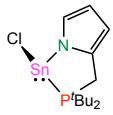
Ms. for Dalton Trans.

ELECTRONIC SUPPLEMENTARY INFORMATION

Stannylenes based on pyrrole-phosphane and dipyrromethane-diphosphane scaffolds: Syntheses and behavior as precursors to PSnP pincer palladium(II), palladium(0) and gold(I) complexes

Javier A. Cabeza,* Israel Fernández, Pablo García-Álvarez, Rubén García-Soriano, Carlos J. Laglera-Gándara and Rubén Toral

NMR spectra



(**1**)

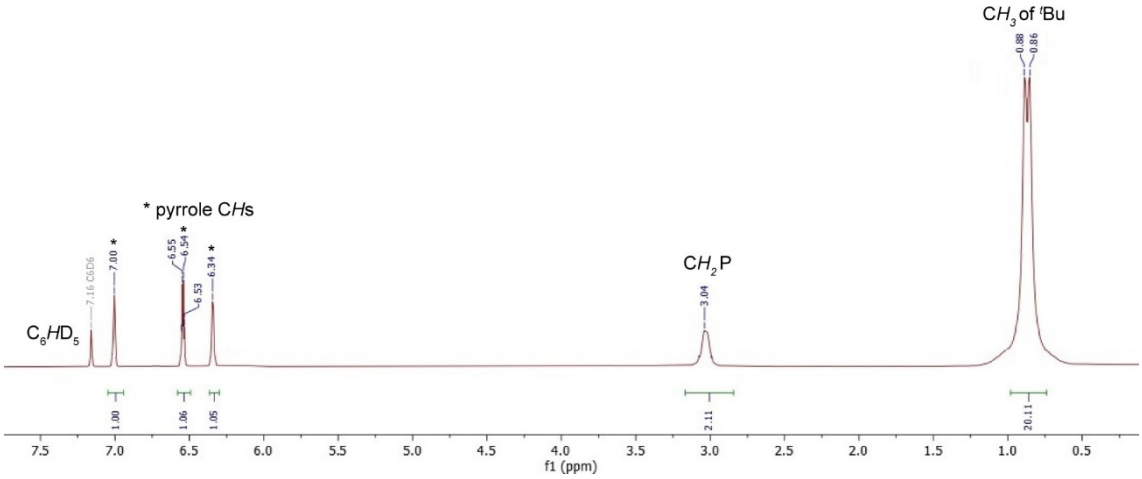


Figure S1. ^{1}H NMR spectrum (400.1 MHz, C_6D_6, 298 K) of SnCl(HpyrmP^{t}Bu$_2$) (**1**).

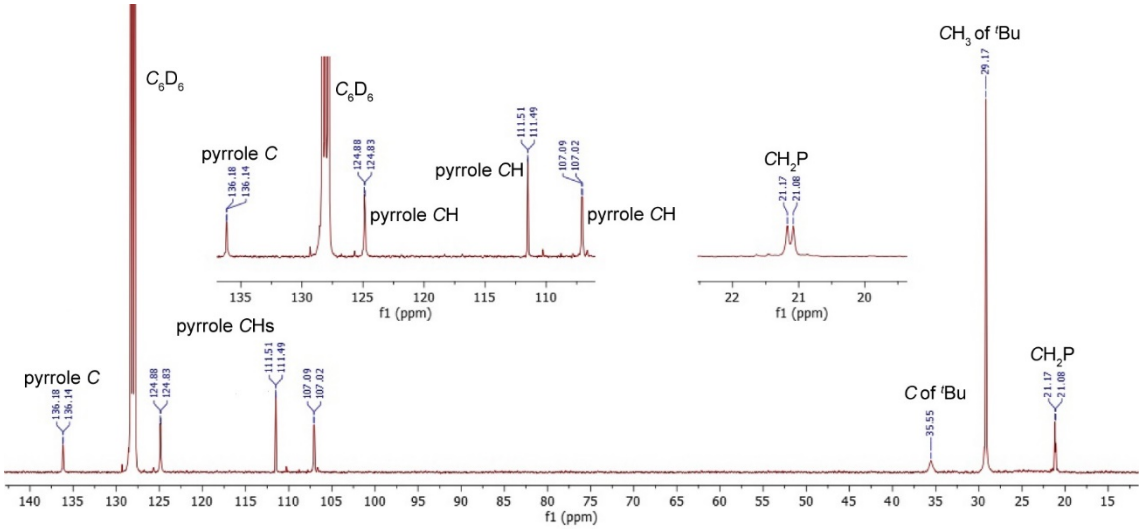
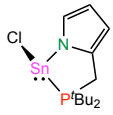


Figure S2. ^{13}C{^{1}H} NMR spectrum (100.6 MHz, C_6D_6, 298 K) of SnCl(HpyrmP^{t}Bu$_2$) (**1**).



(**1**)

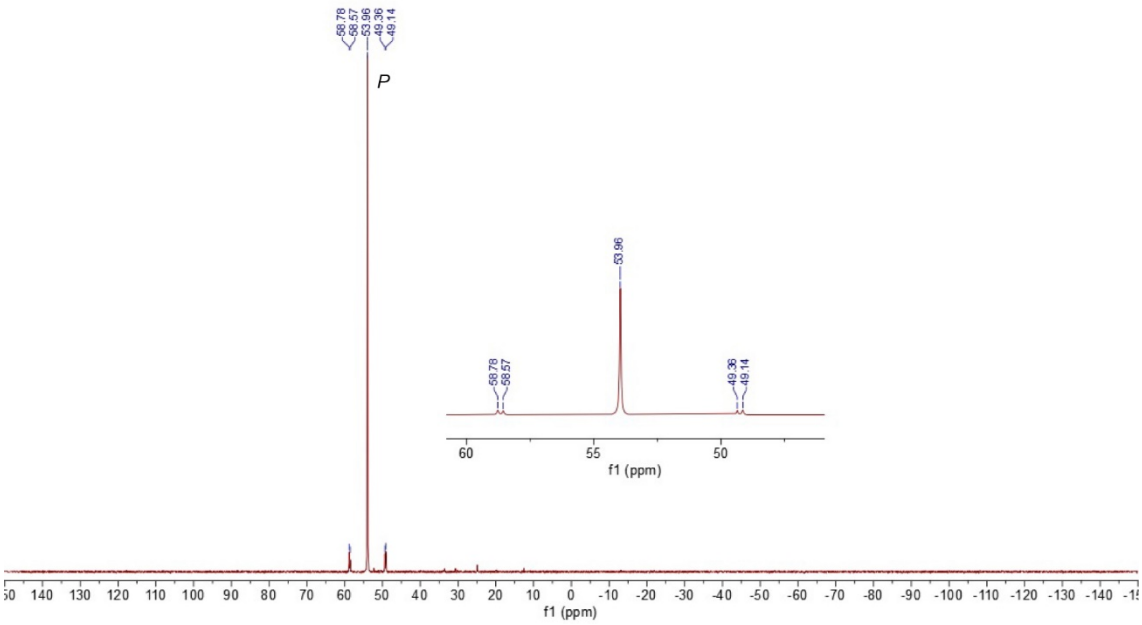


Figure S3. $^{31}P\{^1H\}$ NMR spectrum (162.1MHz, C_6D_6, 298 K) of SnCl(HpyrmP^{t}Bu$_2$) (**1**).

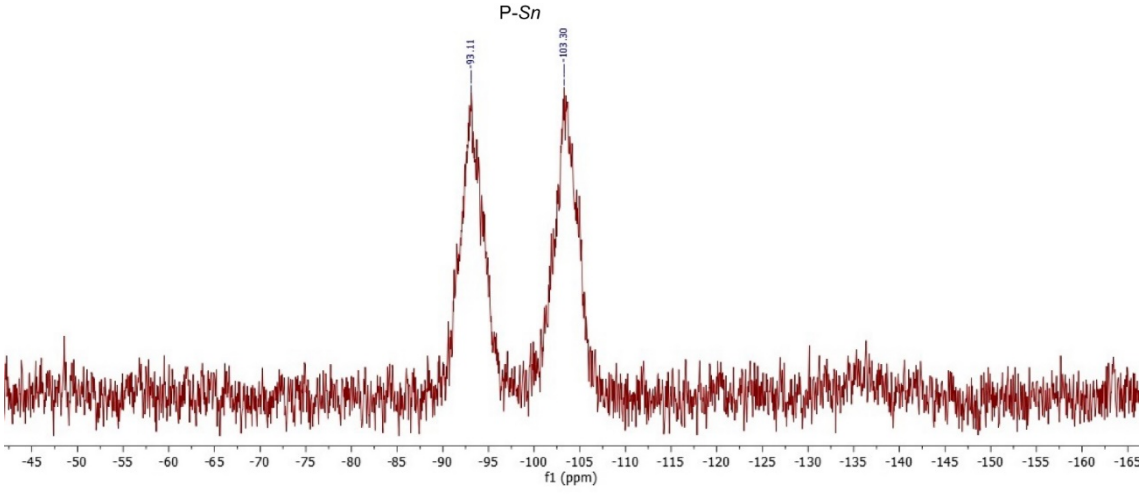
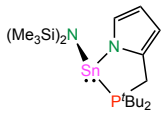


Figure S4. $^{119}Sn\{^1H\}$ NMR spectrum (149.2 MHz, C_6D_6, 298 K) of SnCl(HpyrmP^{t}Bu$_2$) (**1**).



(**2**)

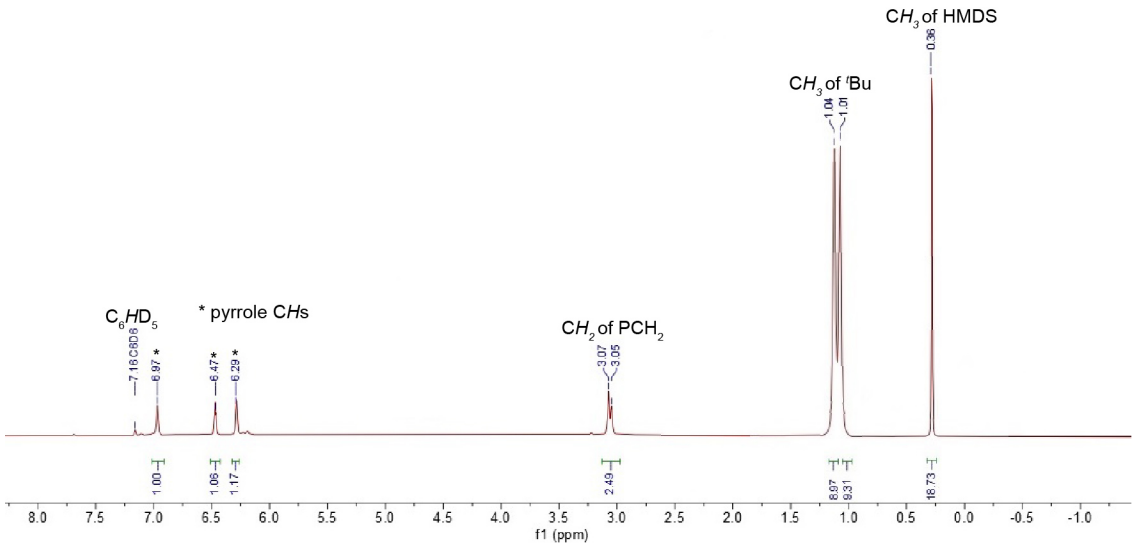


Figure S5. ^{1}H NMR spectrum (400.5 MHz, C_6D_6, 298 K) of Sn{N(SiMe$_3$)$_2$}(HpyrmP^{t}Bu$_2$) (**2**).

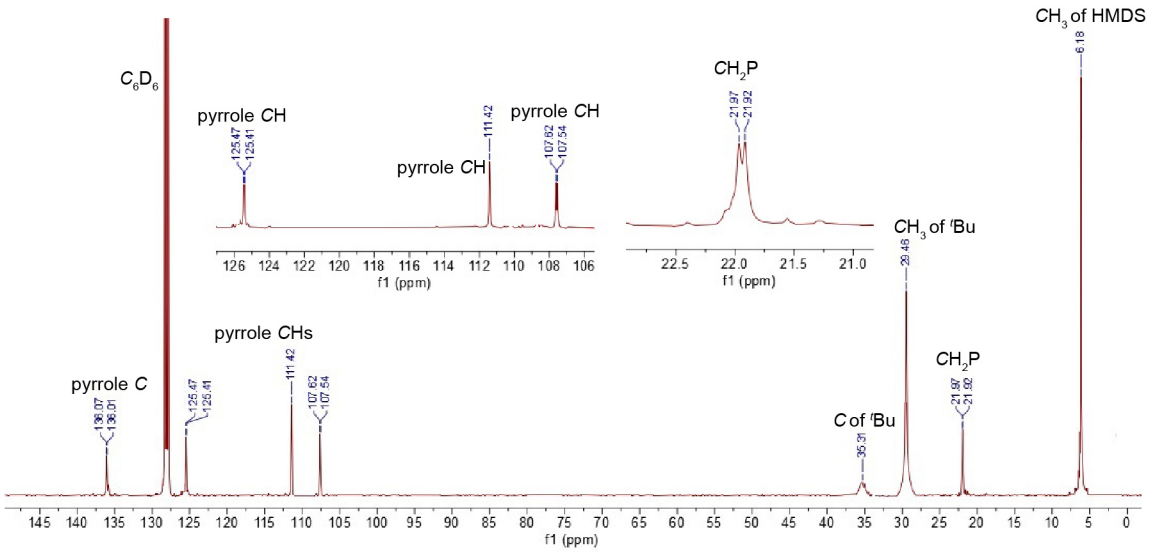
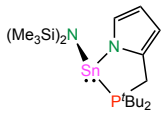


Figure S6. ^{13}C{^{1}H} NMR spectrum (100.6 MHz, C_6D_6, 298 K) of Sn{N(SiMe$_3$)$_2$}(HpyrmP^{t}Bu$_2$) (**2**).



(**2**)

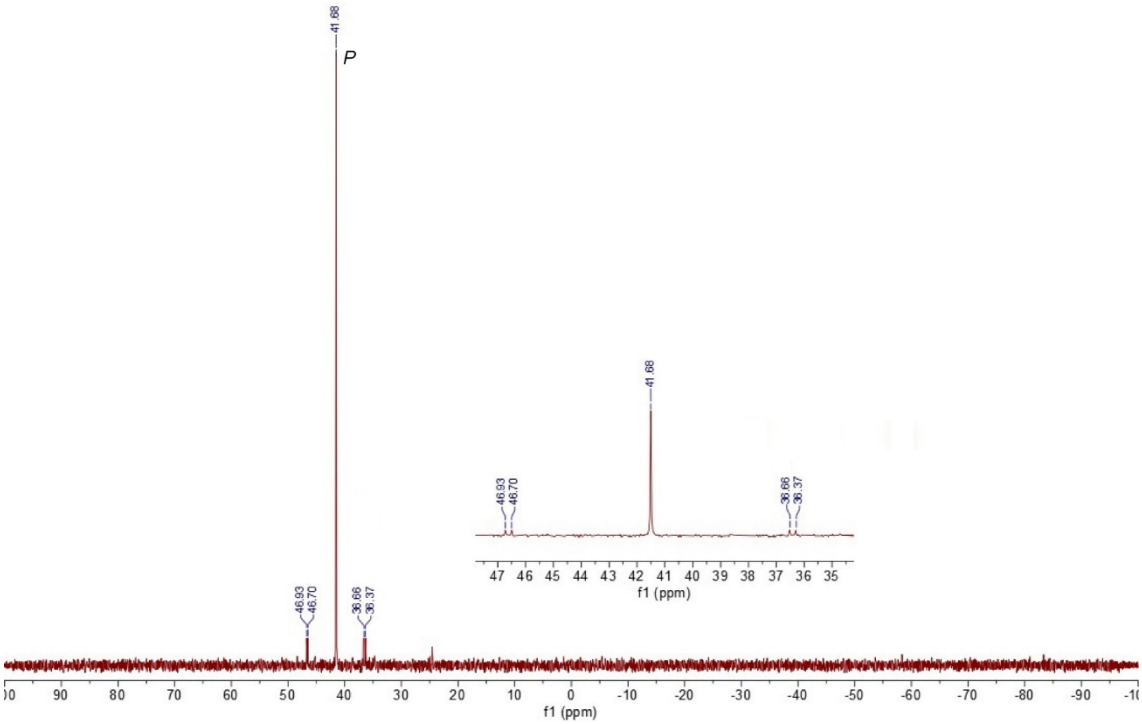


Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum (162.1 MHz, C_6D_6, 298 K) of Sn{N(SiMe$_3$)$_2$}(HpyrmP^{t}Bu$_2$) (**2**).

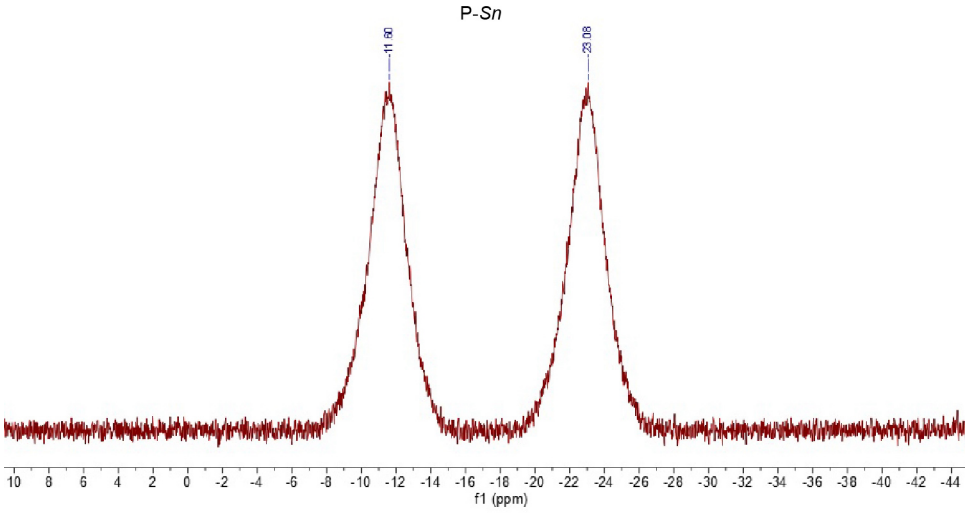


Figure S8. $^{119}Sn\{^{1}H\}$ NMR spectrum (149.2 MHz, C_6D_6, 298 K) of Sn{N(SiMe$_3$)$_2$}(HpyrmP^{t}Bu$_2$) (**2**).

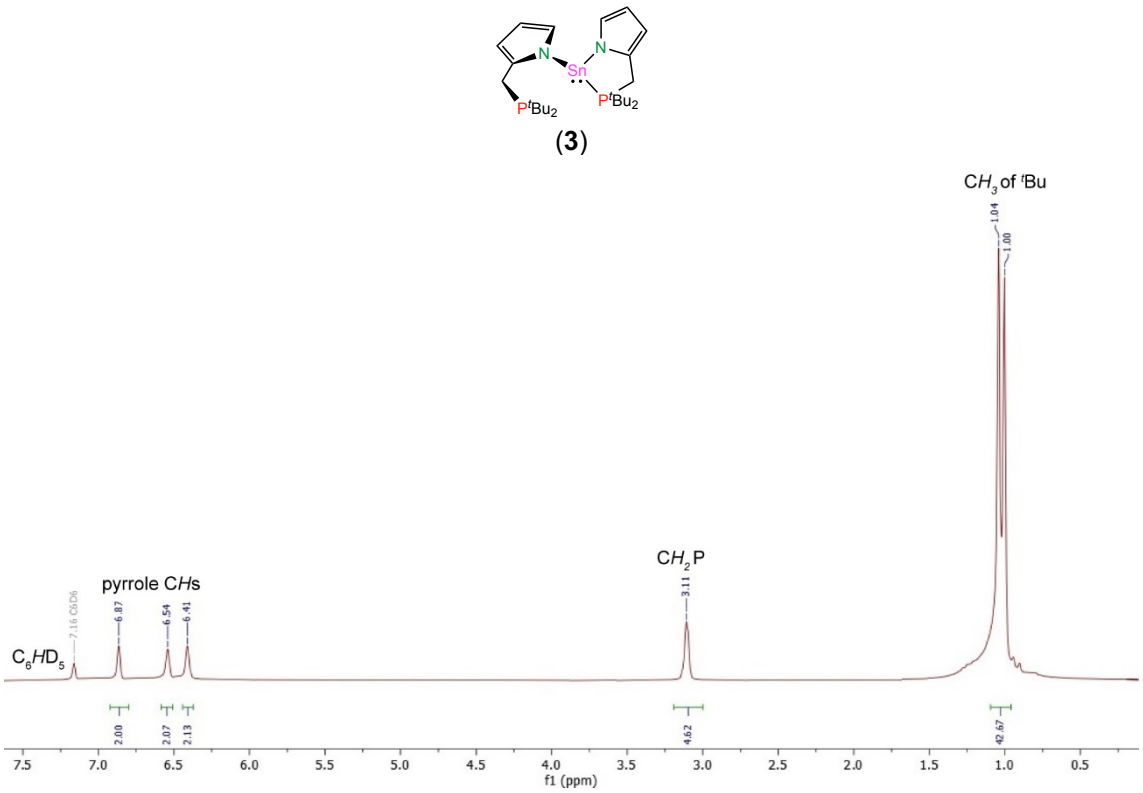


Figure S9. ^{1}H NMR spectrum (300.1 MHz, C_6D_6, 298 K) of Sn(HpyrmP^{t}Bu$_2$)$_2$ (**3**).

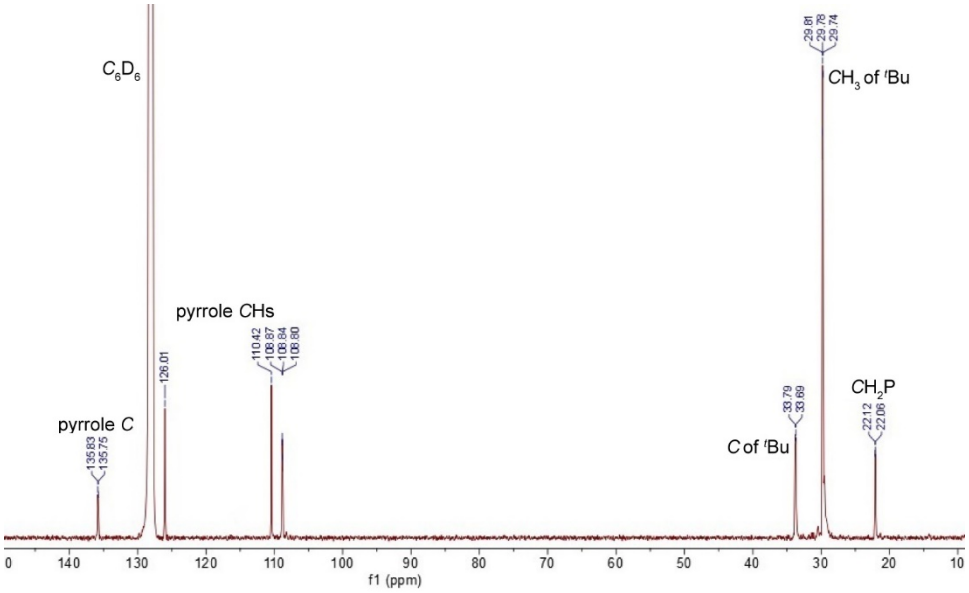


Figure S10. ^{13}C{^{1}H} NMR spectrum (100.6 MHz, C_6D_6, 298 K) of Sn(HpyrmP^{t}Bu$_2$)$_2$ (**3**).

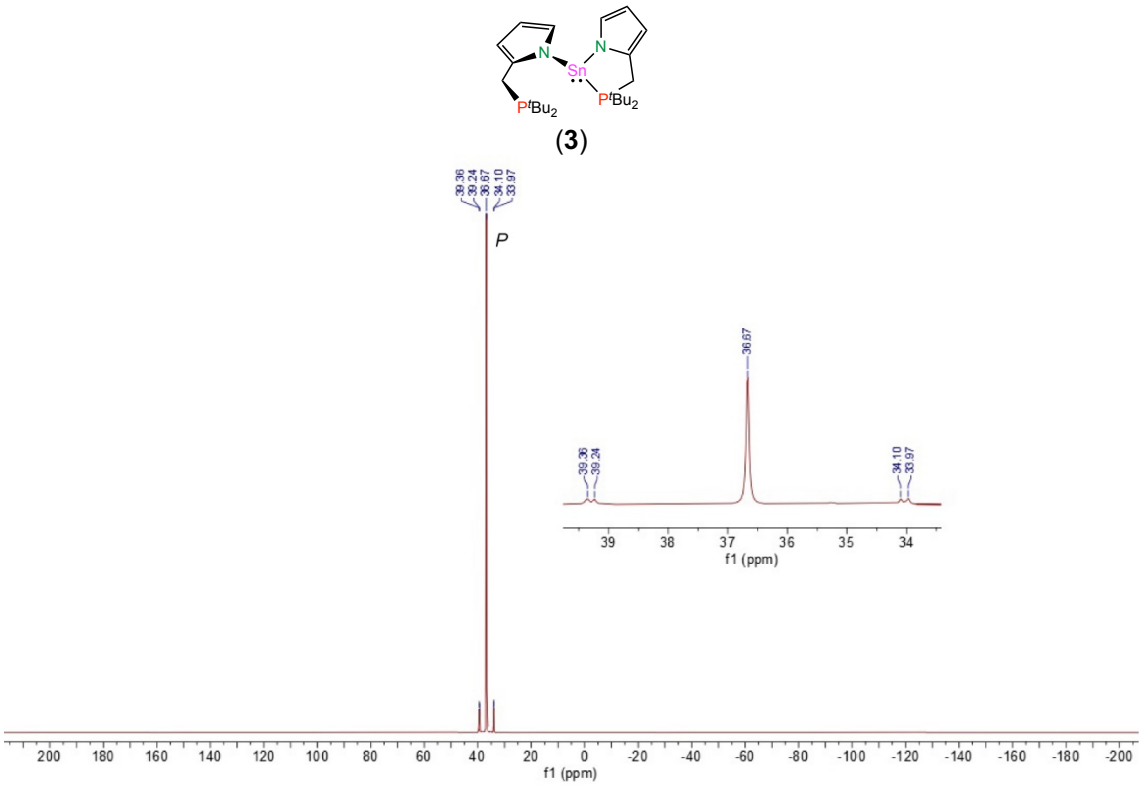


Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum (121.5 MHz, C_6D_6, 298 K) of $Sn(HpyrmP^tBu_2)_2$ (**3**).

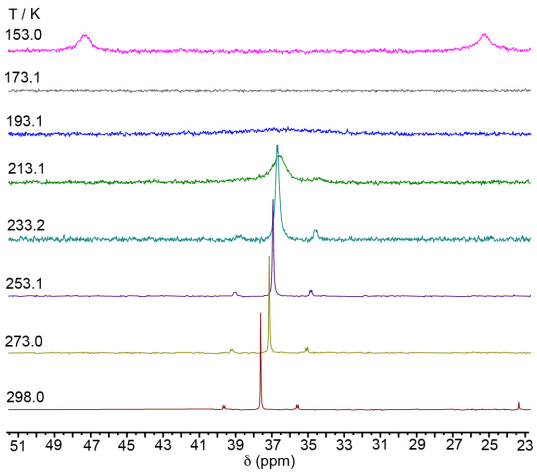
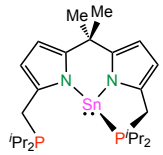


Figure S12. $^{31}P\{^{1}H\}$ NMR (162.0 MHz; 1/1 toluene/dichloromethane-d_2 solution) spectra of stannylene **3** at different temperatures.



(**4**)

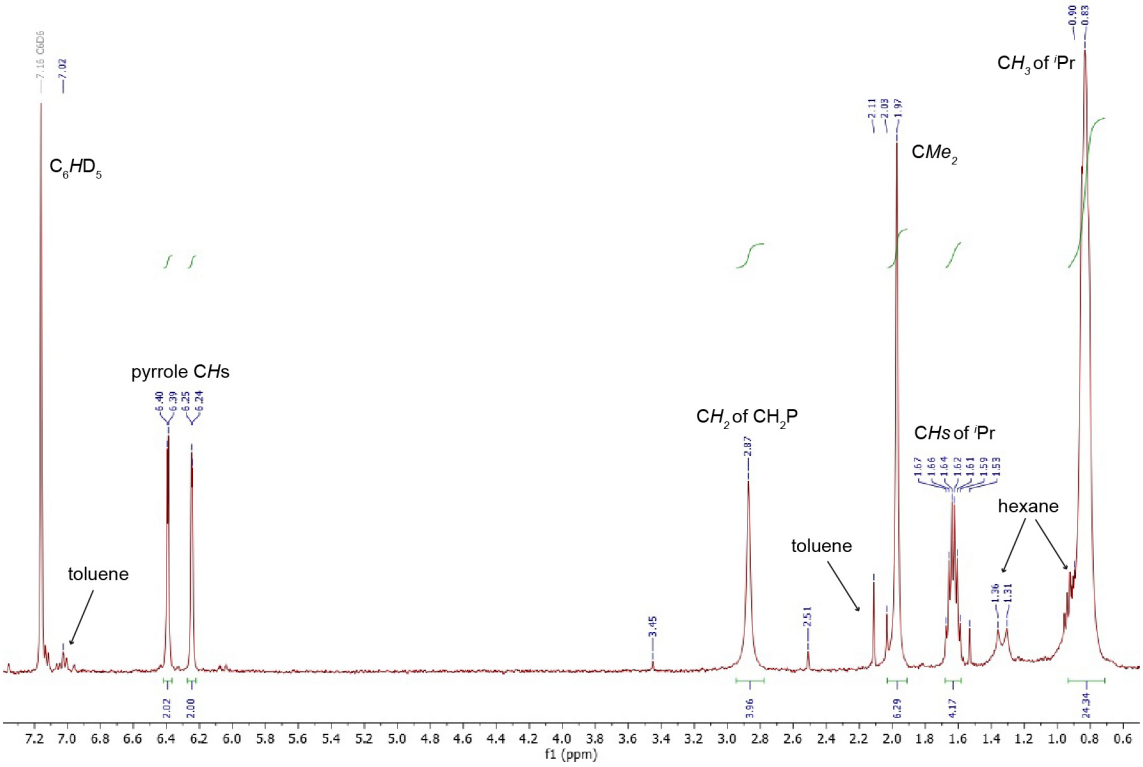


Figure S13. ^{1}H NMR spectrum (400.1 MHz, C_6D_6, 298 K) of Sn(pyrmP^{i}Pr$_2$)$_2$CMe$_2$ (**4**).

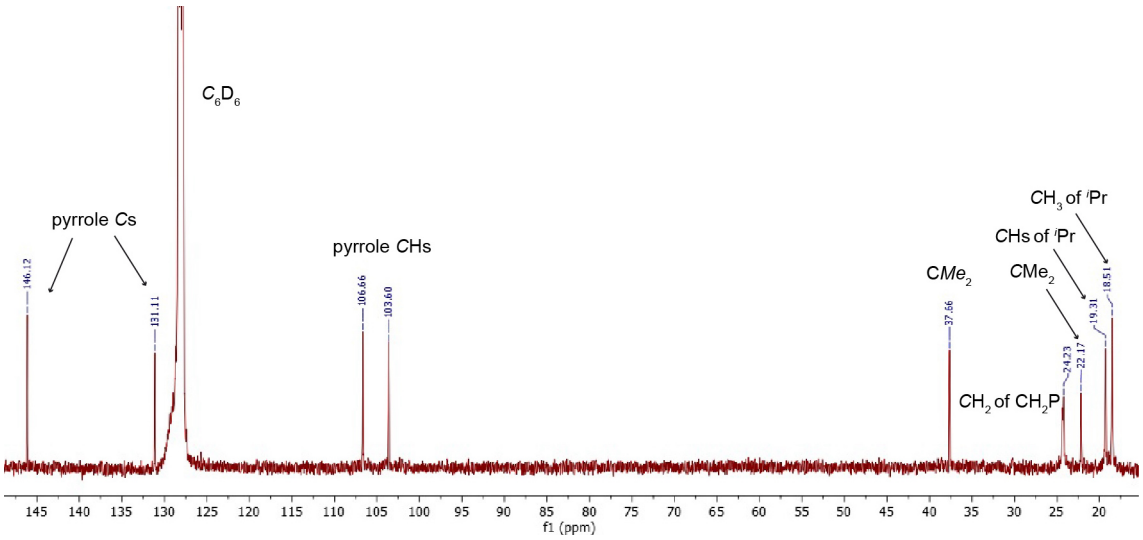


Figure S14. ^{13}C{^{1}H} NMR spectrum (100.6 MHz, C_6D_6, 298 K) of Sn(pyrmP^{i}Pr$_2$)$_2$CMe$_2$ (**4**).

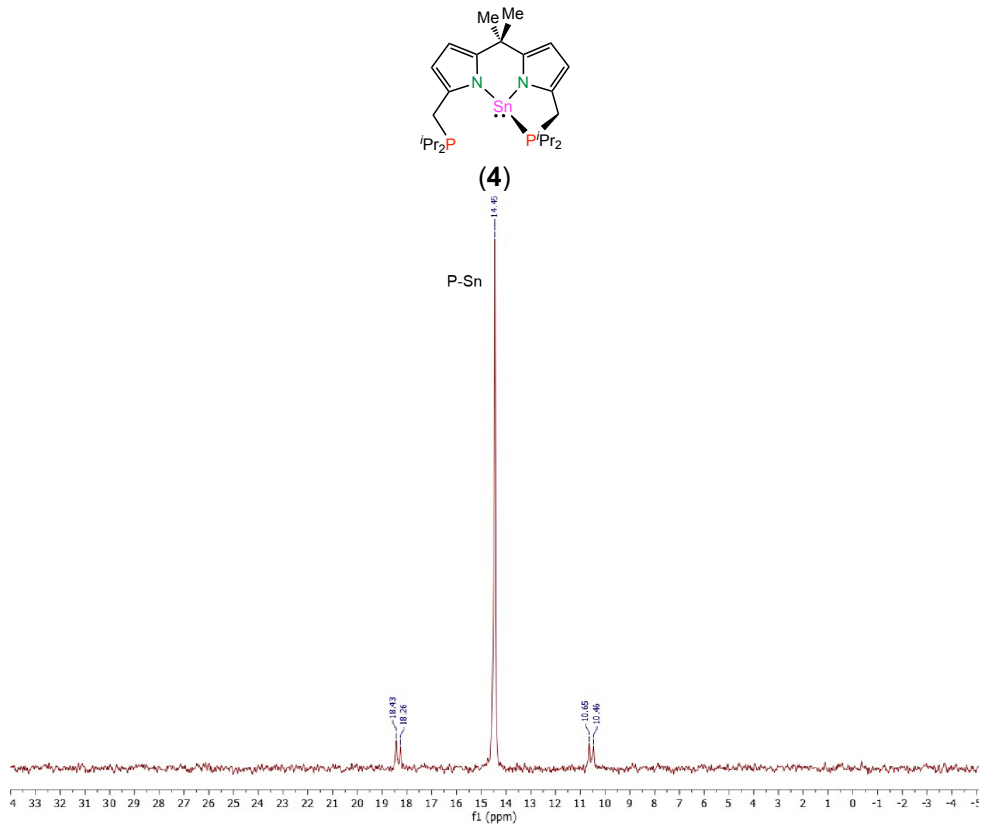


Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum (121.5 MHz, C_6D_6, 298 K) of Sn(pyrmP^{i}Pr$_2$)$_2$CMe$_2$ (**4**).

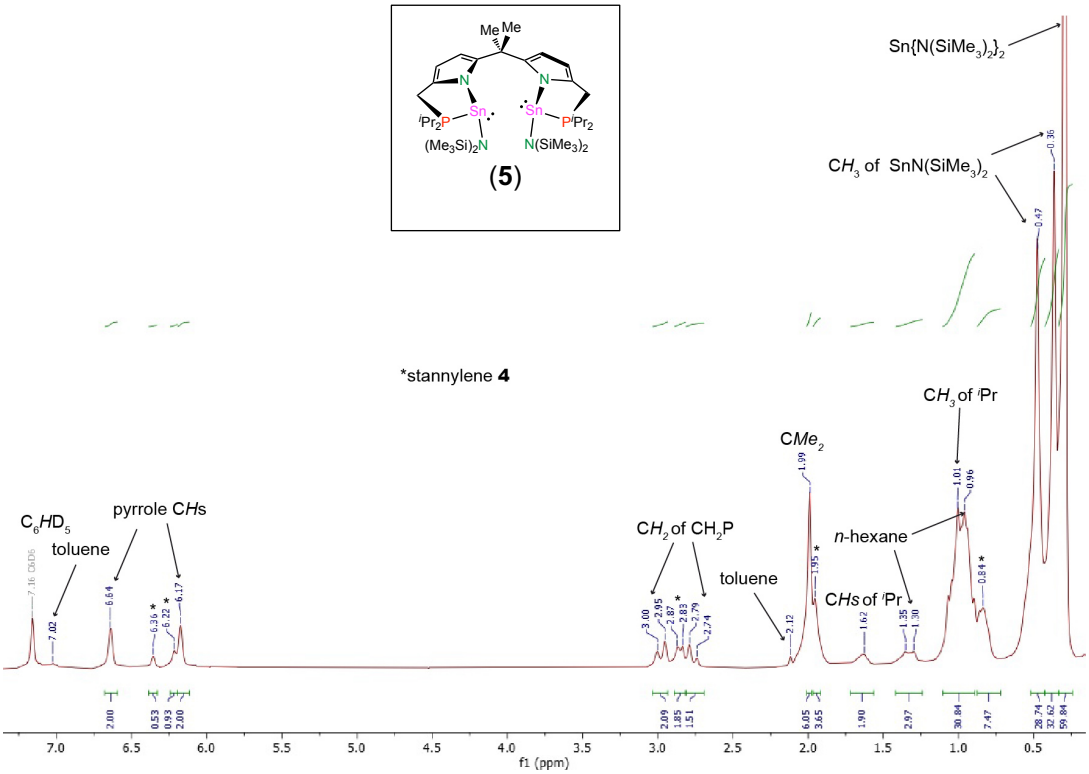


Figure S16. ^{1}H NMR spectrum (300.1 MHz, C_6D_6, 298 K) of a *ca.* 1/4/5 mixture of Sn(pyrmP^{i}Pr$_2$)$_2$CMe$_2$ (**4**), Sn$_2${N(SiMe$_3$)$_2$}$_2${(pyrmP^{i}Pr$_2$)$_2$CMe$_2$} (**5**) and Sn{N(SiMe$_3$)$_2$}$_2$.

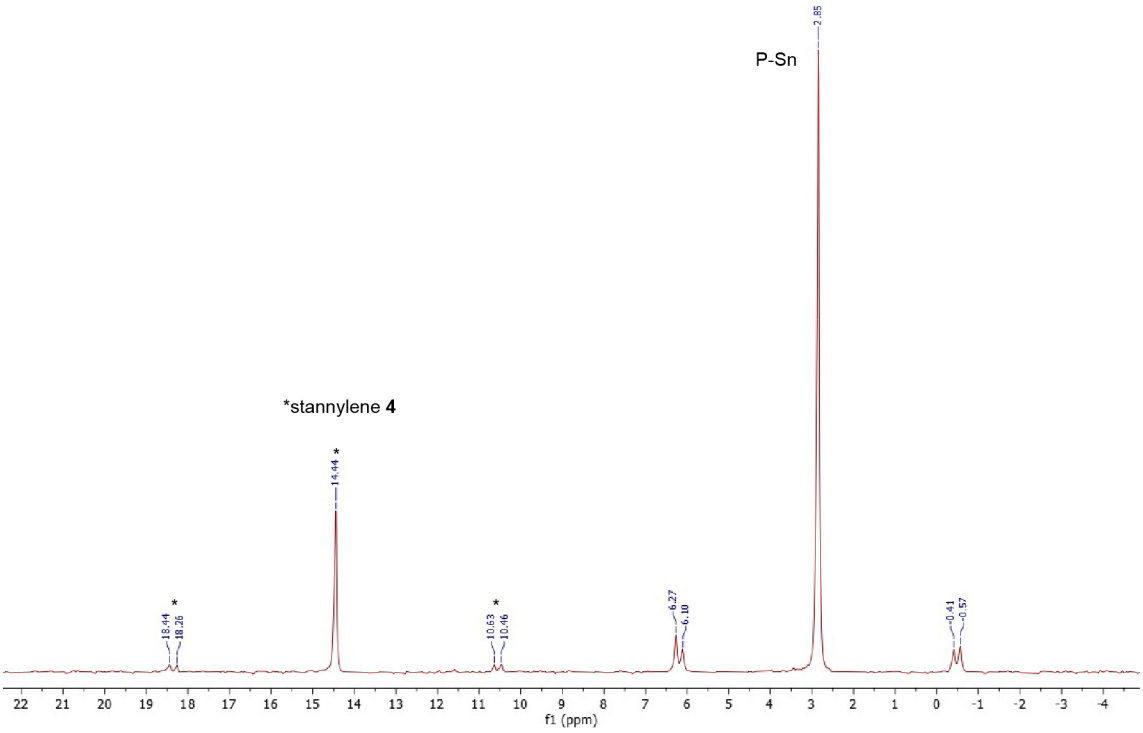


Figure S17. ^{31}P{^{1}H} NMR spectrum (121.5 MHz, C_6D_6, 298 K) of a *ca.* 1/4/5 mixture of Sn(pyrmP^{i}Pr$_2$)$_2$CMe$_2$ (**4**), Sn$_2${N(SiMe$_3$)$_2$}$_2${(pyrmP^{i}Pr$_2$)$_2$CMe$_2$} (**5**) and Sn{N(SiMe$_3$)$_2$}$_2$.

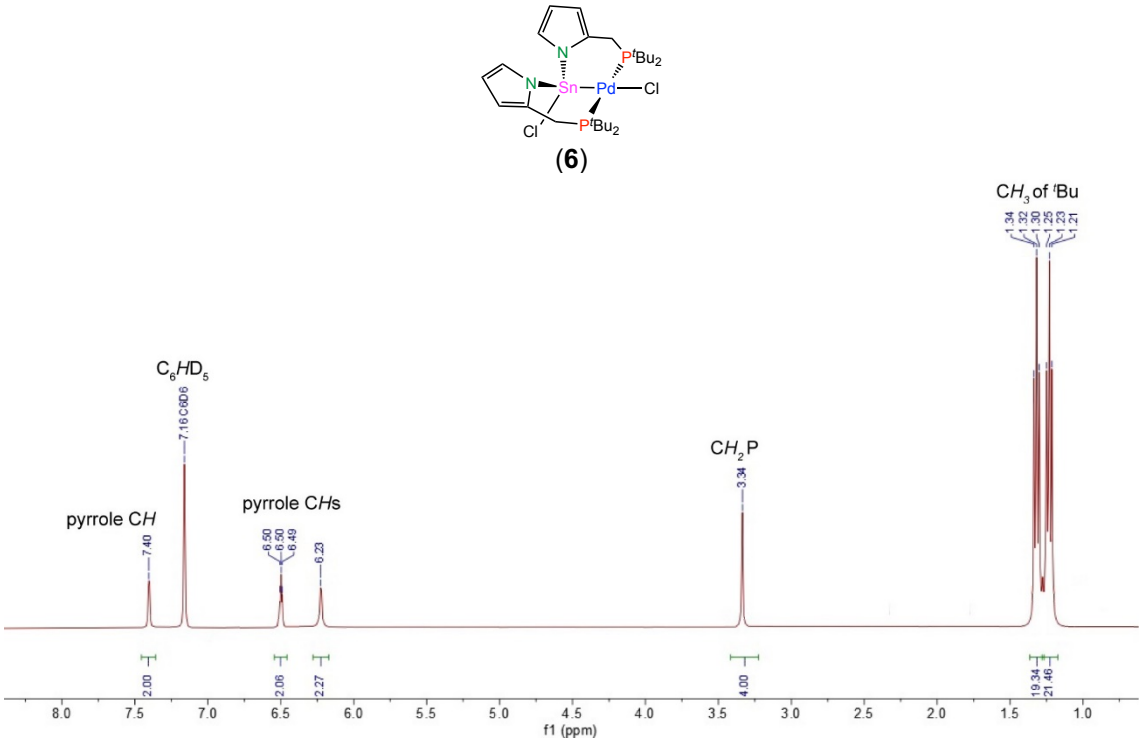


Figure S18. ^{1}H NMR spectrum (400.1 MHz, C_6D_6, 298 K) of [PdCl{κ^3*P*,*Sn*,*P*-SnCl(HpyrmP^{t}Bu$_2$)$_2$] (**6**).

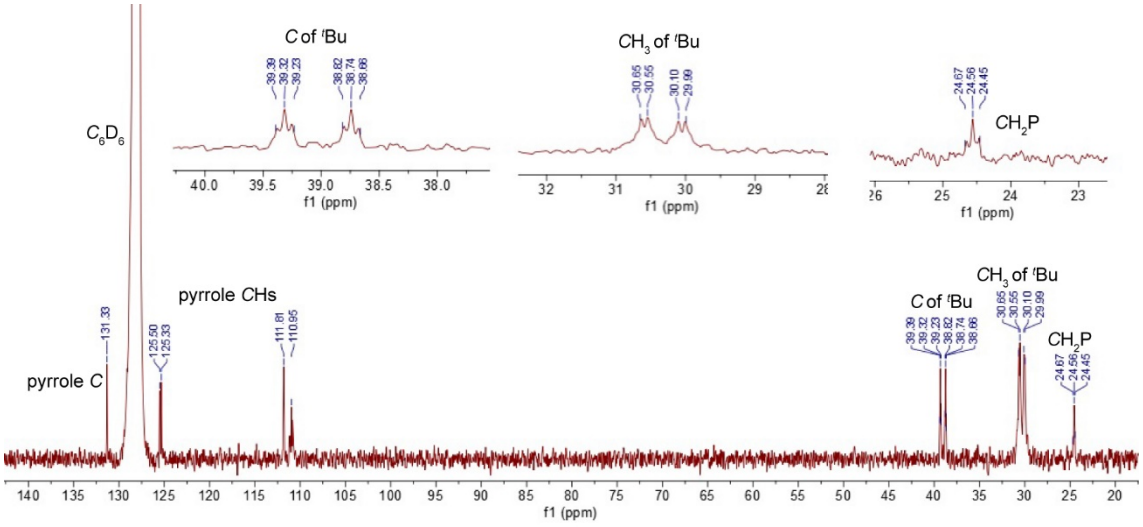


Figure S19. ^{13}C{^{1}H} NMR spectrum (100.6 MHz, C_6D_6, 298 K) of [PdCl{κ^3*P*,*Sn*,*P*-SnCl(HpyrmP^{t}Bu$_2$)$_2$] (**6**).

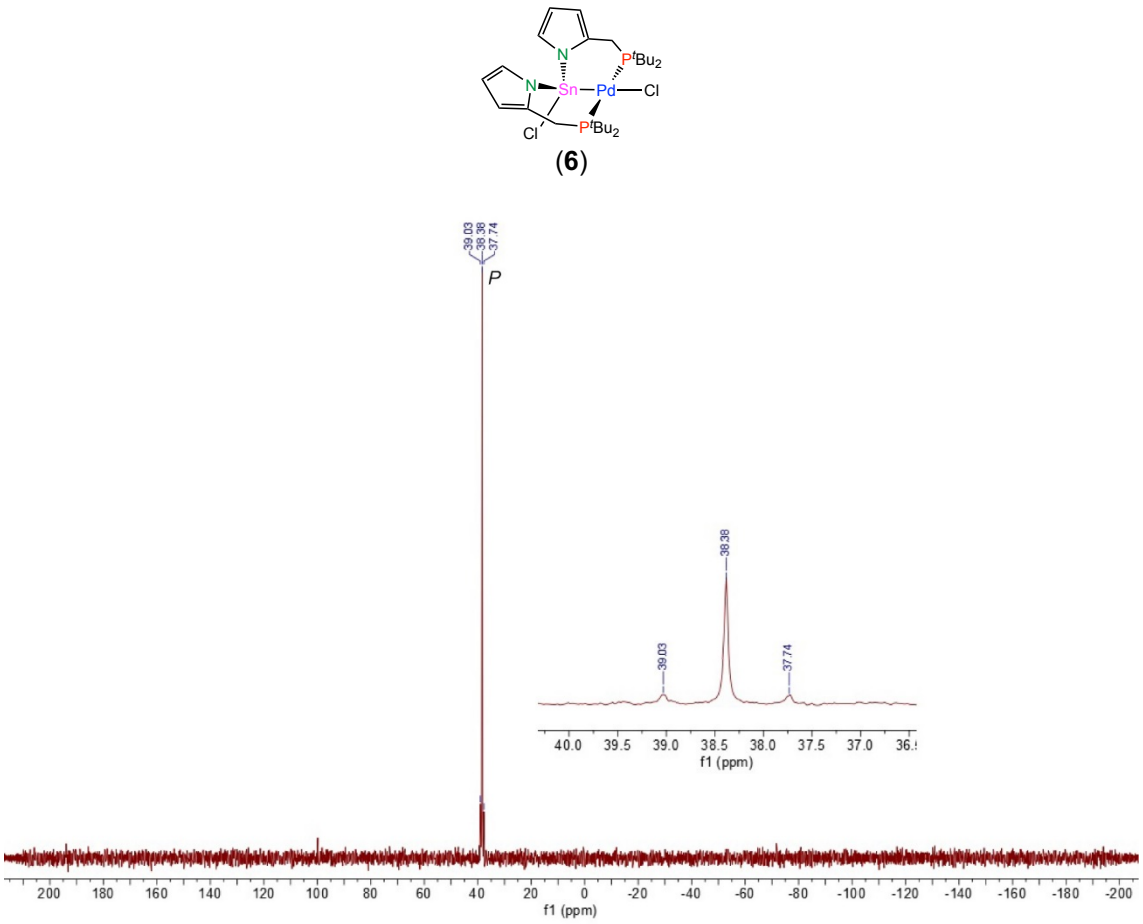


Figure S20. $^{31}P\{^{1}H\}$ NMR spectrum (162.1 MHz, C_6D_6, 298 K) of [PdCl{κ^3*P*,*Sn*,*P*-SnCl(HpyrmP^{t}Bu$_2$)$_2$] (**6**).

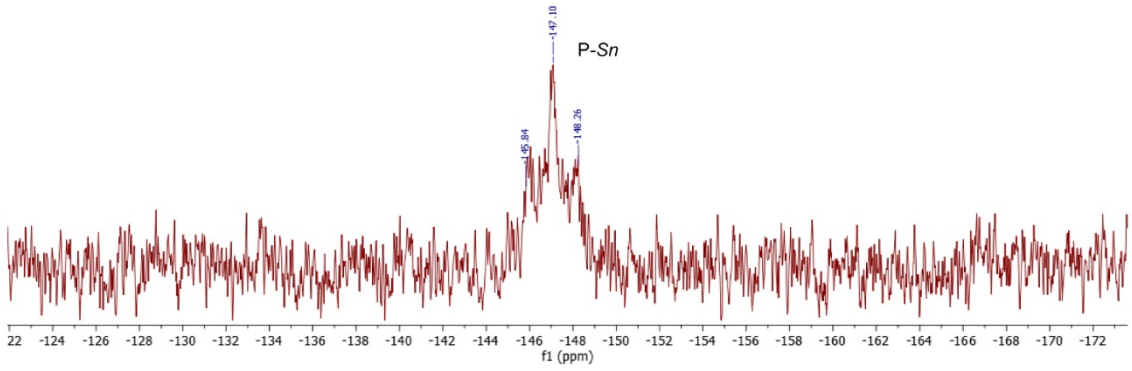


Figure S21. $^{119}Sn\{^{1}H\}$ NMR spectrum (149.2 MHz, C_6D_6, 298 K) of [PdCl{κ^3*P*,*Sn*,*P*-SnCl(HpyrmP^{t}Bu$_2$)$_2$}] (**6**).

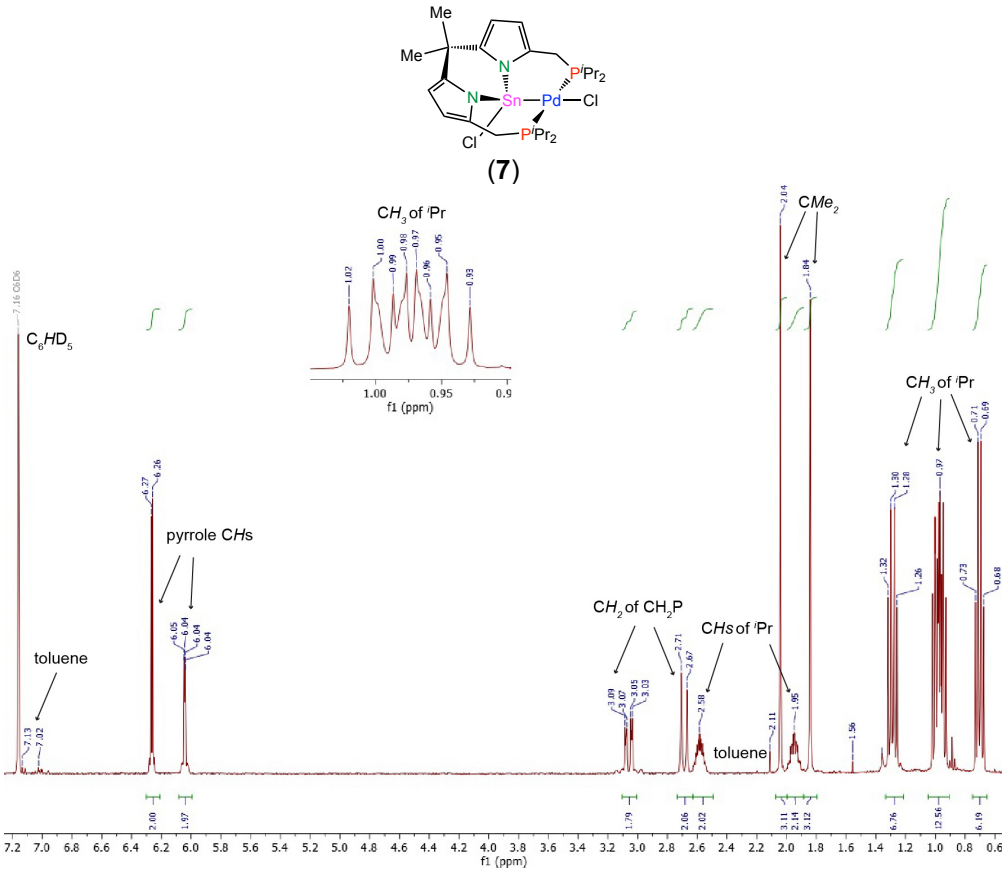


Figure S22. ^{1}H NMR spectrum (400.1 MHz, C_6D_6, 298 K) of [PdCl{κ^3*P*,*Sn*,*P*-SnCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**7**).

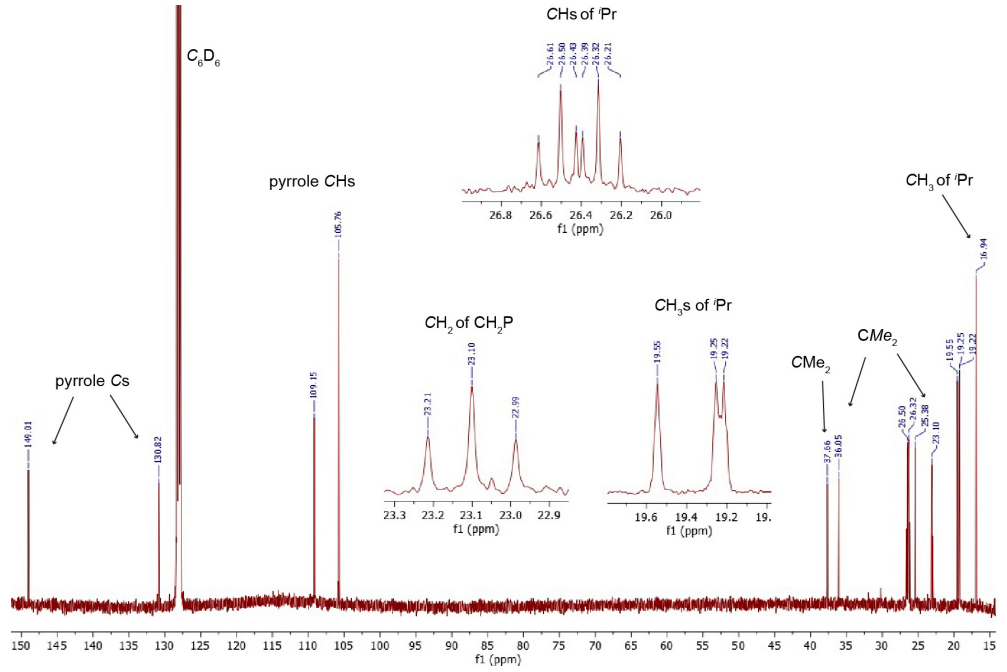


Figure S23. ^{13}C{^{1}H} NMR spectrum (100.7 MHz, C_6D_6, 298 K) of [PdCl{κ^3*P*,*Sn*,*P*-SnCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**7**).

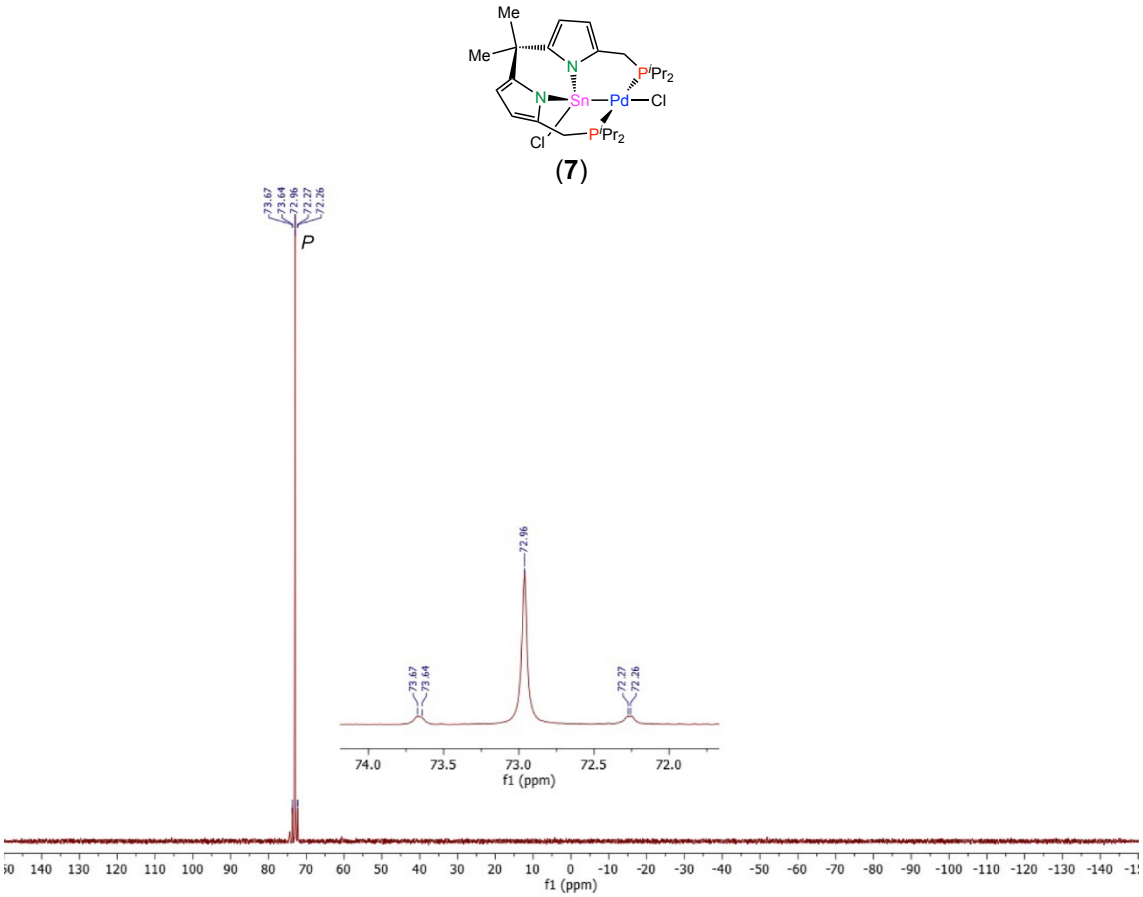


Figure S24. $^{31}P\{^{1}H\}$ NMR spectrum (162.1 MHz, C_6D_6, 298 K) of [PdCl{κ^3*P*,*Sn*,*P*-SnCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**7**).

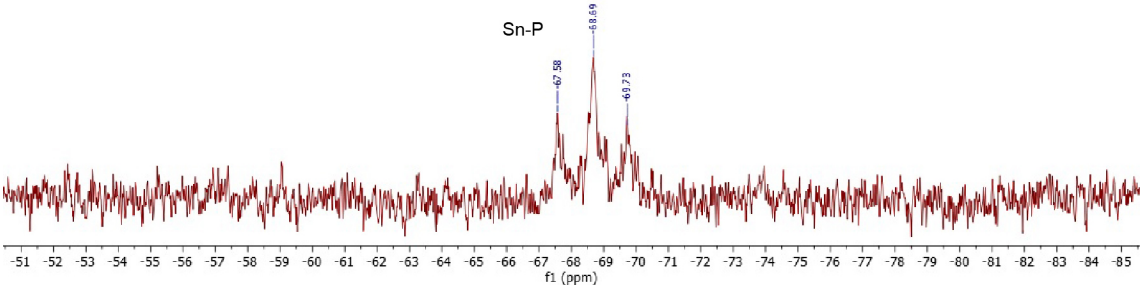


Figure S25. $^{119}Sn\{^{1}H\}$ NMR spectrum (149.2 MHz, CD_2Cl_2, 298 K) of [PdCl{κ^3*P*,*Sn*,*P*-SnCl(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**7**).

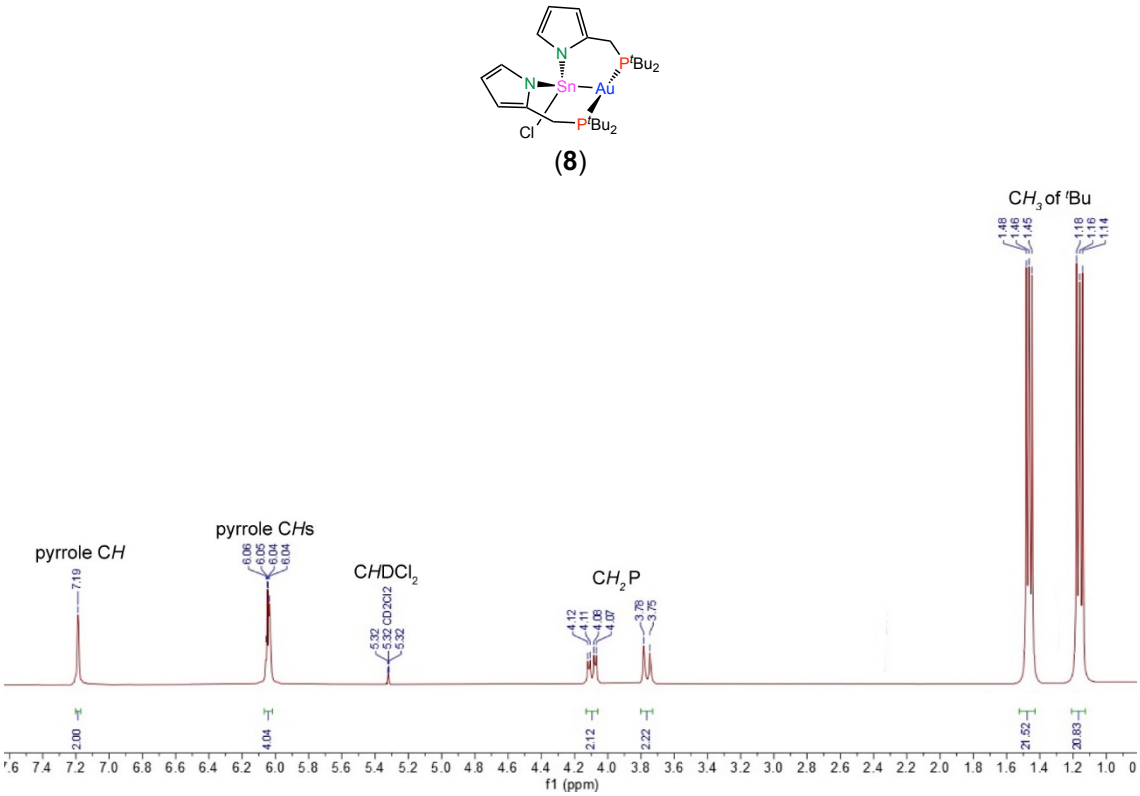


Figure S26. ^{1}H NMR spectrum (400.1 MHz, CD_2Cl_2, 298 K) of [Au{κ^3*P*,*Sn*,*P*-SnCl(HpyrmP^{t}Bu$_2$)$_2$}] (**8**).

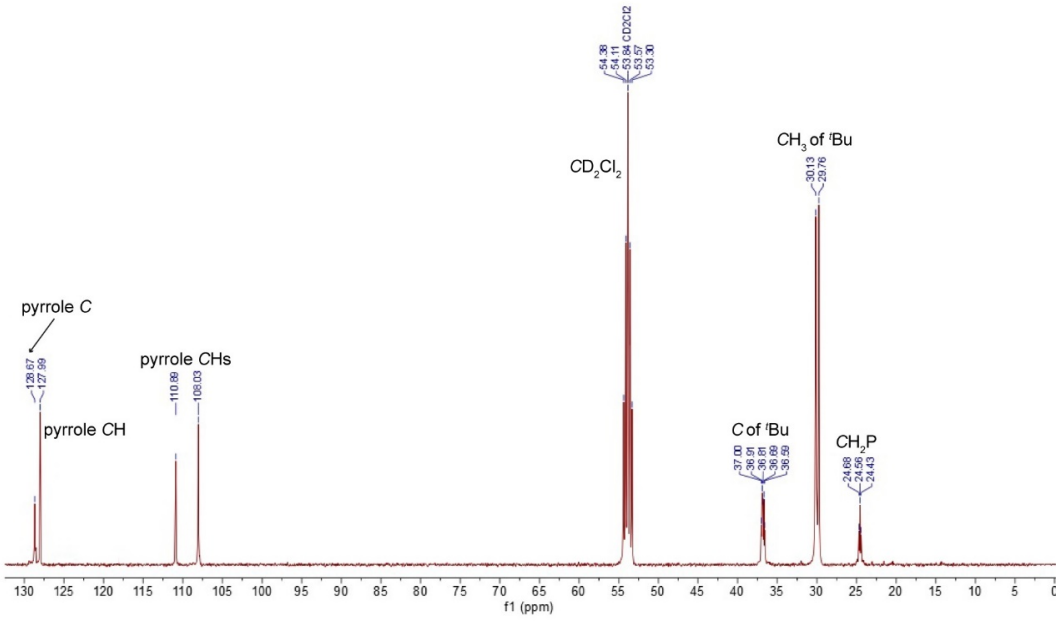


Figure S27. ^{13}C{^{1}H} NMR spectrum (100.6 MHz, CD_2Cl_2, 298 K) of [Au{κ^3*P*,*Sn*,*P*-SnCl(HpyrmP^{t}Bu$_2$)$_2$}] (**8**).

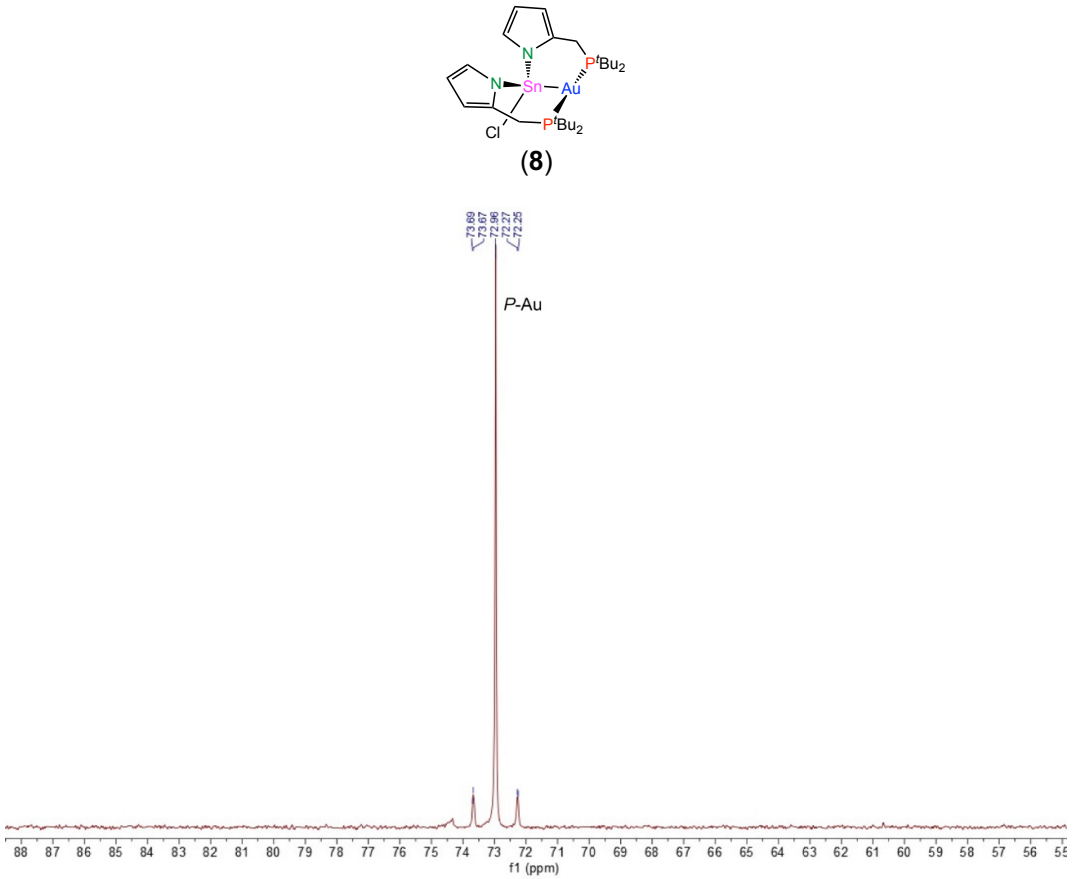
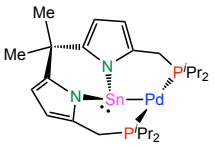


Figure S28. $^{31}P\{^{1}H\}$ NMR spectrum (162.1MHz, CD_2Cl_2, 298 K) of [Au{κ^3*P*,*Sn*,*P*-SnCl(HpyrmP^{t}Bu$_2$)$_2$}] (**8**).



(**9**)

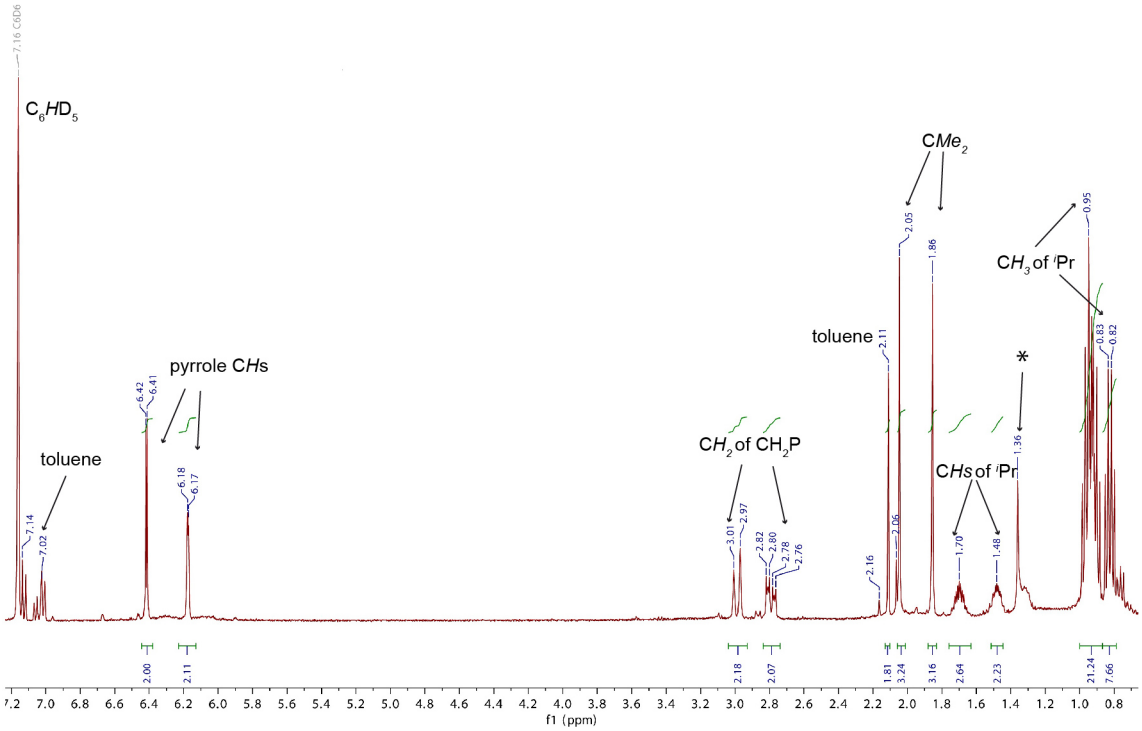


Figure S29. ^{1}H NMR spectrum (400.1 MHz, C_6D_6, 298 K) of [Pd{κ^3*P*,*Sn*,*P*-Sn(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**9**) (* = unknown impurity).

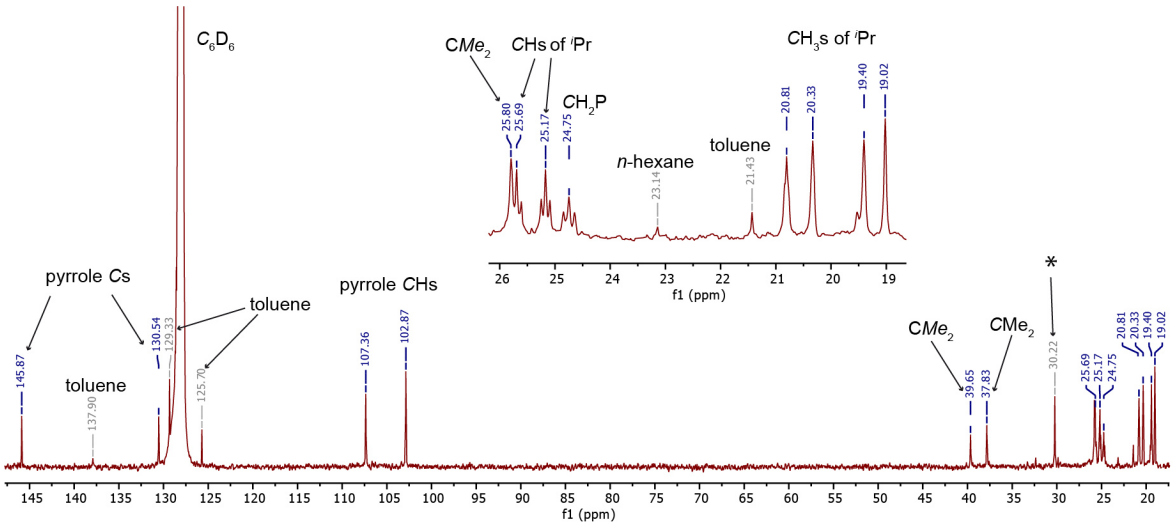


Figure S30. ^{13}C{^{1}H} NMR spectrum (100.6 MHz, C_6D_6, 298 K) of [Pd{κ^3*P*,*Sn*,*P*-Sn(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**9**) (* = unknown impurity).

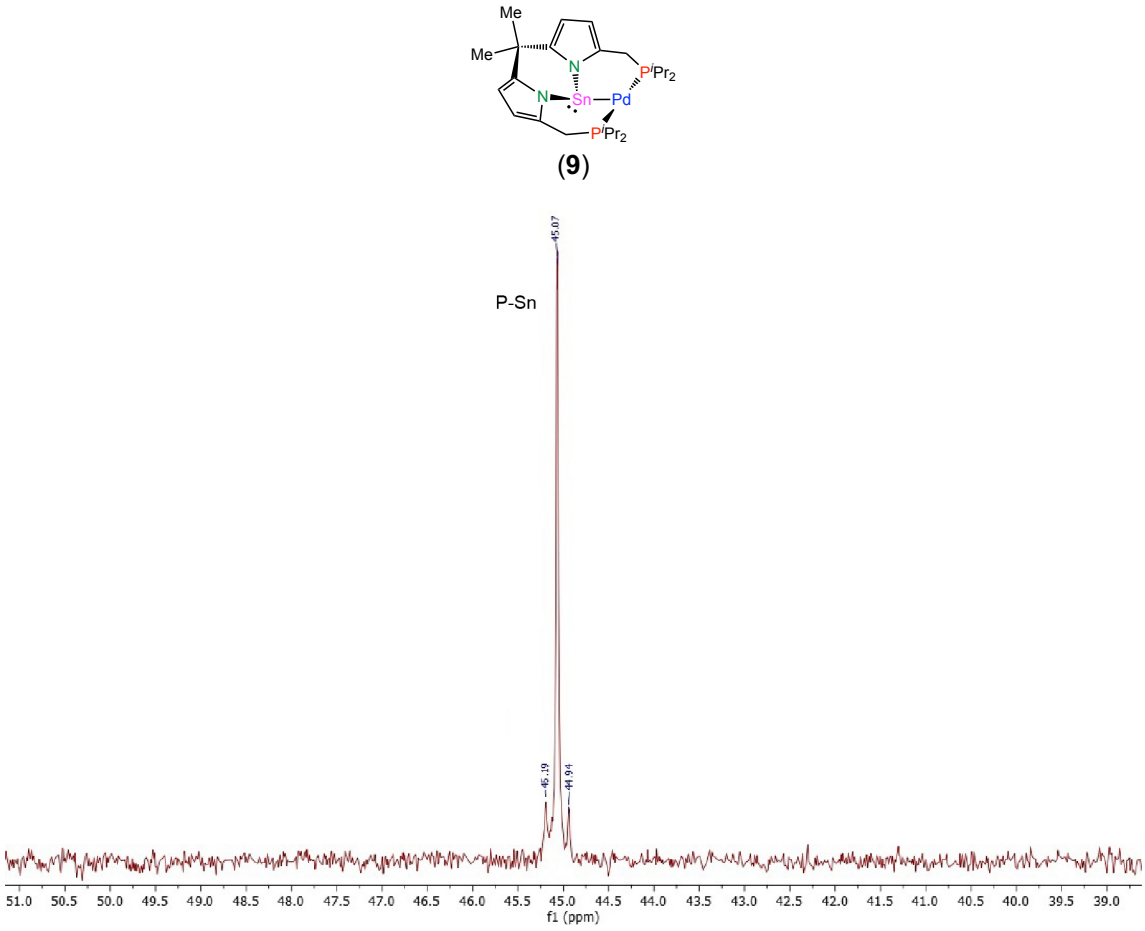


Figure S31. $^{31}P\{^{1}H\}$ NMR spectrum (162.1 MHz, C_6D_6, 298 K) of [Pd{κ^3*P*,*Sn*,*P*-Sn(pyrmP^{i}Pr$_2$)$_2$CMe$_2$}] (**9**).

Images of selected molecular orbitals

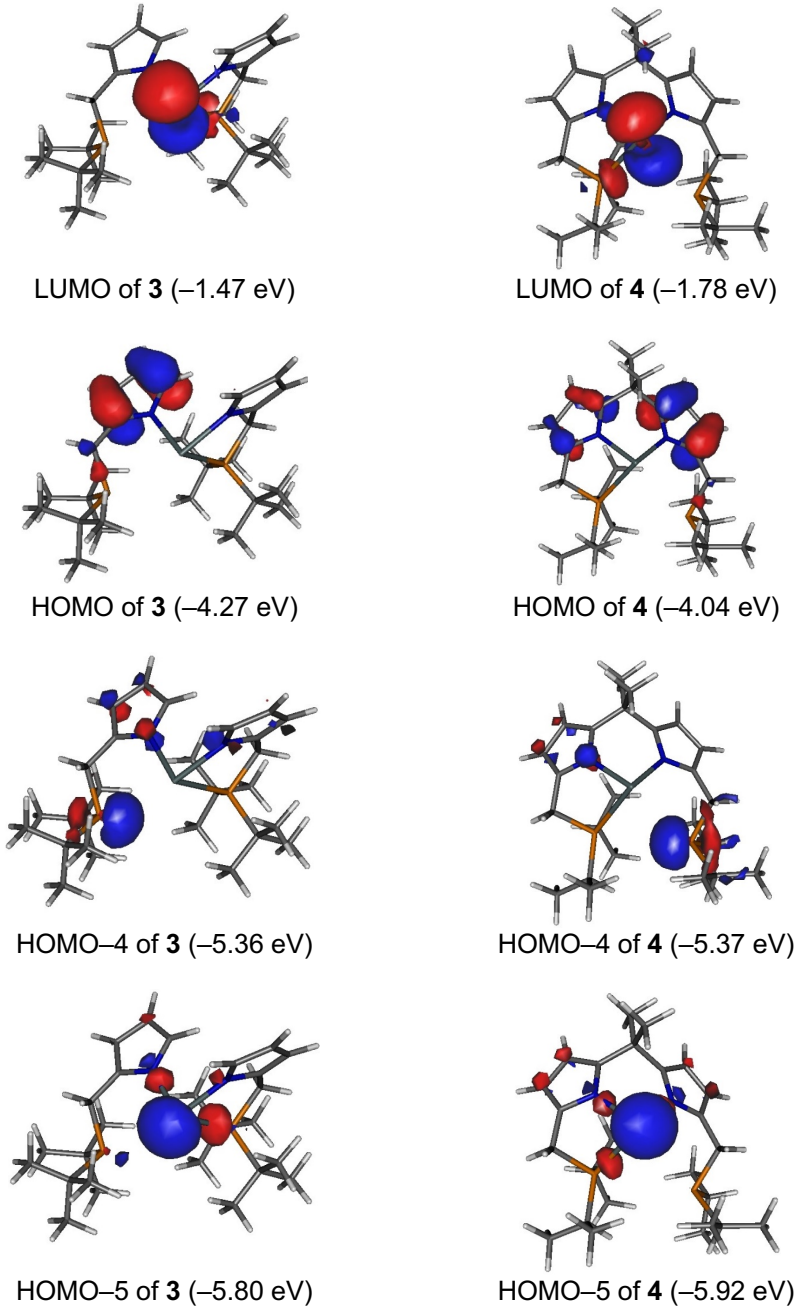
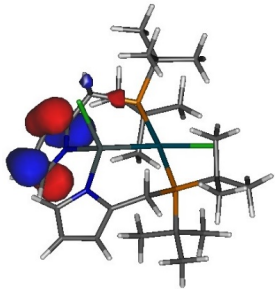
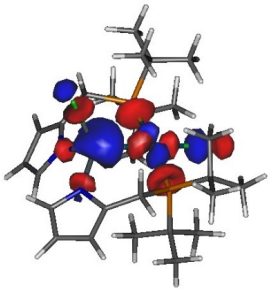


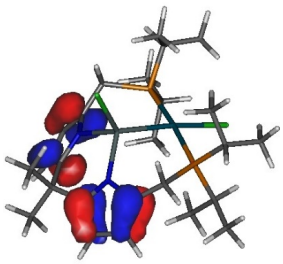
Figure S32. Selected molecular orbitals of stannylenes **3** and **4**.



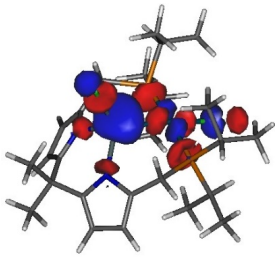
HOMO of **6** (-4.81 eV)



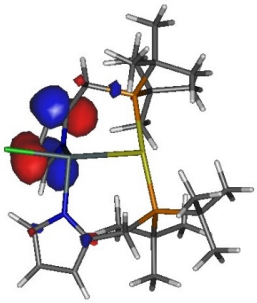
LUMO of **6** (-3.00 eV)



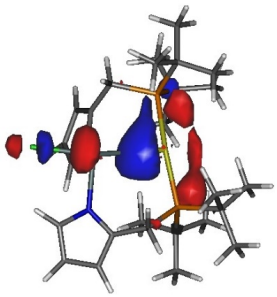
HOMO of **7** (-4.57 eV)



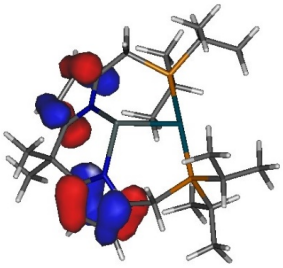
LUMO of **7** (-2.91 eV)



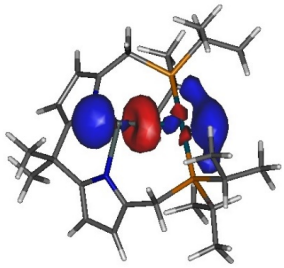
HOMO of **8** (-4.26 eV)



LUMOof **8** (-1.71 eV)



HOMO of **9** (-4.09 eV)



LUMO of **9** (-2.43 eV)

Figure S33. Frontier molecular orbitals of complexes **6**–**9**.

Table S1. Crystal, measurement, and refinement data for the compounds studied by X−ray diffraction.

	3	**4**	**5**	**6**	**7**·0.5(C_6D_6)
formula	$C_{26}H_{46}N_2P_2Sn$	$C_{25}H_{42}N_2P_2Sn$	$C_{37}H_{78}N_4P_4Si_4Sn_4$	$C_{26}H_{46}Cl_2N_2P_2PdSn$	$C_{25}H_{42}Cl_2N_2P_2PdSn\cdot(C_6D_6)_{0.5}$
fw	567.28	551.23	990.71	744.58	770.61
cryst syst	monoclinic	monoclinic	orthorhombic	triclinic	triclinic
space group	P21/n	P21/c	P212121	P−1	P−1
a, Å	12.1119(7)	8.5817(1)	10.5334(9)	11.2189(7)	10.7876(4)
b, Å	20.395(1)	18.7476(1)	16.779(2)	11.5079(6)	12.4560(5)
c, Å	12.8713(8)	16.6005(1)	54.962(5)	12.9008(5)	13.6800(3)
α, ofg	90	90	90	73.449(4)	101.654(3)
β, ofg	116.512(3)	102.959(1)	90	75.271(4)	108.540(3)
γ, ofg	90	90	90	82.184(4)	103.841(3)
V, Å^3	2845.2(3)	2602.77(4)	9714(2)	1540.5(2)	1613.1(1)
Z	4	4	8	2	2
F(000)	1184	1144	4112	752	774
D_{calcd}, g cm^{-3}	1.324	1.407	1.355	1.605	1.586
μ (radiation) mm^{-1}	1.026 (MoKα)	9.064 (CuKα)	1.222 (MoKα)	13.860 (CuKα)	13.258 (CuKα)
cryst size, mm	0.17 x 0.12 x 0.10	0.27 x 0.20 x 0.18	0.07 x 0.07 x 0.02	0.20 x 0.14 x 0.07	0.35 x 0.28 x 0.09
T, K	100(2)	150(2)	100(2)	150(2)	150(2)
θ range, deg	2.67 to 29.57	3.61 to 69.50	1.92 to 26.37	3.67 to 67.68	3.58 to 69.63
min./max. *h*	–16/16	–10/10	–11/13	–12/12	–11/13
min./max. *k*	–28/28	–22/21	–19/20	–13/13	–14/15
min./max. *l*	–17/17	–20/17	–68/68	–14/11	–16/11
no. collected reflns	90483	14699	118636	12021	15094
no. unique reflns	7970	4837	19823	4907	5965
no. reflns with $I > 2\sigma(I)$	7071	4486	15262	4332	5554
no. params/restraints	292/0	281/0	914/0	319/0	344/0
GOF (on F^2)	1.036	1.053	1.060	1.088	1.000
R_1 (on *F*, $I > 2\sigma(I)$)	0.019	0.025	0.094	0.032	0.030
wR_2 (on F^2, all data)	0.044	0.063	0.243	0.083	0.084
min./max. $\Delta\rho$, e Å^{-3}	–0.291/0.373	–0.767/0.400	–1.791/5.930	–1.433/1.211	–1.001/0.519
CCDC dep. no.	2097501	2097502	2097503	2097504	2097505

Table S2. Selected QTAIM parameters for the Sn–M bonds of complexes **6**–**9**.

Complex ($M^{o.e.}$)	ρ(r) / e Å^{-3}	d / Å	$\nabla^2\rho$(r) / e Å^{-5}	ε	q(Sn), q(M)
6 (Pd^{II})	0.066	2.506	+0.120	0.016	+1.36, +0.08
7 (Pd^{II})	0.066	2.495	+0.125	0.020	+1.34, +0.05
8 (Au^{I})	0.027	3.120	+0.038	0.017	+0.94, +0.21
9 (Pd^{0})	0.047	2.660	+0.088	0.020	+0.94, –0.23

Table S3. Cartesian coordinates (in Å) and total energies (in a. u., noncorrected zero-point vibrational energies included) of all the stationary points described in this manuscript (BP86-D3/def2-SVP level).

3: E= -2023.623076

Sn	0.685393000	-1.183780000	-0.748569000
P	-2.713820000	-0.001534000	-0.331186000
P	1.848020000	1.181797000	0.038661000
N	2.784326000	-1.685189000	-0.184518000
N	-0.031219000	-1.630447000	1.281155000
C	2.537770000	2.024787000	-1.535669000
C	-3.698898000	-0.764381000	-1.822643000
C	3.312578000	0.497275000	0.961832000
C	3.716784000	-0.835510000	0.397326000
C	-1.370381000	-1.699559000	3.107936000
C	4.815334000	-2.698500000	-0.301280000
C	1.018239000	2.394539000	1.252936000
C	-2.522312000	-1.541646000	0.766658000
C	-1.354400000	-1.576324000	1.712335000
C	-0.014404000	-1.838927000	3.540558000
C	-3.926328000	1.103879000	0.702224000
C	4.981437000	-1.431130000	0.338686000
C	3.459751000	-2.814497000	-0.612837000
C	0.778181000	-1.794453000	2.394293000
H	1.865768000	-1.888618000	2.280699000
H	0.340669000	-1.978552000	4.569786000
H	-2.273006000	-1.729526000	3.733552000
H	2.927642000	-3.635222000	-1.112959000
H	5.596091000	-3.441445000	-0.509455000
H	5.913562000	-0.999153000	0.726776000
H	-2.445828000	-2.394060000	0.055376000
H	-3.458328000	-1.710293000	1.338601000
H	2.979543000	0.423916000	2.022370000
H	4.158253000	1.217072000	0.938358000
C	-2.628091000	-1.433631000	-2.715685000
H	-1.866588000	-0.706498000	-3.065448000
H	-2.093530000	-2.256093000	-2.195392000
H	-3.114931000	-1.877953000	-3.612473000
C	-4.360379000	0.365238000	-2.639022000
H	-4.730735000	-0.042222000	-3.605872000
H	-5.233475000	0.805861000	-2.117175000
H	-3.645362000	1.182334000	-2.872598000
C	-4.759065000	-1.825227000	-1.456266000
H	-4.322769000	-2.689537000	-0.916814000
H	-5.579421000	-1.417594000	-0.837749000
H	-5.216414000	-2.224287000	-2.389646000
C	-4.036410000	2.482960000	0.013414000
H	-4.609925000	3.178942000	0.665695000
H	-3.037173000	2.932711000	-0.158268000
H	-4.560234000	2.437729000	-0.959918000
C	-5.330775000	0.514186000	0.920244000
H	-5.295751000	-0.495459000	1.380391000
H	-5.905867000	1.168494000	1.613240000
H	-5.910841000	0.446792000	-0.021414000
C	-3.256070000	1.314202000	2.077315000
H	-3.874392000	2.014668000	2.681677000
H	-3.146333000	0.375480000	2.653804000
H	-2.248627000	1.759625000	1.979141000
C	0.410629000	1.524866000	2.377611000
H	1.173484000	0.957820000	2.945425000
H	-0.107586000	2.192049000	3.099946000
H	-0.328063000	0.788501000	2.007281000
C	-0.112256000	3.140447000	0.515981000
H	-0.785481000	2.431738000	-0.012486000
H	-0.724322000	3.701909000	1.254464000
H	0.275160000	3.877977000	-0.215882000
C	2.012129000	3.392012000	1.886430000

H	1.471773000	3.987003000	2.655161000
H	2.848596000	2.878838000	2.403021000
H	2.438533000	4.106509000	1.158250000
C	1.362481000	2.285032000	-2.506412000
H	0.812721000	1.351787000	-2.749580000
H	0.631297000	3.014604000	-2.109195000
H	1.762329000	2.696092000	-3.458797000
C	3.515016000	1.022594000	-2.197144000
H	4.408797000	0.818026000	-1.576006000
H	3.041628000	0.043009000	-2.412134000
H	3.856621000	1.450551000	-3.164883000
C	3.283595000	3.340023000	-1.243128000
H	2.602102000	4.139407000	-0.890557000
H	4.090638000	3.208106000	-0.493157000
H	3.760457000	3.703950000	-2.179457000

4: E= -1983.196969

Sn	-0.789013000	0.166590000	-1.559225000
P	-0.013732000	2.112839000	0.263433000
P	2.579267000	-0.787217000	0.063311000
C	-4.380488000	-2.471244000	0.771517000
H	-4.145886000	-2.389811000	1.851659000
H	-4.385391000	-3.544813000	0.495835000
H	-5.400611000	-2.070223000	0.604938000
C	0.099700000	1.726362000	2.109549000
H	-0.517255000	2.517689000	2.594573000
N	-2.524648000	0.675670000	-0.292211000
N	-0.812113000	-1.718657000	-0.430216000
C	0.276521000	-2.524971000	-0.117334000
C	1.655227000	-2.279886000	-0.655217000
H	1.620131000	-2.108716000	-1.756429000
H	2.269316000	-3.192386000	-0.502734000
C	-2.698575000	1.918557000	0.309072000
C	-1.667824000	2.985866000	0.088215000
H	-1.765494000	3.796798000	0.838888000
H	-1.699819000	3.457942000	-0.922568000
C	3.492183000	-1.616079000	1.508118000
H	3.876404000	-2.589905000	1.124654000
C	-0.531106000	0.350290000	2.401826000
H	-0.010500000	-0.457519000	1.847967000
H	-1.605208000	0.305500000	2.137213000
H	-0.441474000	0.129571000	3.486824000
C	-3.410225000	-0.218244000	0.280406000
C	-3.725143000	1.822570000	1.252039000
H	-4.086007000	2.634881000	1.896527000
C	-1.569866000	-3.391623000	0.892776000
H	-2.236474000	-4.048465000	1.463292000
C	-1.949731000	-2.252442000	0.175406000
C	-4.184853000	0.467717000	1.226596000
H	-4.980861000	0.037457000	1.845561000
C	-0.162803000	-3.563807000	0.708832000
H	0.464777000	-4.372325000	1.107553000
C	-3.355795000	-1.696582000	-0.079075000
C	-3.725683000	-1.891802000	-1.578846000
H	-4.750545000	-1.515831000	-1.779600000
H	-3.664067000	-2.963687000	-1.859110000
H	-3.036239000	-1.336711000	-2.253325000
C	1.295292000	3.388200000	-0.162249000
H	2.247508000	2.902961000	0.147587000
C	3.961608000	-0.575581000	-1.225231000
H	4.644689000	0.160395000	-0.743169000
C	1.116104000	4.717374000	0.593008000
H	1.973588000	5.394113000	0.388067000
H	1.050086000	4.585450000	1.692236000
H	0.196087000	5.242422000	0.260597000
C	1.337050000	3.609482000	-1.685915000
H	0.389950000	4.052082000	-2.061560000
H	1.513718000	2.666768000	-2.242899000
H	2.154585000	4.314459000	-1.948224000
C	1.543432000	1.807965000	2.632242000
H	1.562532000	1.512963000	3.702778000
H	1.981290000	2.823699000	2.562365000
H	2.196586000	1.104946000	2.076288000
C	4.764836000	-1.838008000	-1.571132000
H	4.129491000	-2.602313000	-2.065840000
H	5.223615000	-2.306528000	-0.676530000
H	5.590290000	-1.595420000	-2.275888000
C	2.512178000	-1.905188000	2.660690000
H	3.016533000	-2.506108000	3.448469000

H	1.614859000	-2.461841000	2.323457000
H	2.159488000	-0.966189000	3.133669000
C	3.377488000	0.089736000	-2.483938000
H	4.182804000	0.360555000	-3.200584000
H	2.817349000	1.014248000	-2.233319000
H	2.679603000	-0.587968000	-3.022144000
C	4.682241000	-0.769057000	1.988739000
H	4.358908000	0.250756000	2.291216000
H	5.473363000	-0.660207000	1.218548000
H	5.152626000	-1.239230000	2.879674000

6: E= -3072.033682

Pd	0.071854000	-0.886987000	-0.007562000
Sn	-0.110853000	1.512778000	0.691724000
P	-2.310409000	-1.001441000	-0.055754000
P	2.459304000	-0.579390000	0.051071000
Cl	0.521007000	2.193680000	2.913207000
Cl	0.285924000	-3.128965000	-0.846746000
N	-1.946796000	2.505501000	0.448407000
N	1.214135000	2.640609000	-0.501681000
C	2.553911000	2.267912000	-0.513287000
C	1.010641000	3.604860000	-1.475657000
C	3.295590000	-0.990626000	-1.636524000
C	-2.207120000	3.798132000	0.018152000
C	-3.135768000	1.785713000	0.434948000
C	2.229048000	3.876093000	-2.095237000
C	3.065677000	1.190851000	0.395863000
C	3.192912000	-1.536696000	1.548890000
C	-2.964142000	-2.557527000	0.903227000
C	-3.230954000	0.362814000	0.886865000
C	-2.948509000	-0.847612000	-1.859193000
C	3.209023000	3.033390000	-1.484118000
C	-4.156316000	2.634547000	-0.004207000
C	-3.565645000	3.909702000	-0.268730000
H	4.282055000	3.000756000	-1.711706000
H	2.396539000	4.611706000	-2.891793000
H	0.014558000	4.023479000	-1.659021000
H	-1.414013000	4.554779000	-0.007584000
H	-4.079934000	4.818834000	-0.604042000
H	-5.215944000	2.362651000	-0.095801000
H	4.170452000	1.173144000	0.360103000
H	2.787133000	1.397257000	1.452205000
H	-2.878774000	0.244008000	1.937203000
H	-4.301608000	0.088933000	0.884445000
C	2.413435000	-1.041287000	2.791282000
H	2.822150000	-1.546662000	3.693034000
H	2.484201000	0.050504000	2.964425000
H	1.336349000	-1.301234000	2.720196000
C	4.701222000	-1.260723000	1.717474000
H	4.929798000	-0.190650000	1.894552000
H	5.071659000	-1.822866000	2.602335000
H	5.286444000	-1.607914000	0.841872000
C	2.955579000	-3.056378000	1.423007000
H	3.579205000	-3.522432000	0.638881000
H	3.227641000	-3.531892000	2.390537000
H	1.898627000	-3.295691000	1.197780000
C	2.288316000	-0.497192000	-2.704540000
H	1.354888000	-1.095258000	-2.675465000
H	2.037343000	0.576248000	-2.572646000
H	2.743971000	-0.615193000	-3.711948000
C	4.639299000	-0.252189000	-1.815057000
H	4.513039000	0.842366000	-1.894363000
H	5.361592000	-0.475946000	-1.004420000
H	5.098179000	-0.597490000	-2.766676000
C	3.543438000	-2.502714000	-1.806892000
H	3.846734000	-2.687062000	-2.860771000
H	4.373043000	-2.857141000	-1.161949000
H	2.637021000	-3.102044000	-1.601411000
C	-2.994071000	-3.812757000	0.008025000
H	-2.032443000	-3.974459000	-0.513775000
H	-3.186222000	-4.696942000	0.654661000
H	-3.815530000	-3.766643000	-0.735168000
C	-4.377413000	-2.350070000	1.493999000
H	-4.708451000	-3.312911000	1.939536000
H	-4.405335000	-1.596384000	2.305043000
H	-5.128267000	-2.072824000	0.726110000
C	-1.957185000	-2.767445000	2.059210000
H	-1.831530000	-1.855418000	2.681260000
H	-2.330243000	-3.575844000	2.725485000

H	-0.963171000	-3.068025000	1.672438000
C	-4.484856000	-0.722936000	-1.889808000
H	-4.985139000	-1.613191000	-1.456610000
H	-4.843425000	0.185790000	-1.367231000
H	-4.816571000	-0.643341000	-2.947947000
C	-2.301210000	0.436547000	-2.439263000
H	-2.577448000	1.350444000	-1.879004000
H	-1.194436000	0.353452000	-2.475975000
H	-2.659132000	0.566715000	-3.483490000
C	-2.494200000	-2.040038000	-2.726296000
H	-1.411972000	-2.247692000	-2.617130000
H	-3.042989000	-2.970505000	-2.493756000
H	-2.699524000	-1.791589000	-3.790248000

7: E= -3031.622192

Pd	-1.312931000	0.071811000	-0.072635000
Sn	0.931393000	-0.079344000	1.006325000
P	-1.080836000	2.410430000	-0.078062000
P	-1.365813000	-2.279246000	-0.105890000
Cl	-3.333437000	0.213682000	-1.352975000
Cl	1.254287000	-0.186035000	3.379995000
N	2.250460000	1.387437000	0.285874000
N	2.082976000	-1.626455000	0.179952000
C	1.475152000	-2.811750000	-0.225504000
C	-2.627089000	-2.934539000	1.123837000
C	-2.352337000	3.246785000	1.025886000
C	1.789822000	2.665191000	-0.019398000
C	3.236730000	-1.417764000	-0.571939000
C	3.385653000	1.111817000	-0.471651000
C	3.378706000	-2.508670000	-1.435709000
C	0.179048000	-3.256024000	0.379755000
C	2.268515000	-3.387592000	-1.218576000
C	0.516873000	3.185686000	0.571499000
C	3.668959000	2.250165000	-1.234150000
C	-1.282697000	3.058017000	-1.820595000
C	4.144303000	-0.209723000	-0.324834000
C	-1.833434000	-2.897912000	-1.807728000
C	2.663305000	3.229635000	-0.950119000
H	2.075856000	-4.345413000	-1.719261000
H	4.206466000	-2.670985000	-2.135300000
H	4.522837000	2.375547000	-1.909591000
H	2.587044000	4.240209000	-1.372205000
H	-1.944083000	4.267240000	1.210939000
H	-2.344169000	2.804886000	-2.036062000
H	-2.849523000	-2.464136000	-1.937346000
H	-2.404753000	-4.022138000	1.221972000
H	-0.018425000	-4.315012000	0.117560000
H	0.215974000	-3.207701000	1.491898000
H	0.436494000	4.277882000	0.398187000
H	0.484425000	3.036341000	1.675031000
C	4.727415000	-0.299891000	1.118341000
H	5.401524000	0.560118000	1.311841000
H	3.930403000	-0.283720000	1.889167000
H	5.297812000	-1.243699000	1.242145000
C	5.310820000	-0.237756000	-1.331394000
H	5.893618000	-1.173926000	-1.220756000
H	4.944121000	-0.173917000	-2.375644000
H	5.998703000	0.611770000	-1.148596000
C	-2.402147000	-2.250057000	2.486441000
H	-2.654663000	-1.170142000	2.425422000
H	-3.056621000	-2.711798000	3.255632000
H	-1.356393000	-2.322802000	2.850982000
C	-4.071309000	-2.744186000	0.633641000
H	-4.290215000	-3.333350000	-0.279635000
H	-4.778888000	-3.076401000	1.422933000
H	-4.275062000	-1.678040000	0.402047000
C	-2.417624000	2.483214000	2.363810000
H	-3.047878000	3.038721000	3.090055000
H	-2.870398000	1.480076000	2.213491000
H	-1.421291000	2.331748000	2.829805000
C	-3.738142000	3.360744000	0.372623000
H	-4.118414000	2.363008000	0.072182000
H	-4.452826000	3.808870000	1.095564000
H	-3.727473000	4.006091000	-0.528849000
C	-1.894683000	-4.429173000	-1.906080000
H	-2.520241000	-4.888858000	-1.112610000
H	-2.332246000	-4.722057000	-2.884061000
H	-0.882790000	-4.883614000	-1.855885000
C	-0.914780000	-2.270662000	-2.872669000

H	0.146597000	-2.558796000	-2.726407000
H	-1.231223000	-2.609362000	-3.882022000
H	-0.985104000	-1.164668000	-2.850761000
C	-1.065675000	4.574430000	-1.934198000
H	-1.363946000	4.918769000	-2.947234000
H	-1.662090000	5.154085000	-1.198699000
H	0.003455000	4.841221000	-1.802272000
C	-0.394507000	2.260385000	-2.795460000
H	-0.667208000	1.186079000	-2.794690000
H	-0.540443000	2.644563000	-3.827439000
H	0.682129000	2.350371000	-2.542339000

8: E= -2619.754829

Au	-0.388119000	-0.813694000	-0.190105000
Sn	0.631011000	1.974114000	-1.152719000
P	1.778214000	-1.729122000	-0.069450000
P	-2.629131000	-0.081908000	-0.010118000
Cl	0.883157000	4.405542000	-1.415617000
N	2.648572000	1.714794000	-0.261956000
N	-0.328212000	2.219884000	0.880221000
C	-1.698519000	2.328898000	1.076521000
C	0.291578000	2.659741000	2.031960000
C	-3.357692000	-0.718008000	1.641445000
C	3.345450000	2.720211000	0.381551000
C	3.474552000	0.600478000	-0.315680000
C	-0.668923000	3.050884000	2.969203000
C	-2.676298000	1.796894000	0.074488000
C	-3.660581000	-0.575630000	-1.542821000
C	1.772136000	-3.392514000	-1.024582000
C	3.080486000	-0.695885000	-0.950856000
C	2.293625000	-1.884342000	1.760326000
C	-1.943595000	2.842862000	2.358294000
C	4.695016000	0.905636000	0.307953000
C	4.608883000	2.256983000	0.755858000
H	-2.931262000	3.041742000	2.796405000
H	-0.472536000	3.455206000	3.970509000
H	1.386125000	2.687558000	2.099337000
H	2.902096000	3.719570000	0.478612000
H	5.388013000	2.837585000	1.265830000
H	5.558495000	0.231564000	0.393924000
H	-3.709416000	2.126327000	0.303975000
H	-2.444699000	2.140109000	-0.955908000
H	2.655021000	-0.541554000	-1.965844000
H	3.979884000	-1.335614000	-1.063909000
C	-3.122772000	0.279486000	-2.716620000
H	-3.552519000	-0.103498000	-3.667109000
H	-3.410312000	1.346512000	-2.634199000
H	-2.016394000	0.224090000	-2.798366000
C	-5.165583000	-0.310392000	-1.353238000
H	-5.369283000	0.743203000	-1.070696000
H	-5.699073000	-0.505456000	-2.309070000
H	-5.614212000	-0.970848000	-0.584759000
C	-3.401739000	-2.061197000	-1.880221000
H	-3.777615000	-2.752290000	-1.103797000
H	-3.918001000	-2.314418000	-2.831800000
H	-2.317616000	-2.258378000	-2.018463000
C	-2.232770000	-0.618480000	2.702645000
H	-1.399625000	-1.313834000	2.470703000
H	-1.819740000	0.406039000	2.795079000
H	-2.652179000	-0.910469000	3.690259000
C	-4.566748000	0.124049000	2.096393000
H	-4.269492000	1.163711000	2.333966000
H	-5.383062000	0.149194000	1.348570000
H	-4.983557000	-0.316561000	3.028061000
C	-3.750008000	-2.201241000	1.491448000
H	-4.011257000	-2.606464000	2.493059000
H	-4.631915000	-2.350630000	0.836363000
H	-2.904580000	-2.804634000	1.097756000
C	0.541236000	-4.233710000	-0.617816000
H	-0.405034000	-3.675314000	-0.776484000
H	0.506478000	-5.151048000	-1.245200000
H	0.572064000	-4.554596000	0.439917000
C	3.060787000	-4.209462000	-0.814463000
H	3.061188000	-5.080424000	-1.505828000
H	3.977856000	-3.622428000	-1.026931000
H	3.134858000	-4.610107000	0.216231000
C	1.624127000	-3.015819000	-2.519037000
H	2.540209000	-2.552286000	-2.935671000
H	1.424236000	-3.937342000	-3.107223000

H	0.772950000	-2.319993000	-2.683601000
C	3.792962000	-2.202302000	1.923279000
H	4.079499000	-3.174525000	1.479080000
H	4.422401000	-1.402808000	1.489142000
H	4.028713000	-2.251058000	3.008594000
C	1.984012000	-0.517049000	2.423019000
H	2.589177000	0.303801000	1.993282000
H	0.915083000	-0.231422000	2.340287000
H	2.231092000	-0.590457000	3.504373000
C	1.435196000	-2.976323000	2.429691000
H	0.351370000	-2.824038000	2.241349000
H	1.711603000	-3.996448000	2.094442000
H	1.594488000	-2.935304000	3.528722000

9: E= -2111.320798

Pd	-1.128068000	0.779117000	-0.045204000
Sn	0.584003000	-0.473132000	-1.650504000
P	-2.490572000	-1.095588000	0.146945000
P	0.306372000	2.595232000	0.192048000
N	0.696849000	-2.271593000	-0.396479000
N	2.394675000	0.141329000	-0.561470000
C	2.804550000	1.457701000	-0.397932000
C	-0.466982000	4.249520000	-0.264496000
C	-4.142602000	-0.976071000	-0.751309000
C	-0.406292000	-3.010098000	0.008979000
C	3.316986000	-0.688737000	0.060090000
C	1.810696000	-2.719002000	0.302585000
C	4.329935000	0.109910000	0.609860000
C	1.919012000	2.602625000	-0.781953000
C	4.004262000	1.471740000	0.320231000
C	-1.779985000	-2.712458000	-0.506691000
C	1.406641000	-3.748908000	1.162589000
C	-2.933916000	-1.459065000	1.944207000
C	3.217074000	-2.211421000	-0.012580000
C	0.813714000	2.755542000	1.998783000
C	0.000014000	-3.932833000	0.977754000
H	4.564500000	2.366861000	0.622027000
H	5.212334000	-0.245530000	1.154302000
H	2.053942000	-4.325613000	1.833265000
H	-0.646504000	-4.659821000	1.487588000
H	-4.627749000	-1.975702000	-0.671806000
H	-3.639006000	-0.633727000	2.190672000
H	-0.159235000	2.996030000	2.484734000
H	0.326491000	5.020685000	-0.136717000
H	2.438318000	3.566949000	-0.606177000
H	1.626646000	2.580535000	-1.857122000
H	-2.479482000	-3.534521000	-0.253508000
H	-1.790808000	-2.615943000	-1.616272000
C	3.604403000	-2.669979000	-1.453401000
H	3.552145000	-3.775611000	-1.537925000
H	2.915942000	-2.243768000	-2.214218000
H	4.631046000	-2.330092000	-1.703558000
C	4.222369000	-2.838249000	0.974252000
H	5.256435000	-2.521855000	0.731413000
H	3.998878000	-2.536076000	2.017037000
H	4.189645000	-3.944432000	0.912641000
C	-0.901646000	4.212757000	-1.741057000
H	-1.650032000	3.407920000	-1.908338000
H	-1.364852000	5.179954000	-2.031614000
H	-0.051916000	4.031638000	-2.430554000
C	-1.652328000	4.579557000	0.657438000
H	-1.344119000	4.721889000	1.713144000
H	-2.148384000	5.517232000	0.326850000
H	-2.412314000	3.767965000	0.628865000
C	-3.892002000	-0.655144000	-2.236497000
H	-4.855411000	-0.606542000	-2.787713000
H	-3.381983000	0.326218000	-2.344525000
H	-3.261676000	-1.416810000	-2.739381000
C	-5.048366000	0.084196000	-0.103767000
H	-4.533555000	1.069330000	-0.062072000
H	-5.976575000	0.214847000	-0.700286000
H	-5.354120000	-0.186896000	0.927110000
C	1.805139000	3.897756000	2.267141000
H	1.447254000	4.878143000	1.889051000
H	1.972119000	4.004833000	3.360423000
H	2.790344000	3.680188000	1.807081000
C	1.304787000	1.409812000	2.569671000
H	2.302192000	1.135410000	2.173324000
H	1.378840000	1.479579000	3.676111000

H	0.611875000	0.581232000	2.319038000
C	-3.653593000	-2.801314000	2.148152000
H	-4.023792000	-2.877559000	3.192952000
H	-4.528934000	-2.929402000	1.476939000
H	-2.962404000	-3.653514000	1.985705000
C	-1.699495000	-1.315654000	2.854362000
H	-1.262811000	-0.298892000	2.779924000
H	-1.988513000	-1.491016000	3.913103000
H	-0.905708000	-2.042806000	2.585357000