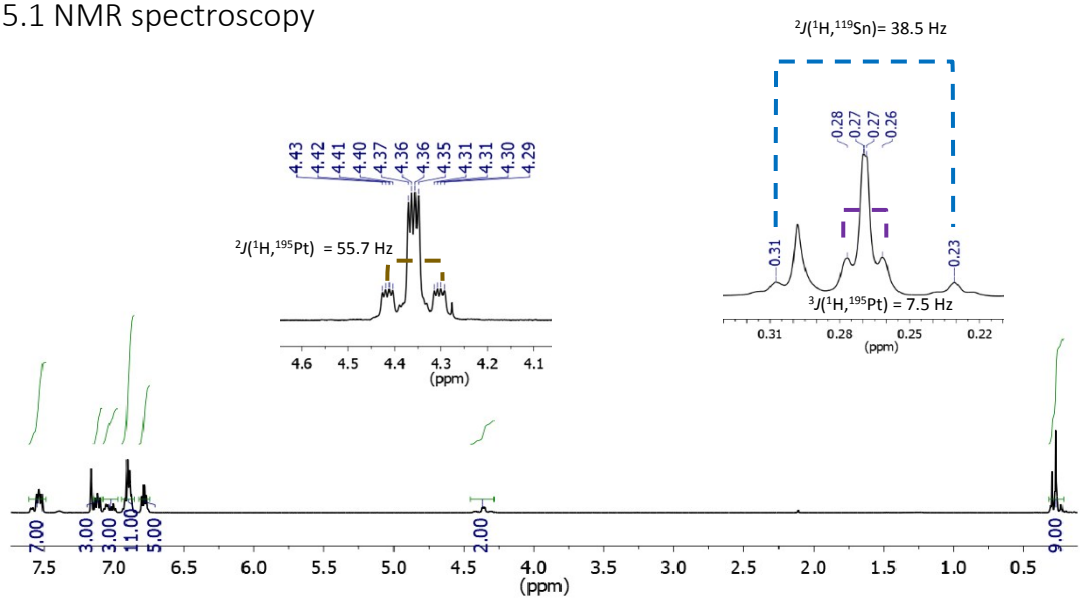


Figure S21. ^1H NMR spectrum (500 MHz, C_6D_6, 298 K) for **5**.

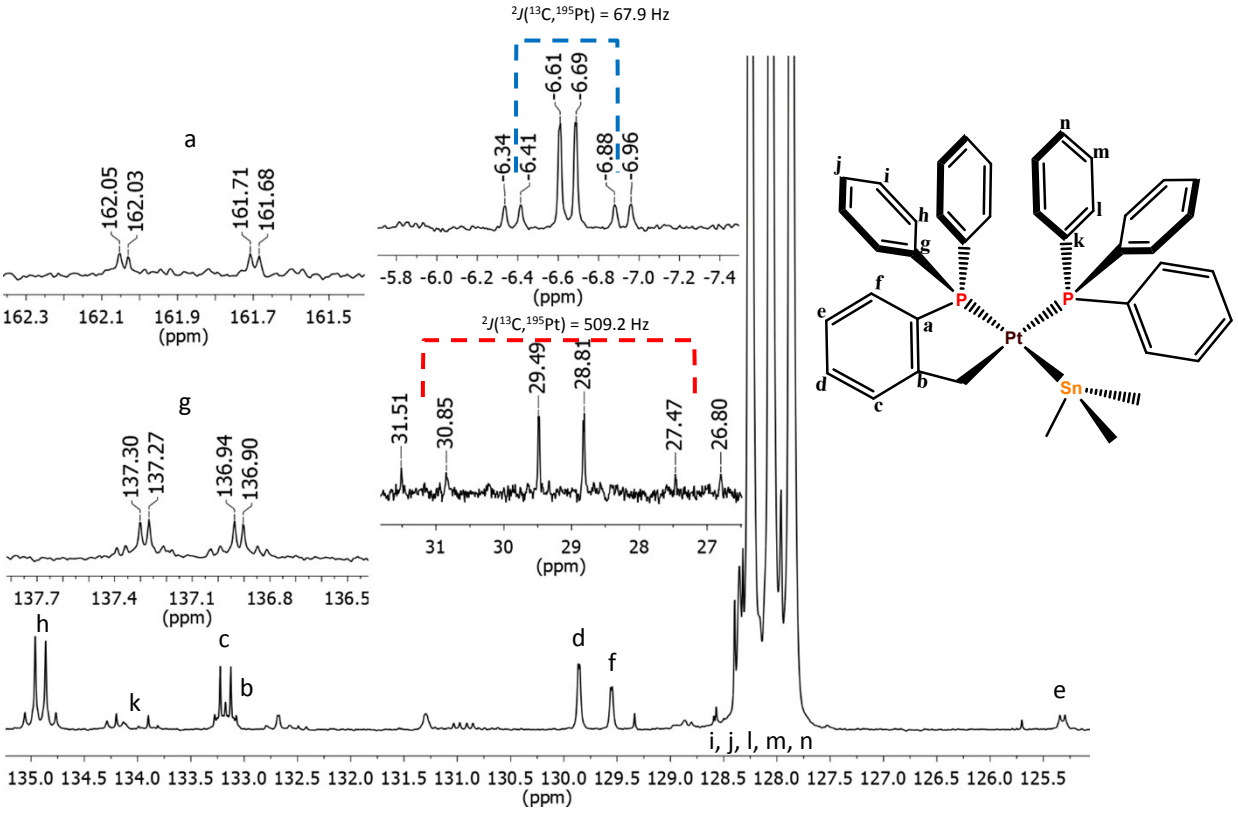


Figure S22. $^{13}C\{^1H\}$ NMR spectrum for **5** (125.75 MHz, C_6D_6, 298 K).

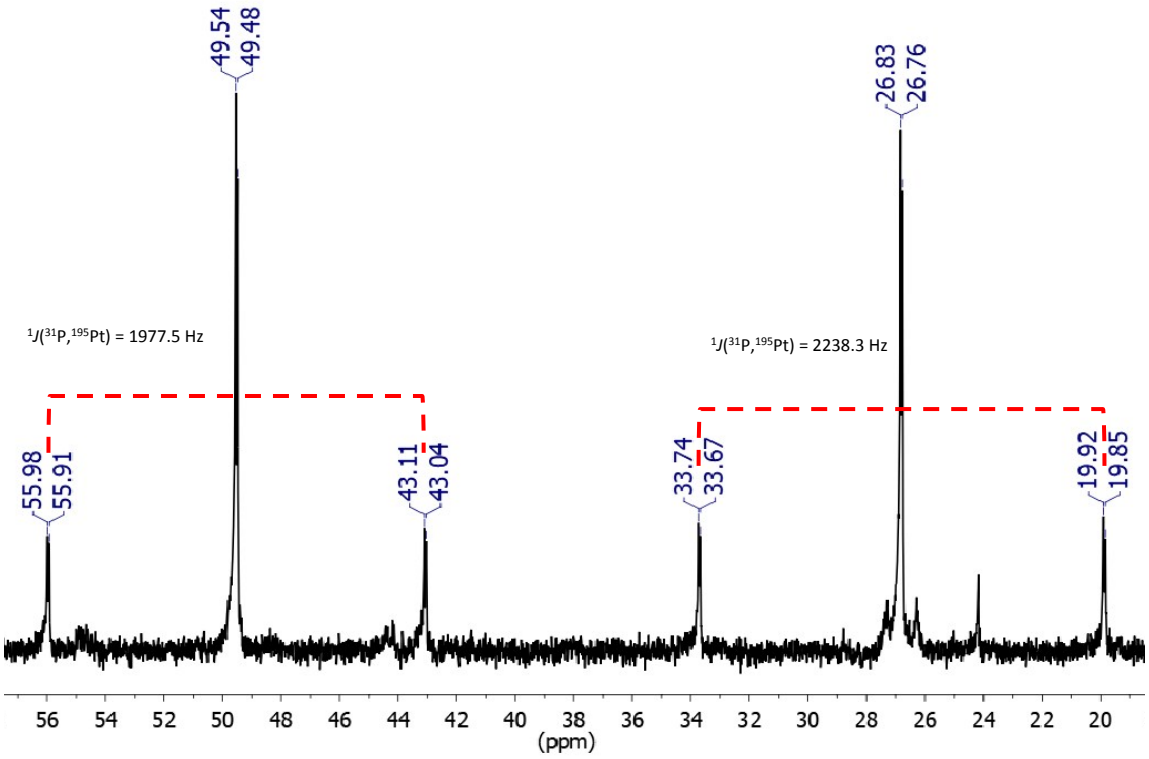


Figure S23. $^{31}P\{^1H\}$ NMR spectrum for **5** (161.97 MHz, C_6D_6, 298 K).

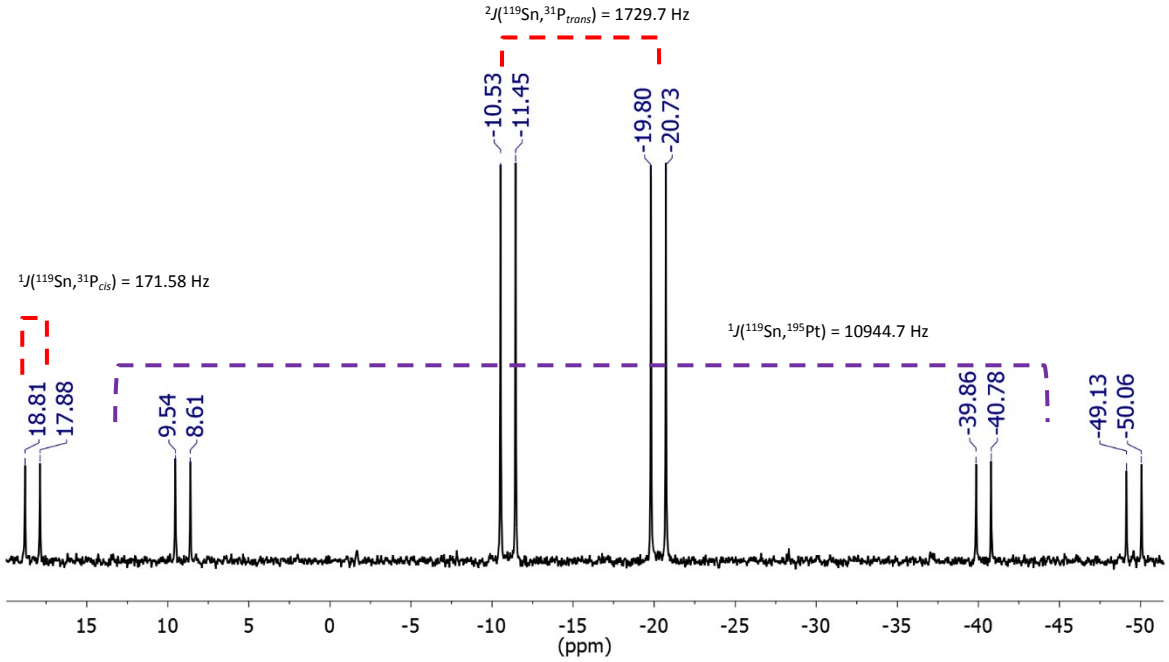


Figure S24. $^{119}Sn\{^1H\}$ NMR spectrum for **5** (186.50 MHz, C_6D_6, 298 K).

6. Spectroscopic characterization of complex **6**

6.1 NMR spectroscopy

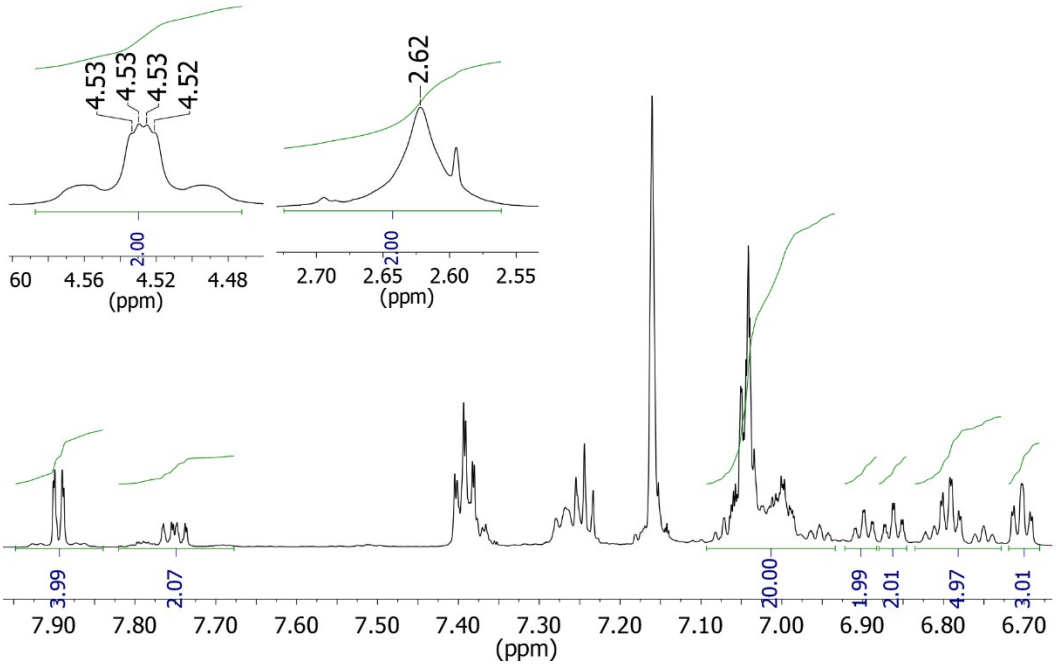


Figure S25. ^{1}H NMR spectrum for **6** (700 MHz, C_6D_6, 298 K).

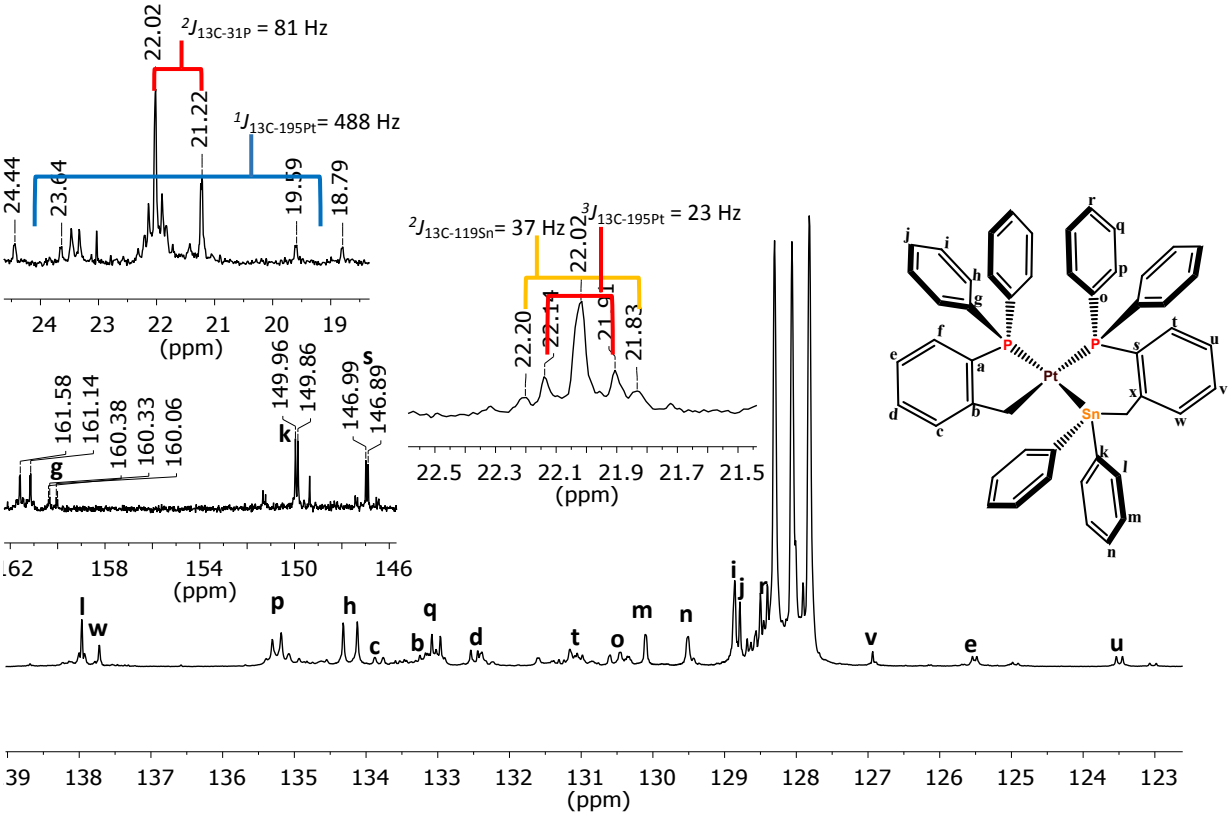


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum for **6** (100.61 MHz, C_6D_6, 298 K).

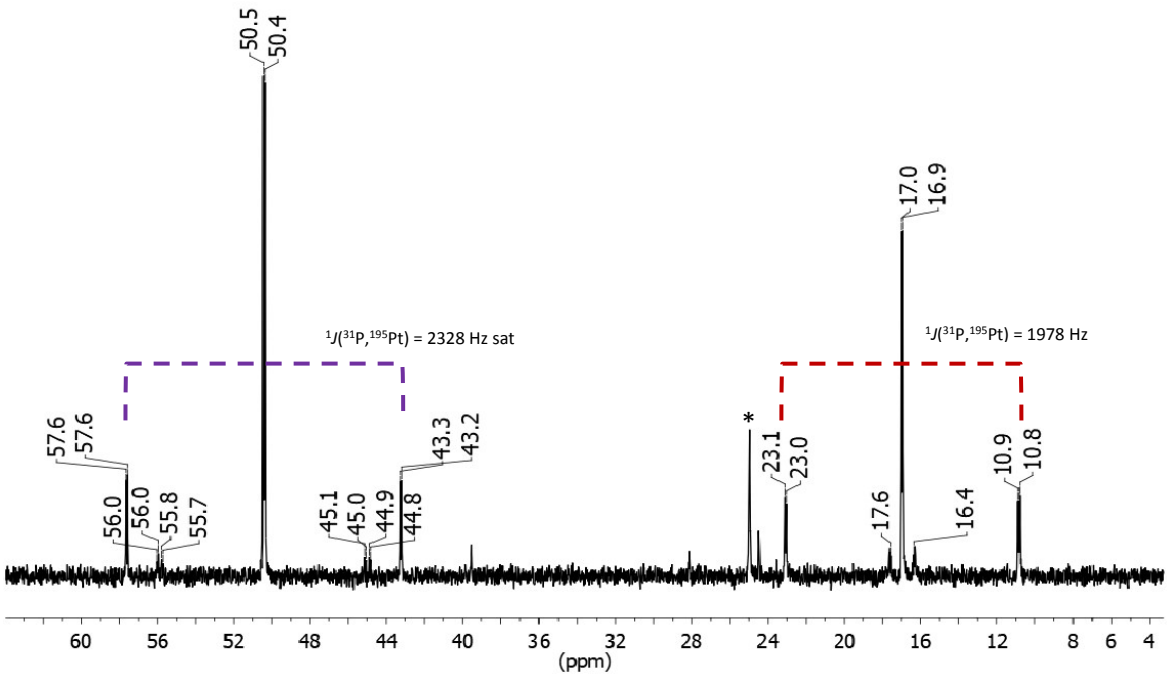


Figure S27. $^{31}P\{^1H\}$ NMR spectrum for **6** (161.97 MHz, C_6D_6, 298 K).

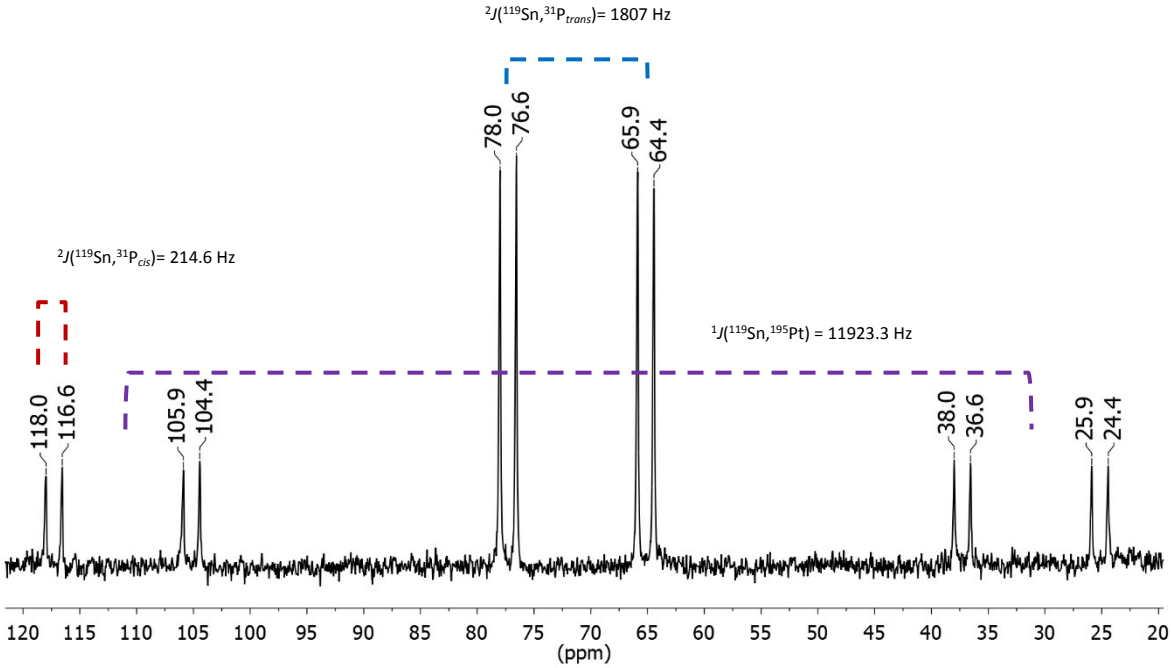


Figure S28. $^{119}Sn\{^1H\}$ NMR spectrum of complex **6** (149.21 MHz, C_6D_6, 298 K).

6.2 FT-IR spectroscopy

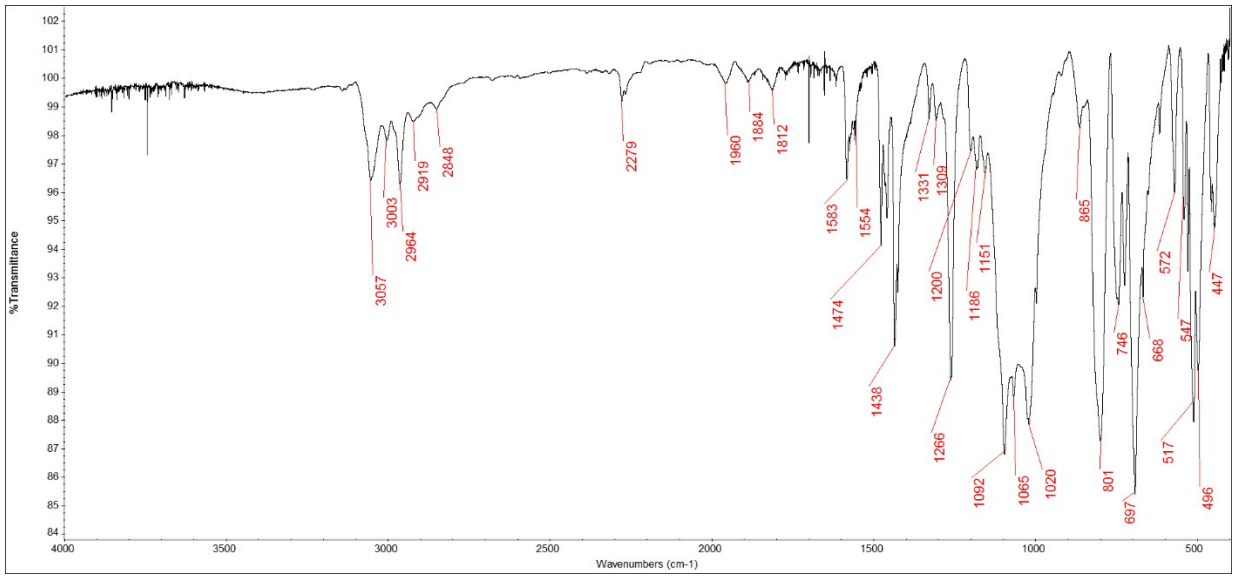


Figure S29. FT- IR spectrum of complex **6** as KBr pellet.

7. Summary of crystal data and molecular structures for 1-6.

Table S1. Crystal data and structure refinement

Complex	1	2	3	4	5	6
Molecular formula	$C_{37}H_{31}PSn$	$C_{22}H_{25}PSn$	$C_{50}H_{42}P_2Sn$	$C_{55}H_{46}P_2PtSn$	$C_{40}H_{40}P_2PtSn$	$C_{50}H_{42}P_2PtSn$
Formula Weight	625.28	439.08	823.46	1082.64	896.44	1018.55
T/K	100(2)	100(3)	100(2)	100(2)	100(2)	100(2)
λ(Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Monoclinic	Triclinic
Space group	P1	P-1	P-1	P-1	P2(1)/c	P-1
a(Å)	11.44027(17)	10.7778(3)	11.0985(7)	10.1200(6)	9.9322(2)	10.1448(3)
b(Å)	11.6827(18)	10.9555(3)	11.5385(5)	13.4335(11)	28.0658(3)	12.7959(4)
c(Å)	12.1997(19)	19.6759(4)	16.3580(11)	16.6547(13)	28.8753(6)	17.5669(5)
α(°)	103.668(3)	77.307(2)	100.250(5)	87.478(7)	90	93.852(2)
β(°)	94.851(2),	85.848(2)	103.764(6)	80.408(6)	120.936(3)	99.343(2)
γ (°)	101.453(2)	62.788(2)	92.688(4)	76.369(6)	90	112.307(3)
Volume [Å^3]	1532.9(4)	2014.57(10)	1993.4(2)	2169.6(3)	6904.1(3)	2060.91(10)
Z	2	4	2	2	8	2
ρ_{calcd}(g/cm^3)	1.355	1.448	1.372	1.657	1.725	1.641
Abs. Coeff(mm^{-1})	0.909	1.348	0.756	3.908	4.892	4.108
Reflections collected	26528	31457	25938	19226	35608	41885
Independent reflns [R_{int}]	7475 [0.0368]	9697[0.0303]	7012[0.1509]	10111 [0.0611]	15653[0.0336]	8961 [0.0519]
Completeness to θmax	97.70 %	99.89%	99.80 %	99.70 %	83.70%	99.60 %
Data/restraints/parameters	7475/0/352	9697/0/439	7012/72/478	10111/0/532	15653/0/799	8961/0/487
GOF[a] on F^2	1.017	1.026	1.066	0.864	1.057	1.029
R_1[b] (I>2σ)	0.0439	0.0255	0.0779	0.0483	0.333	0.0341
wR_2[c](I>2σ)	0.0998	0.0531	0.1824	0.0607	0.0768	0.0801
R_1 (all data)	0.0465	0.0314	0.0952	0.0893	0.0415	0.0413
wR_2(all data)	0.1016	0.0558	0.1987	0.0721	0.0807	0.0854
Largest diff. Peak, hole	1.062 & -0.730	0.45& -0.49	3.18 & -1.54	1.43 & -1.34	1.66 & -1.36	1.97 & -2.38

[a]GOF = $(\Sigma w(F_o^2 - F_c^2)^2/(n - p))^{1/2}$ where n is the number of data and p is the number of parameters refined. [b]$R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [c]w$R2 = (\Sigma\ (w(F_o^2 - F_c^2)^2)/\Sigma\ (w(F_o^2)^2))^{1/2}$

7.1. X-Ray diffraction of complex 1

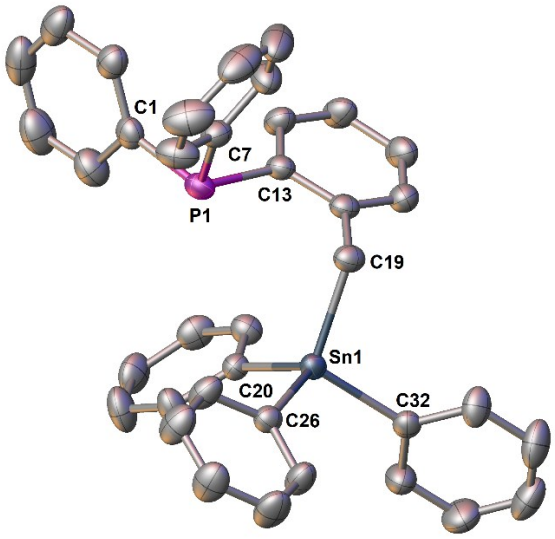


Figure S30. ORTEP drawing for **1** showing ellipsoids at 30% probability level.

Table S2. X-Ray diffraction bond distances and angles for 1.

Bond Distances (Angstrom)

C19 Sn1 2.168(3)

C20 Sn1 2.127(3)

C26 Sn1 2.134(3)

C32 Sn1 2.133(3)

C1 P1 1.827(4)

C7 P1 1.832(3)

C13 P1 1.827(3)

Bond Angles (Degrees)

C20 Sn1 C19 113.77(12)

C20 Sn1 C26 109.35(12)

C20 Sn1 C32 108.12(12)

C26 Sn1 C19 108.98(13)

C26 Sn1 C32 109.68(11)

C32 Sn1 C19 106.87(13)

C24 C25 P1 122.0(6)

C20 C25 P1 118.2(5)

C31 C26 P1 126.6(8)

C27 C26 P1 119.3(9)

C37 C32 P1 127.6(8)

C33 C32 P1 111.3(8)

7.2. X-Ray diffraction of complex 2.

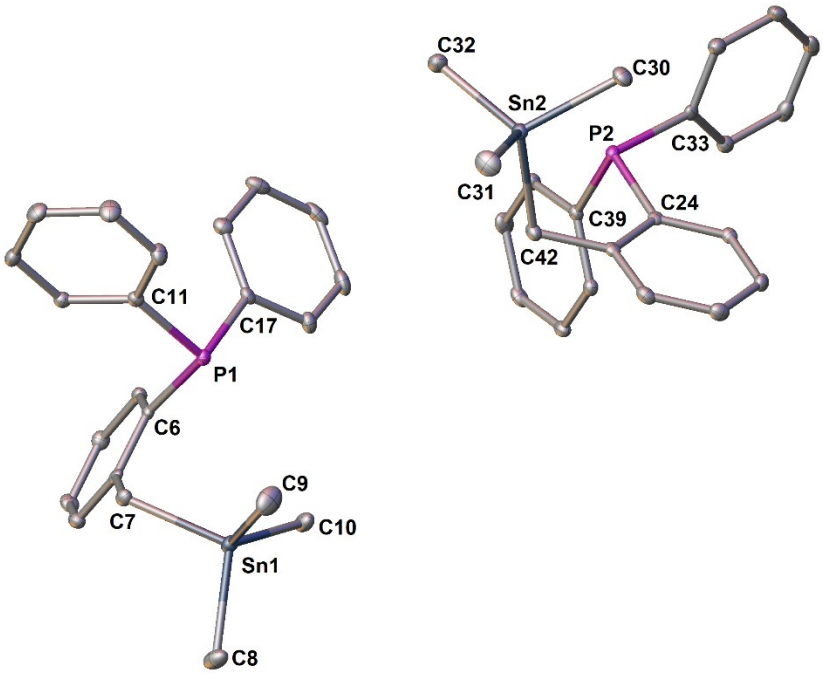


Figure S31. ORTEP drawing for **2** showing ellipsoids at 30% probability level.

Table S3. X-Ray diffraction bond distances and angles for **2**.

Bond Distances (Angstrom)

Sn1	C7	2.176(2)		Sn2	C29	2.1768(19)	
Sn1	C8	2.147(2)		Sn2	C30	2.142(2)	
Sn1	C9	2.140(2)		Sn2	C31	2.138(2)	
Sn1	C10	2.136(2)		Sn2	C32	2.137(2)	
P1	C6	1.8436(19)		P2	C24	1.8383(19)	
P1	C11	1.837(2)		P2	C33	1.839(2)	
P1	C17	1.8335(19)		P2	C39	1.840(2)	

Bond Angles (Degrees)

C8	Sn1	C7	107.47(9)	C30	Sn2	C29	108.32(8)
C9	Sn1	C7	109.54(9)	C31	Sn2	C29	105.63(9)
C9	Sn1	C8	109.12(10)	C31	Sn2	C30	109.98(9)
C10	Sn1	C7	110.41(8)	C32	Sn2	C29	112.27(8)
C10	Sn1	C8	109.52(8)	C32	Sn2	C30	111.12(8)
C10	Sn1	C9	110.72(10)	C32	Sn2	C31	109.37(10)
C11	P1	C6	102.71(9)	C24	P2	C33	102.49(9)
C17	P1	C6	100.74(9)	C24	P2	C39	101.80(8)
C17	P1	C11	103.27(9)	C33	P2	C39	101.58(9)

7.3 X-Ray diffraction of complex 3

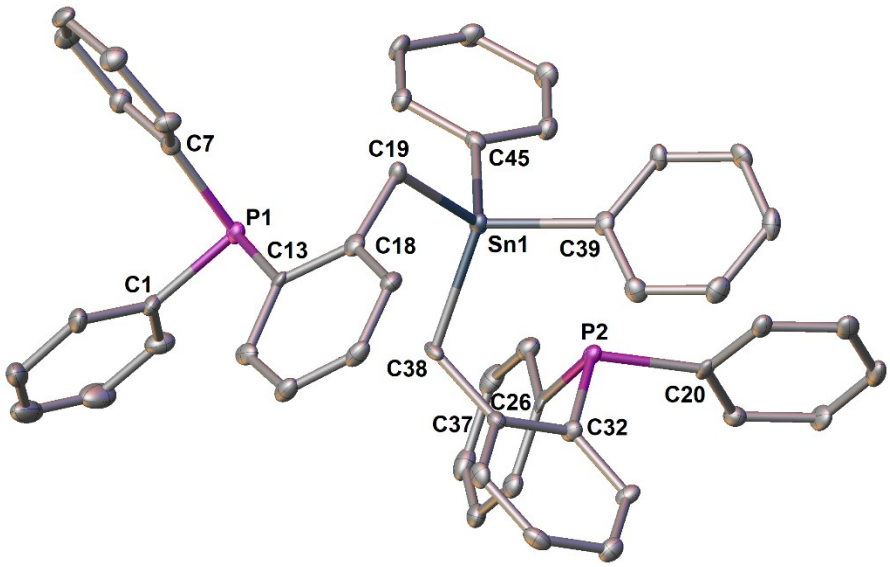


Figure S32. ORTEP drawing for **3** showing ellipsoids at 30% probability level.

7.4 X-Ray diffraction of complex 4

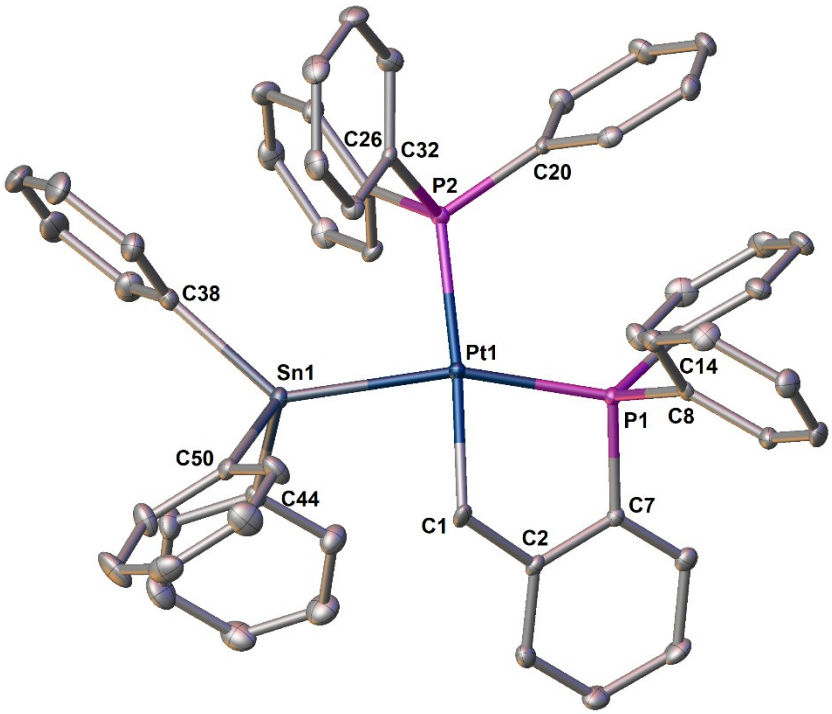


Figure S33. ORTEP drawing for **4** showing ellipsoids at 30% probability level.

Table S4. X-Ray diffraction bond lengths and angles for 4.

Bond Distances (Angstrom)
Pt1 C1 2.128(5)

Pt1 P2 2.2791(14)

Pt1 P1 2.2822(17)

Pt1 Sn1 2.6036(5)

Sn1 C38 2.165(7)

Sn1 C44 2.172(6)

Sn1 C50 2.180(6)

P2 C26 1.819(6)

P2 C20 1.834(6)

P2 C32 1.840(6)

P1 C7 1.813(6)

P1 C14 1.828(6)

P1 C8 1.831(6)

Bond Angles (Degrees)

C1 Pt1 P2 175.04(19)

C1 Pt1 P1 80.27(18)

P2 Pt1 P1 104.14(5)

C1 Pt1 Sn1 84.46(17)

P2 Pt1 Sn1 91.71(4)

P1 Pt1 Sn1 160.19(4)

C38 Sn1 C44 101.7(2)

C38 Sn1 C50 100.4(2)

C44 Sn1 C50 104.4(2)

C38 Sn1 Pt1 129.58(14)

C44 Sn1 Pt1 106.99(18)

C50 Sn1 Pt1 111.18(17)

C26 P2 C20 102.0(2)

C26 P2 C32 107.8(3)

C20 P2 C32 101.2(3)

C26 P2 Pt1 113.29(17)

C20 P2 Pt1 118.9(2)

C32 P2 Pt1 112.37(17)

C7 P1 C14 103.8(3)

C7 P1 C8 105.1(3)

C14 P1 C8 106.4(3)

C7 P1 Pt1 101.6(2)

C14 P1 Pt1 119.3(2)

C8 P1 Pt1 118.5(2)

7.5 X-Ray diffraction of complex 5

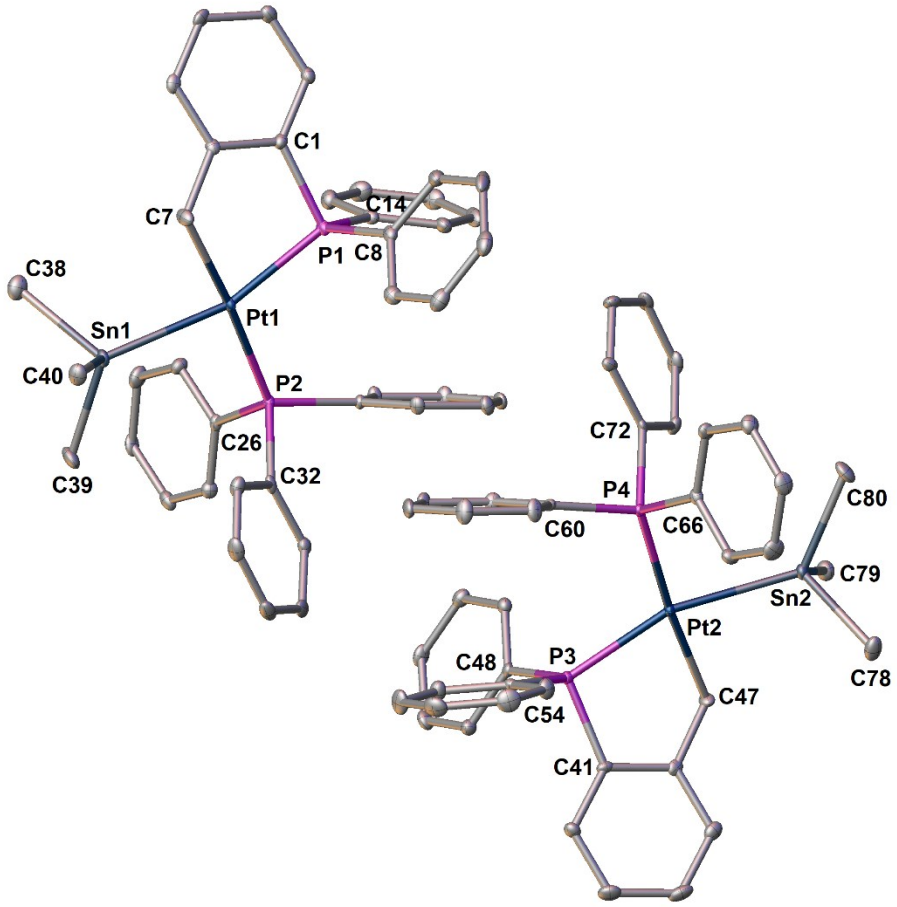


Figure S34. ORTEP drawing for **5** showing ellipsoids at 30% probability level.

Table S5. X-Ray diffraction bond lengths and angles for 5.

Bond Distances (Angstrom)

Pt1	Sn1	2.6026(3)	Pt2	Sn2	2.6019(3)
Pt1	P1	2.2850(11)	Pt2	P3	2.3044(10)
Pt1	P2	2.2775(11)	Pt2	P4	2.2699(11)
Pt1	C1	2.120(4)	Pt2	C47	2.132(4)
Sn1	C38	2.169(5)	Sn2	C78	2.162(4)
Sn1	C39	2.169(5)	Sn2	C79	2.172(4)
Sn1	C40	2.173(4)	Sn2	C80	2.160(5)
P1	C1	1.822(4)	P3	C41	1.822(4)

P1	C8	1.827(4)
P1	C14	1.825(4)
P2	C20	1.832(4)
P2	C26	1.838(4)
P2	C32	1.830(4)
P3	C48	1.829(4)
P3	C54	1.828(4)
P4	C60	1.835(4)
P4	C66	1.833(4)
P4	C72	1.846(4)

P1	Pt1	Sn1	163.77(3)
P2	Pt1	Sn1	92.79(3)
P2	Pt1	P1	102.62(4)
C7	Pt1	Sn1	83.17(11)
C7	Pt1	P1	81.49(12)
C7	Pt1	P2	175.86(11)
C38	Sn1	Pt1	113.51(14)
C38	Sn1	C40	101.94(17)
C39	Sn1	Pt1	122.24(12)
C39	Sn1	C38	101.60(19)
C39	Sn1	C40	103.27(19)
C40	Sn1	Pt1	111.90(12)
C1	P1	Pt1	102.09(13)
C8	P1	Pt1	116.42(14)
C14	P1	Pt1	120.51(14)
C20	P2	Pt1	118.96(14)
C26	P2	Pt1	112.70(14)
C32	P2	Pt1	115.30(14)
P3	Pt2	Sn2	161.31(3)
P4	Pt2	Sn2	93.73(3)
P4	Pt2	P3	104.49(4)
C41	P3	Pt2	100.95(13)
C48	P3	Pt2	117.48(13)
C54	P3	Pt2	121.38(14)
C60	P4	Pt2	117.66(14)
C66	P4	Pt2	112.74(14)
C72	P4	Pt2	115.40(14)

7.6 X-Ray diffraction of complex6

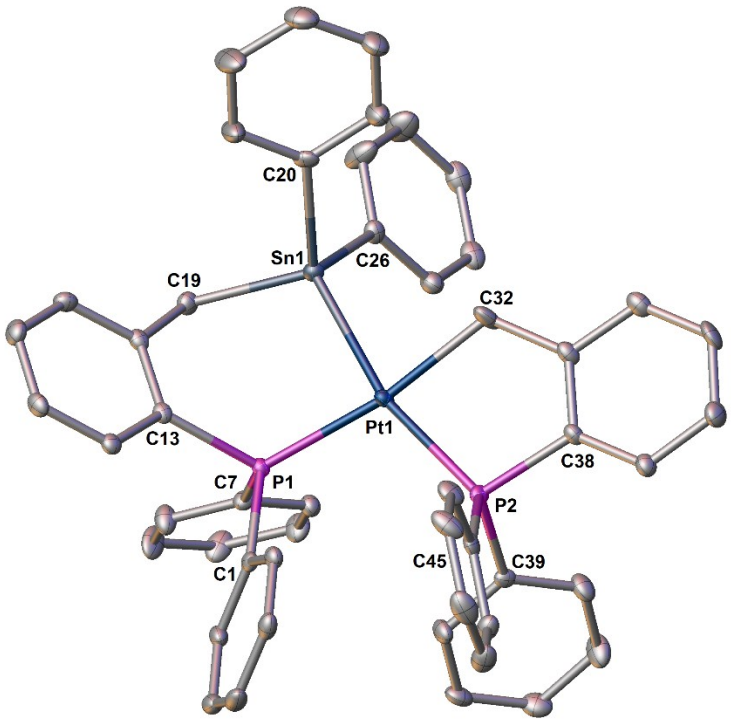


Figure S35. ORTEP drawing for **6** showing ellipsoids at 30% probability level.

Table S6. X-ray diffraction bond distances and angles for 6.

Bond Distances (Angstrom)

Pt1 Sn1 2.5693(4)	P1 C1 1.831(5)
Pt1 P1 2.3007(11)	P1 C7 1.826(4)
Pt1 P2 2.3059(11)	P1 C13 1.863(4)
Pt1 C32 2.117(5)	P2 C38 1.824(5)
Sn1 C19 2.187(5)	P2 C39 1.840(4)
Sn1 C20 2.166(5)	P2 C45 1.821(5)
Sn1 C26 2.152(5)	

Bond Angles (Degrees)

P1 Pt1 Sn1 87.79(3)	C32 Pt1 Sn1 82.23(15)
P1 Pt1 P2 106.37(4)	C32 Pt1 P1 170.01(15)
P2 Pt1 Sn1 164.48(3)	C32 Pt1 P2 83.52(15)

C19 Sn1 Pt1 110.03(13)

C20 Sn1 Pt1 118.35(13)

C20 Sn1 C19 106.96(18)

C26 Sn1 Pt1 112.15(13)

C26 Sn1 C19 105.54(18)

C26 Sn1 C20 102.85(18)

C1 P1 Pt1 116.11(15)

C7 P1 Pt1 111.32(16)

C13 P1 Pt1 119.55(15)

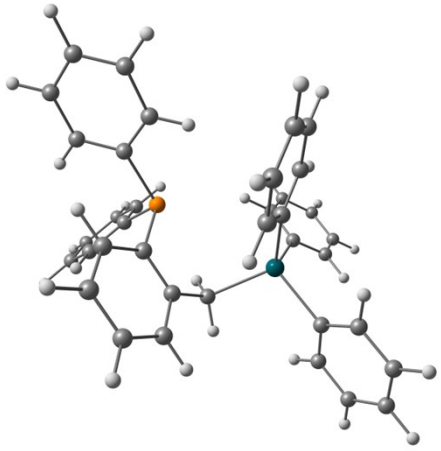
C38 P2 Pt1 103.32(15)

C39 P2 Pt1 116.63(14)

C45 P2 Pt1 122.31(15)

8. DFT computations for **1**, **3**, and PPh_3 and complexes **4**, **4B**, **6**, **6B**, and $[Pt(PPh_3)_3]$.

8.1 Cartesian coordinates for **1**.



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1	-0.081597000	2.060958000	1.803721000
6	1.058803000	3.593841000	2.786174000
1	0.187501000	4.024971000	3.273531000
6	2.322313000	4.153367000	2.990666000
1	2.437317000	5.020130000	3.636679000
6	3.436896000	3.595327000	2.361220000
1	4.422945000	4.026760000	2.516071000
6	3.286880000	2.480083000	1.531530000
1	4.167645000	2.060307000	1.050219000
6	3.750356000	-0.283927000	-0.838381000
6	4.338416000	0.565801000	-1.792376000
1	3.824843000	1.471019000	-2.112699000
6	5.587097000	0.274515000	-2.348847000
1	6.023677000	0.946175000	-3.084142000
6	6.272080000	-0.879519000	-1.961265000
1	7.242771000	-1.108952000	-2.393511000
6	5.703845000	-1.737475000	-1.017264000
1	6.231469000	-2.638239000	-0.712900000
6	4.455371000	-1.440215000	-0.462544000
1	4.027861000	-2.123822000	0.267939000
6	1.172686000	-1.536139000	1.189348000
6	1.028433000	-1.429905000	2.583657000
1	1.220554000	-0.481415000	3.080512000
6	0.635323000	-2.528561000	3.353988000

1	0.532011000	-2.425438000	4.431543000
6	0.378561000	-3.756866000	2.739977000
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6	0.516472000	-3.880831000	1.355572000
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6	0.454730000	0.628255000	-1.671439000
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6	-0.005797000	-1.386752000	-3.089111000
1	0.935707000	-1.179086000	-3.593297000
6	-0.762092000	-2.493061000	-3.473131000
1	-0.407024000	-3.139664000	-4.271556000
6	-1.972919000	-2.760532000	-2.833165000
1	-2.574698000	-3.617231000	-3.124558000
6	-2.411147000	-1.913978000	-1.814255000
1	-3.353778000	-2.124583000	-1.319247000
6	-1.658925000	-0.798618000	-1.413736000
6	-3.566630000	-0.649717000	0.773463000
6	-3.224654000	-1.556869000	1.792272000
1	-2.181939000	-1.684805000	2.073189000
6	-4.210317000	-2.292532000	2.451461000
1	-3.927561000	-2.992787000	3.233145000
6	-5.555904000	-2.119743000	2.117083000
1	-6.324906000	-2.684958000	2.637084000
6	-5.908742000	-1.211615000	1.116644000
1	-6.953910000	-1.069212000	0.853760000
6	-4.921897000	-0.483487000	0.447262000
1	-5.209409000	0.217922000	-0.330132000
6	-3.048067000	1.685318000	-0.867985000
6	-3.238757000	2.873496000	-0.141133000
1	-2.881469000	2.938951000	0.884126000
6	-3.877192000	3.971925000	-0.718250000
1	-4.017986000	4.880948000	-0.139352000
6	-4.321703000	3.906502000	-2.041192000
1	-4.810723000	4.764038000	-2.495693000
6	-4.128417000	2.736588000	-2.778812000
1	-4.468988000	2.680021000	-3.809583000
6	-3.498825000	1.633485000	-2.196828000
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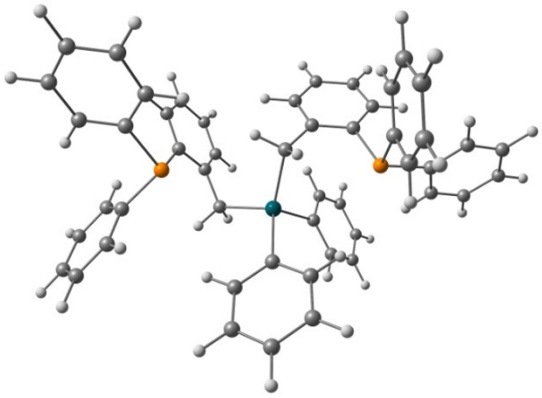
15	-2.178277000	0.293180000	-0.006609000

8.2 Cartesian coordinates for **3**.



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6	6.859597000	-1.338451000	-0.345494000
1	7.105936000	-2.369204000	-0.586869000
6	7.872172000	-0.381821000	-0.235175000
1	8.910133000	-0.664387000	-0.390338000
6	7.544366000	0.937815000	0.082473000
1	8.326855000	1.687001000	0.173494000
6	6.210559000	1.303356000	0.282064000
1	5.968751000	2.333680000	0.524705000
6	3.418707000	2.371064000	1.275948000
6	3.491653000	2.399316000	2.679641000
1	3.529662000	1.464423000	3.234163000
6	3.510017000	3.610753000	3.371907000
1	3.569675000	3.612484000	4.457132000
6	3.437355000	4.817236000	2.671057000
1	3.442115000	5.761762000	3.208630000
6	3.350540000	4.803656000	1.277293000
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6	3.343455000	3.590565000	0.584187000
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6	2.758566000	1.089025000	-1.239606000
6	3.620036000	1.304547000	-2.327463000
1	4.693526000	1.291155000	-2.167379000
6	3.127509000	1.532564000	-3.612520000
1	3.815848000	1.697611000	-4.437203000
6	1.748213000	1.548956000	-3.824108000

1	1.346187000	1.727557000	-4.818256000
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6	1.355121000	1.103982000	-1.451600000
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1	-0.610299000	1.290190000	-0.619521000
1	0.660761000	1.324337000	0.597526000
6	-0.182697000	-1.624971000	2.244133000
6	-1.380701000	-2.064242000	2.832504000
1	-2.268465000	-2.220714000	2.224190000
6	-1.465043000	-2.303995000	4.207382000
1	-2.402671000	-2.643913000	4.640733000
6	-0.347835000	-2.108141000	5.021677000
1	-0.411409000	-2.294538000	6.090828000
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1	1.725199000	-1.514859000	5.083527000
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1	1.874368000	-1.086304000	2.659733000
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1	3.533466000	-5.151164000	0.272945000
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6	2.846019000	-3.395082000	-2.558917000
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1	-3.700247000	1.341810000	-4.816715000
6	-3.698714000	0.955149000	-2.696743000
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6	-3.265838000	0.131759000	-1.644411000
6	-4.969752000	-0.660913000	0.570671000
6	-5.210543000	-0.885208000	1.937732000

1	-4.608638000	-0.367337000	2.680955000
6	-6.208866000	-1.768214000	2.352389000
1	-6.384186000	-1.926020000	3.413349000
6	-6.972514000	-2.455193000	1.405318000
1	-7.744503000	-3.149484000	1.726231000
6	-6.734624000	-2.251248000	0.044323000
1	-7.322772000	-2.785628000	-0.697378000
6	-5.742567000	-1.359242000	-0.370901000
1	-5.565377000	-1.208333000	-1.431698000
6	-4.515531000	2.146775000	0.042227000
6	-3.749060000	3.312851000	0.210497000
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1	-3.736279000	5.464496000	0.299105000
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1	-6.193228000	5.668807000	-0.043572000
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6	-5.901145000	2.275738000	-0.146366000
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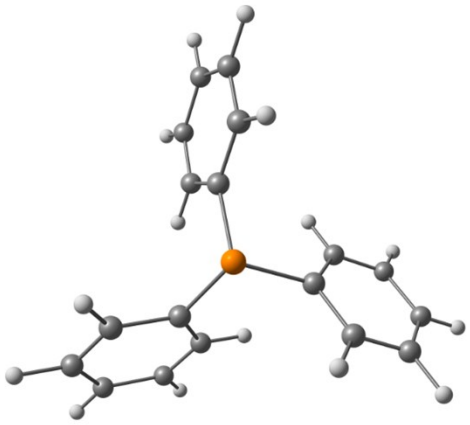
8.3 Cartesian coordinates for PPh_3.



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6	0.053533000	-2.780678000	-1.034749000
6	-0.221208000	-4.043191000	-0.507918000
6	-0.990341000	-4.164251000	0.652264000
6	-1.477700000	-3.017009000	1.281762000
6	-1.193030000	-1.752524000	0.759993000
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1	0.155750000	-4.931445000	-1.008097000
1	-1.213926000	-5.146977000	1.058846000
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1	-1.578226000	-0.868306000	1.258657000
6	2.387329000	1.431520000	-1.038479000
6	3.618097000	1.824063000	-0.511264000
6	4.103414000	1.223521000	0.653209000
6	3.349279000	0.233568000	1.286769000
6	2.111869000	-0.151407000	0.764436000
1	2.025150000	1.891491000	-1.955168000
1	4.201932000	2.590376000	-1.014428000
1	5.066244000	1.520982000	1.060050000
1	3.722986000	-0.241033000	2.190513000
1	1.535233000	-0.922259000	1.266611000
6	-0.922679000	1.912229000	0.758063000
6	-1.876365000	2.790343000	1.279242000
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6	-3.393535000	2.210362000	-0.508419000
6	-2.436629000	1.341883000	-1.034801000
1	0.035945000	1.806094000	1.256661000
1	-1.650575000	3.357993000	2.178402000

1	-3.854566000	3.623127000	1.056972000
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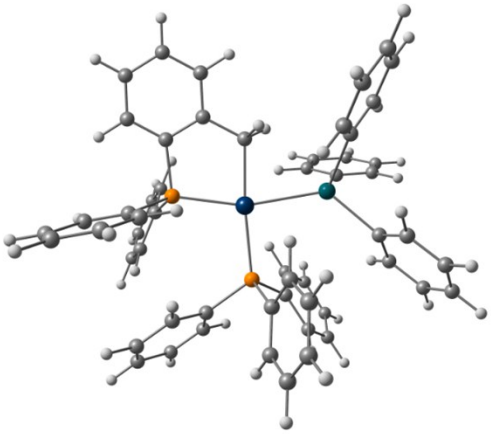
1	-2.655599000	0.792872000	-1.947921000

8.4 Cartesian coordinates for **4**.



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15	0.478285000	1.889383000	0.032878000
15	2.634804000	-1.145134000	0.042733000
6	-3.740319000	1.074664000	0.382604000
6	-1.345747000	2.343898000	-3.619428000
1	-1.435887000	1.736852000	-4.515738000
6	-1.064502000	2.593694000	3.799282000
1	-1.548468000	1.997706000	4.568145000
6	6.022142000	-0.306272000	2.310678000
1	7.100456000	-0.286492000	2.176731000
6	-1.924696000	3.613799000	-3.565366000
1	-2.463521000	4.004706000	-4.424273000
6	-5.631929000	3.131779000	0.844484000
1	-6.359574000	3.920490000	1.021035000
6	4.259438000	0.301552000	-1.794096000
1	4.376810000	1.045961000	-1.014664000
6	2.110512000	2.736184000	-0.255983000
6	5.198019000	-0.619581000	1.227180000
1	5.646048000	-0.834502000	0.262129000
6	-3.355981000	-2.989974000	3.694555000
1	-3.061378000	-2.962365000	4.741539000
6	3.694997000	-3.799069000	0.213047000
1	4.690141000	-3.369390000	0.134679000
6	0.199309000	4.103559000	1.822135000
1	0.720999000	4.696257000	1.077106000
6	-0.674003000	1.991412000	2.600915000
1	-0.843514000	0.931160000	2.442883000
6	3.542891000	-5.177186000	0.321460000
1	4.415424000	-5.824690000	0.328894000

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6	2.434020000	3.350275000	-1.474567000
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1	2.831956000	2.298908000	1.736060000
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1	2.127783000	-6.798468000	0.502610000
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6	-4.301723000	-1.265058000	-2.367713000
1	-5.058604000	-0.853860000	-1.702695000
6	-3.749946000	-2.251372000	-4.510030000
1	-4.055107000	-2.615063000	-5.488330000
6	-4.698116000	-1.733442000	-3.625067000
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6	3.253061000	-0.359286000	2.640926000
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1	-0.003641000	5.764215000	3.173898000
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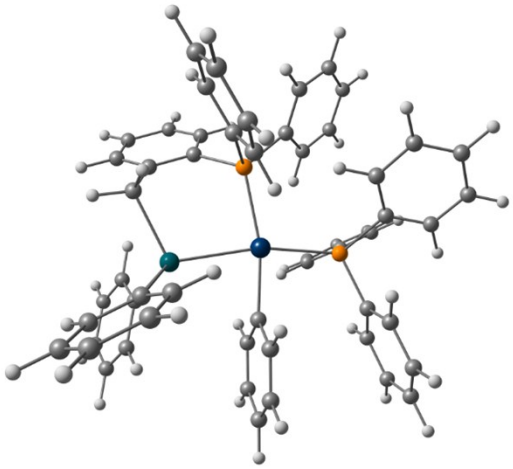
8.5 Cartesian coordinates for **4B**.



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1	-4.455122000	-5.080969000	0.593776000
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6	2.070673000	-3.104523000	-1.071809000
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6	4.399435000	1.766987000	-1.592389000
1	4.328958000	2.377992000	-0.695682000
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6	5.026339000	0.599100000	1.774540000
1	5.564899000	0.494312000	0.834743000
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6	3.705365000	0.892069000	4.209568000
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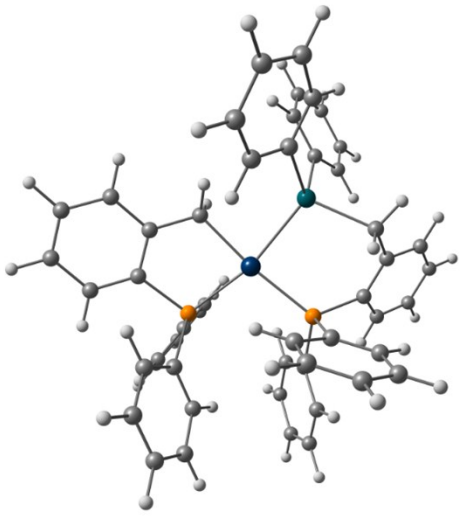
8.6 Cartesian coordinates for **6**.



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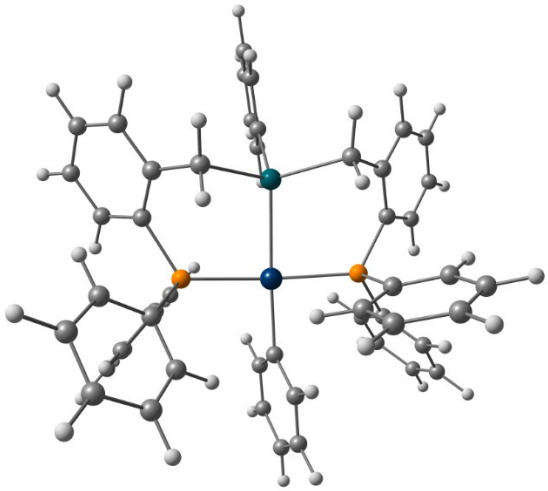
8.7 Cartesian coordinates for 6B.



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6	5.042258000	-2.551959000	-2.839249000
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6	1.614174000	2.662265000	1.681156000
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6	-1.403416000	5.862015000	-2.358899000
1	-1.642881000	6.693781000	-3.016903000
6	-1.031249000	4.627226000	-2.893686000
1	-0.978939000	4.494655000	-3.972034000
6	-0.724821000	3.559575000	-2.043431000
1	-0.437313000	2.605678000	-2.482181000
6	-2.002275000	1.816738000	2.075173000
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1	-2.110159000	2.646527000	2.778662000
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6	-4.175761000	2.717805000	1.257423000
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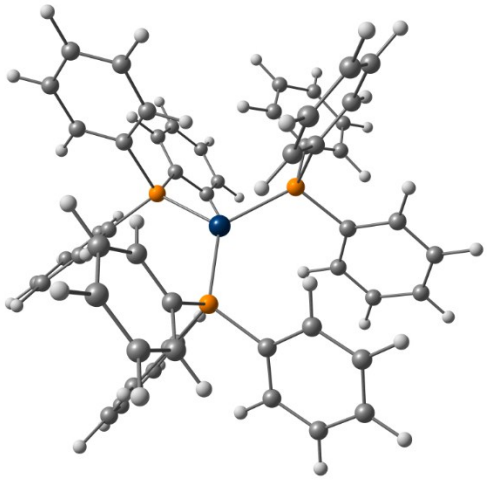
6	-5.315924000	2.711312000	0.461973000
1	-6.034295000	3.523514000	0.538047000
6	-5.531762000	1.654484000	-0.421630000
1	-6.421823000	1.620757000	-1.043540000
6	-4.591849000	0.629474000	-0.500932000
1	-4.780196000	-0.187486000	-1.185954000
6	-3.422741000	0.625693000	0.283685000
6	-2.668645000	-1.848645000	1.581448000
6	-3.756688000	-1.535938000	2.412262000
1	-4.366021000	-0.662563000	2.208659000
6	-4.067302000	-2.343618000	3.508968000
1	-4.909969000	-2.082675000	4.143617000
6	-3.304628000	-3.478838000	3.786034000
1	-3.549100000	-4.107131000	4.638403000
6	-2.227010000	-3.803971000	2.958765000
1	-1.630199000	-4.689656000	3.160102000

6	-1.906276000	-2.993497000	1.868702000
1	-1.069594000	-3.255160000	1.231596000
6	-2.939823000	-1.716053000	-1.338893000
6	-3.678723000	-2.898804000	-1.214732000
1	-3.860152000	-3.329077000	-0.235337000
6	-4.186288000	-3.536187000	-2.351036000
1	-4.753452000	-4.456465000	-2.240596000
6	-3.971481000	-2.993067000	-3.617796000
1	-4.370237000	-3.488333000	-4.498945000
6	-3.238229000	-1.809874000	-3.749642000
1	-3.064024000	-1.381583000	-4.733060000
6	-2.719149000	-1.180377000	-2.619552000
1	-2.140719000	-0.266217000	-2.729488000
6	0.486184000	-2.512267000	-0.705169000
6	0.184550000	-2.924874000	-2.019586000
6	1.107968000	-3.482644000	0.108627000
6	0.471299000	-4.211598000	-2.488747000
6	1.394553000	-4.776094000	-0.345287000
6	1.075650000	-5.150981000	-1.651083000
1	-0.291298000	-2.230004000	-2.706365000
1	1.390083000	-3.235362000	1.129756000
1	0.216147000	-4.479664000	-3.512735000
1	1.874199000	-5.487404000	0.325223000
1	1.297222000	-6.153252000	-2.010358000

8.8 Cartesian coordinates for $[Pt(PPh_3)_3]$.



6	3.222147000	-1.042986000	1.114359000
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6	4.565133000	-1.263208000	0.775083000
6	3.954149000	-0.045586000	3.211541000
6	5.590786000	-0.871434000	1.640355000
6	5.288684000	-0.266315000	2.861520000
1	1.895109000	-0.219309000	2.598184000
1	4.817132000	-1.737532000	-0.168334000
1	3.709339000	0.434148000	4.155546000
1	6.626630000	-1.043273000	1.358372000
1	6.087160000	0.037052000	3.533556000
6	1.526429000	-3.298085000	0.564879000
6	2.314493000	-3.948469000	1.526120000
6	0.477957000	-4.015393000	-0.036457000
6	2.062123000	-5.279706000	1.874459000
6	0.234998000	-5.346229000	0.299845000
6	1.025934000	-5.983385000	1.260783000
1	3.132695000	-3.421651000	2.005635000
1	-0.157754000	-3.524243000	-0.767964000
1	2.682870000	-5.764352000	2.624065000
1	-0.580990000	-5.881419000	-0.178274000
1	0.831483000	-7.018126000	1.530695000
6	2.545082000	-1.767347000	-1.634506000
6	2.387958000	-0.753228000	-2.594058000
6	3.265577000	-2.919962000	-1.990409000
6	2.948629000	-0.878882000	-3.867337000
6	3.824101000	-3.046773000	-3.264265000
6	3.669278000	-2.026164000	-4.205447000
1	1.809056000	0.130627000	-2.339782000

1	3.388174000	-3.725542000	-1.272827000
1	2.813088000	-0.083460000	-4.595654000
1	4.378682000	-3.945742000	-3.521001000
1	4.102023000	-2.127901000	-5.197244000
15	1.783979000	-1.526584000	0.044083000
78	-0.003925000	-0.011231000	0.050495000
15	-2.215979000	-0.780059000	0.035838000
6	-2.799351000	-1.303415000	-1.648717000
6	-1.838674000	-1.674267000	-2.604148000
6	-2.222649000	-2.089608000	-3.881360000
1	-1.463392000	-2.370833000	-4.606548000
1	-0.785550000	-1.619802000	-2.341820000
6	-3.574843000	-2.132240000	-4.226933000
6	-4.155890000	-1.339334000	-2.013222000
6	-4.539745000	-1.752965000	-3.290696000
1	-3.875317000	-2.451098000	-5.221564000
1	-5.594074000	-1.775740000	-3.554291000
1	-4.484420000	-0.942608000	2.055675000
6	-4.544002000	0.014549000	1.548396000
6	-3.612968000	0.341643000	0.551851000
6	-3.727547000	1.589714000	-0.084349000
1	-3.005525000	1.873452000	-0.845146000
6	-4.750261000	2.475099000	0.251545000
6	-5.670140000	2.139286000	1.249721000
1	-6.461935000	2.833084000	1.520049000
6	-5.560562000	0.909578000	1.898419000
1	-6.269393000	0.637158000	2.676540000
1	-4.916914000	-1.037589000	-1.299783000
6	-2.543990000	-2.266178000	1.100233000
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1	-3.955964000	-3.276631000	-0.188024000
6	-3.617953000	-4.385257000	1.622016000
1	-4.296741000	-5.185390000	1.337216000
6	-2.950591000	-4.436476000	2.847170000
1	-3.105539000	-5.276726000	3.518899000
6	-2.075810000	-3.406026000	3.201471000
1	-1.543322000	-3.442413000	4.148220000
6	-1.867288000	-2.336884000	2.329545000
1	-1.159781000	-1.552769000	2.589241000
1	-4.820335000	3.433504000	-0.255922000
15	0.429114000	2.295260000	0.038893000
6	-0.702091000	3.313900000	1.103366000
6	-1.121157000	2.748326000	2.318994000
6	-1.947427000	3.456814000	3.191866000

1	-2.261654000	3.001344000	4.127309000
1	-0.810948000	1.735841000	2.565984000
6	-2.386306000	4.739480000	2.852968000
6	-1.147495000	4.603362000	0.774817000
6	-1.988351000	5.307555000	1.641200000
1	-3.039420000	5.289017000	3.525817000
1	-2.329634000	6.302843000	1.367511000
1	1.543421000	4.776953000	-1.281318000
6	0.909318000	4.267275000	-2.000280000
6	0.269214000	3.067854000	-1.644776000
6	-0.523873000	2.422425000	-2.607831000
1	-1.000210000	1.479612000	-2.353882000
6	-0.688847000	2.968140000	-3.883048000
6	-0.055279000	4.165859000	-4.219906000
1	-0.178887000	4.589667000	-5.213077000
6	0.746166000	4.812195000	-3.275884000
1	1.248497000	5.741601000	-3.531794000
1	-0.843195000	5.063048000	-0.160175000
6	2.092840000	2.953750000	0.560313000
6	2.268205000	3.915921000	1.565671000
1	1.406384000	4.331642000	2.076802000
6	3.548980000	4.355266000	1.917721000
1	3.663064000	5.100099000	2.701504000
6	4.671671000	3.848425000	1.264032000
1	5.666183000	4.192270000	1.536061000
6	4.508926000	2.890176000	0.258635000
1	5.376728000	2.481563000	-0.252246000
6	3.234141000	2.441529000	-0.080311000
1	3.122851000	1.680218000	-0.847570000
1	-1.305659000	2.451034000	-4.613555000

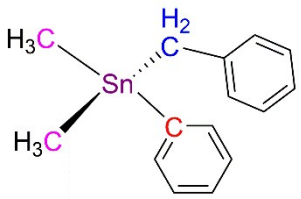
Table S9. Optimized B3LYP/6-31G(d) potential energies and computed Gibbs free energies at 298 K.

Compound	G_{h298K}	ΔG_{298K}(kcalmol^{-1})
1	-1772.810855	
[Pt(PPh$_3$)$_3$]	-3228.340302	
PPh$_3$	-1036.056388	
4	-2928.332466	945.94
4B (not observed)	-2928.320688	953.33
3	-2615.980361	
6	-2735.474907	304.11
6B (not observed)	-2735.452620	941.53

Formally complexes **4** and **6** can be described as Sn(III)-Pt(I) species with a X-type stannyl ligand.

9. Computations on model molecule A

The Sn-C bond polarity was analyzed for Sn-C methyl, Sn-C benzyl and Sn-C phenyl using the following model molecule:



A

The geometry was optimized at the B3LYP/6-31G** level and a Natural Population Analysis was performed leading to the following results. Below C1 and C2 belong to the equivalent methyl groups, C3 to the phenyl and C4 to the benzyl group.

Atomic Natural charges

Sn +1.862

C1 -1.199

C2 -1.197

C3 -0.493

C4 -0.922

Sn-C bond Natural Bond analysis

Sn-C bonds	Sn contribution %	C contribution %
Sn-C1 Methyl	26	74
Sn-C2 Methyl	26	74
Sn-C3 Phenyl	25	75
Sn-C4 Benzyl	24	76