Supporting Information for

Insertion of $SnCl_2$ into the Pd–Cl Bond: Mechanistic Elucidation and Antitumor Evaluation of Trichlorostannyl Palladium-NHC Allyl Complexes in Ovarian Cancer Models

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† Electronic Supplementary Information (ESI) available: Experimental procedures, analytical data and spectra. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/x0xx00000x

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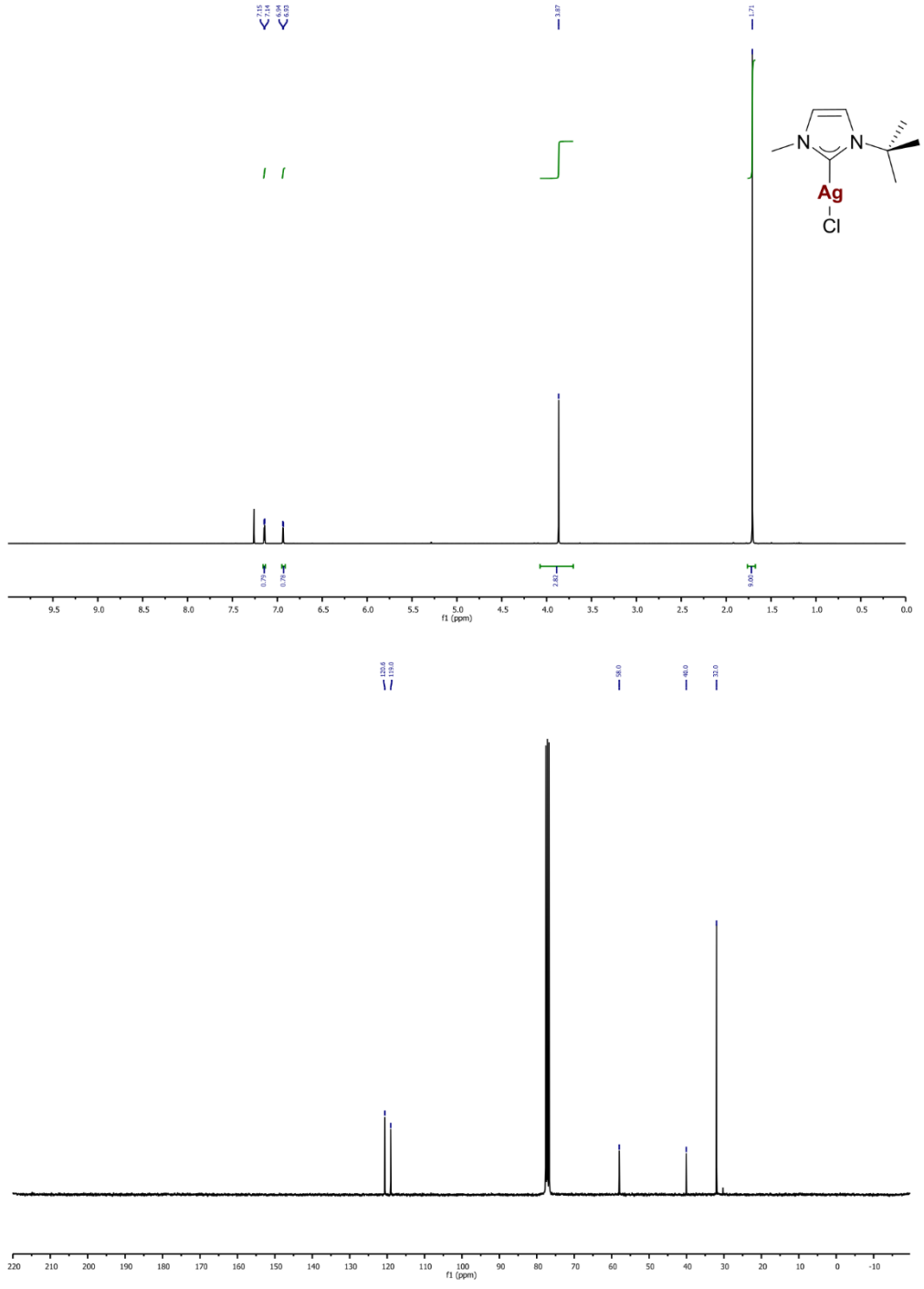
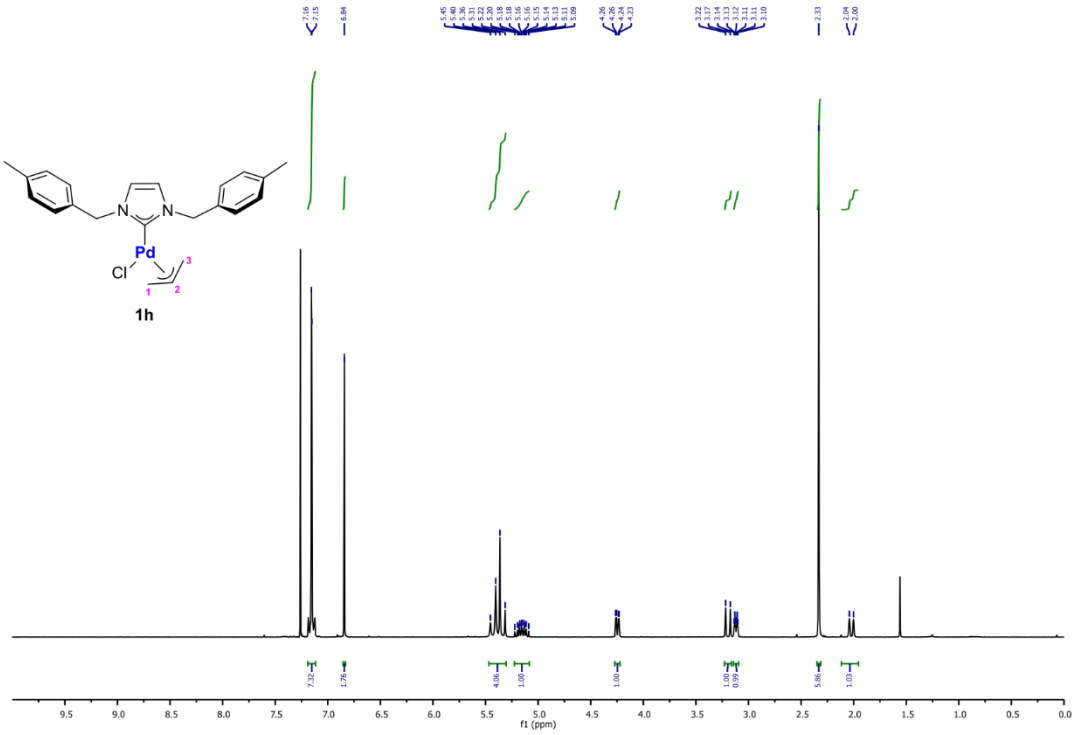
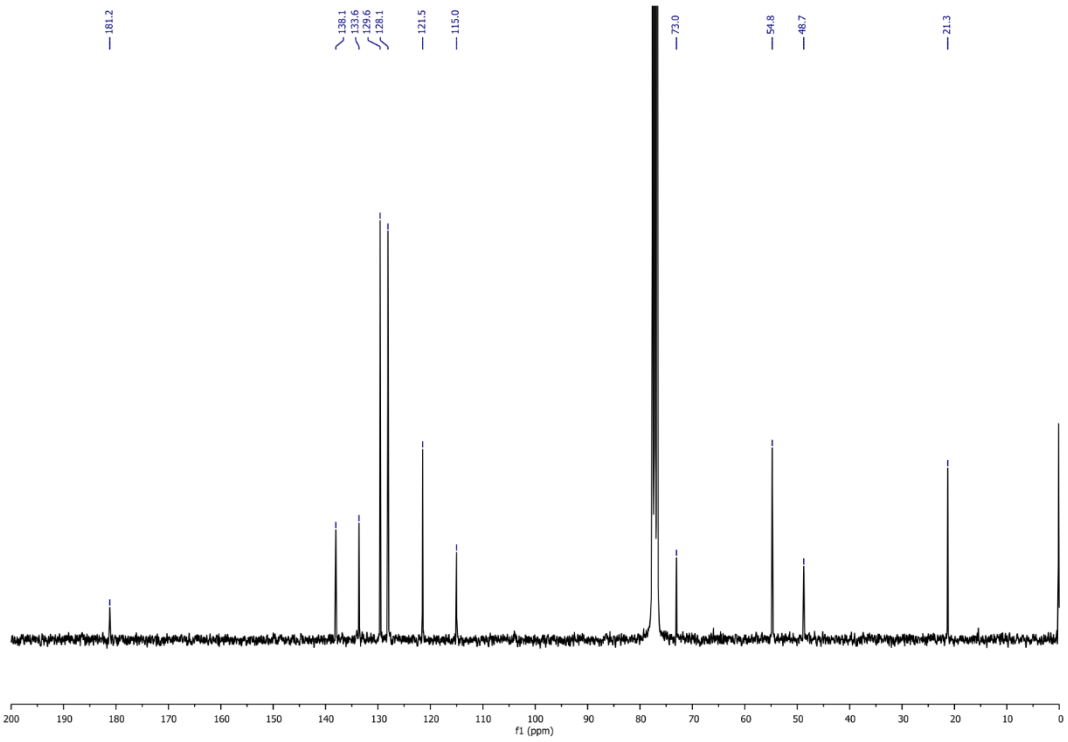
NMR Spectra

^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of [Ag(Me-Im-^{t}Bu)Cl]



*^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of [Pd(allyl)(Tol-CH_2-Im-CH_2-Tol)Cl] (**1h**)*





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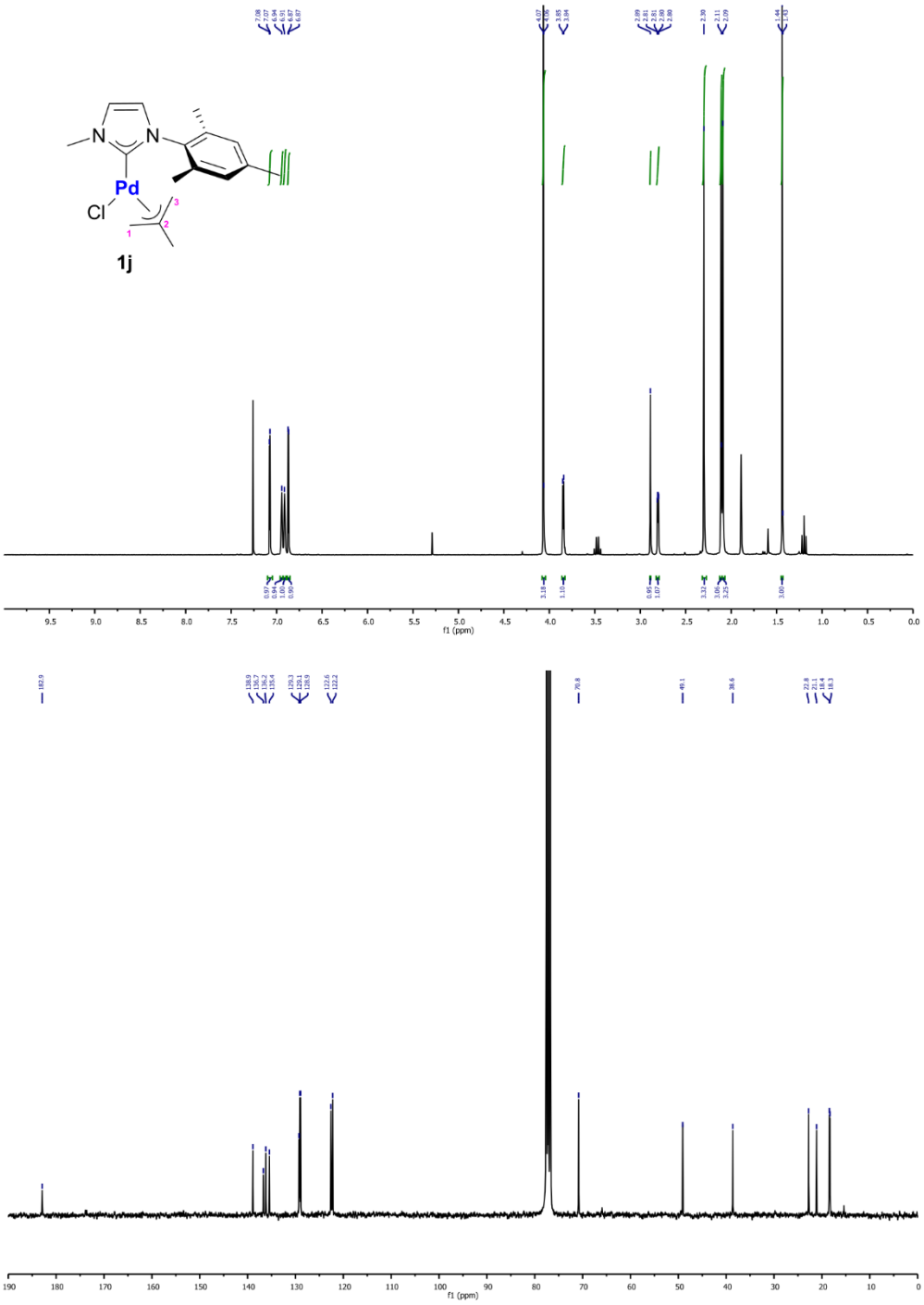

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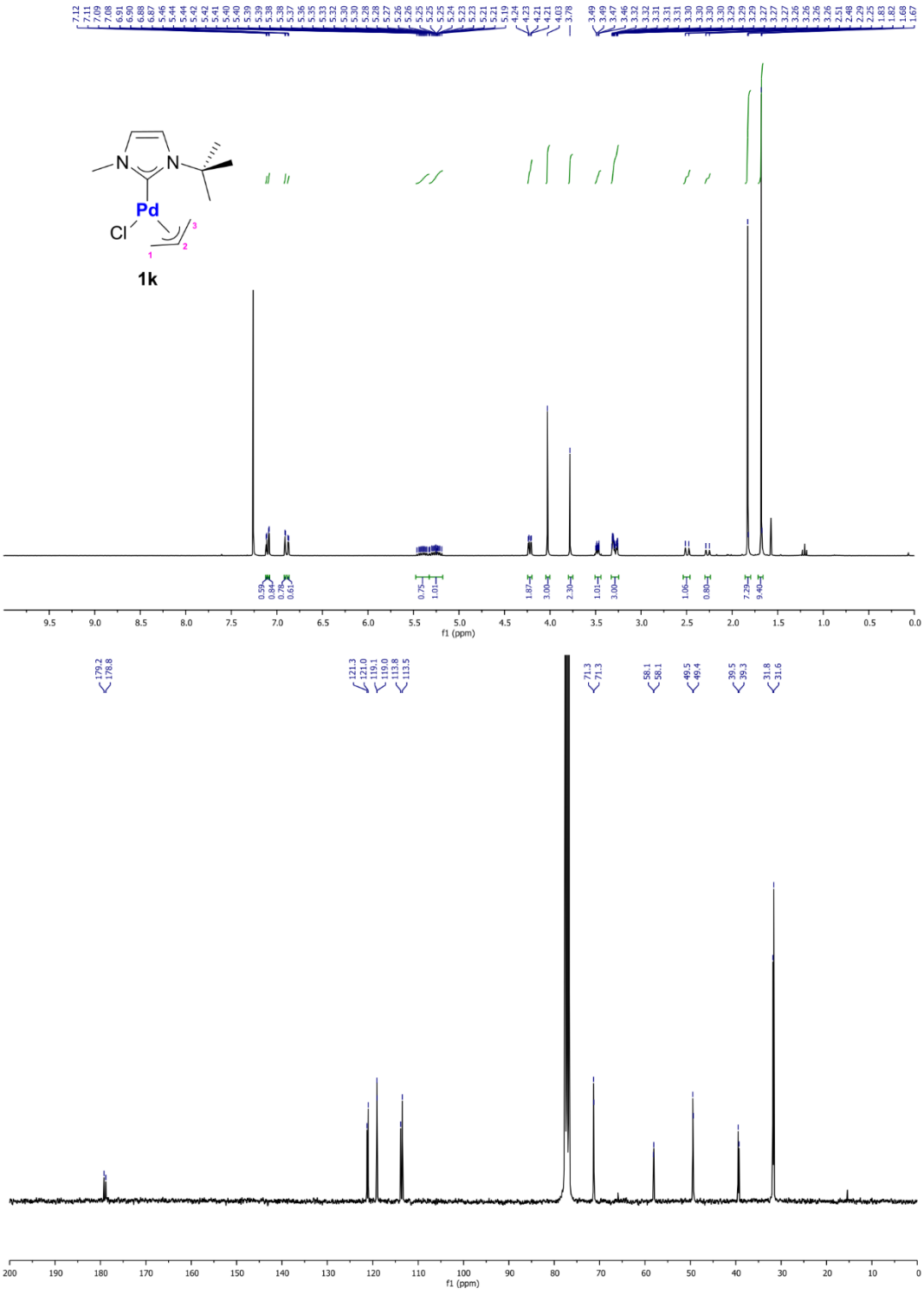
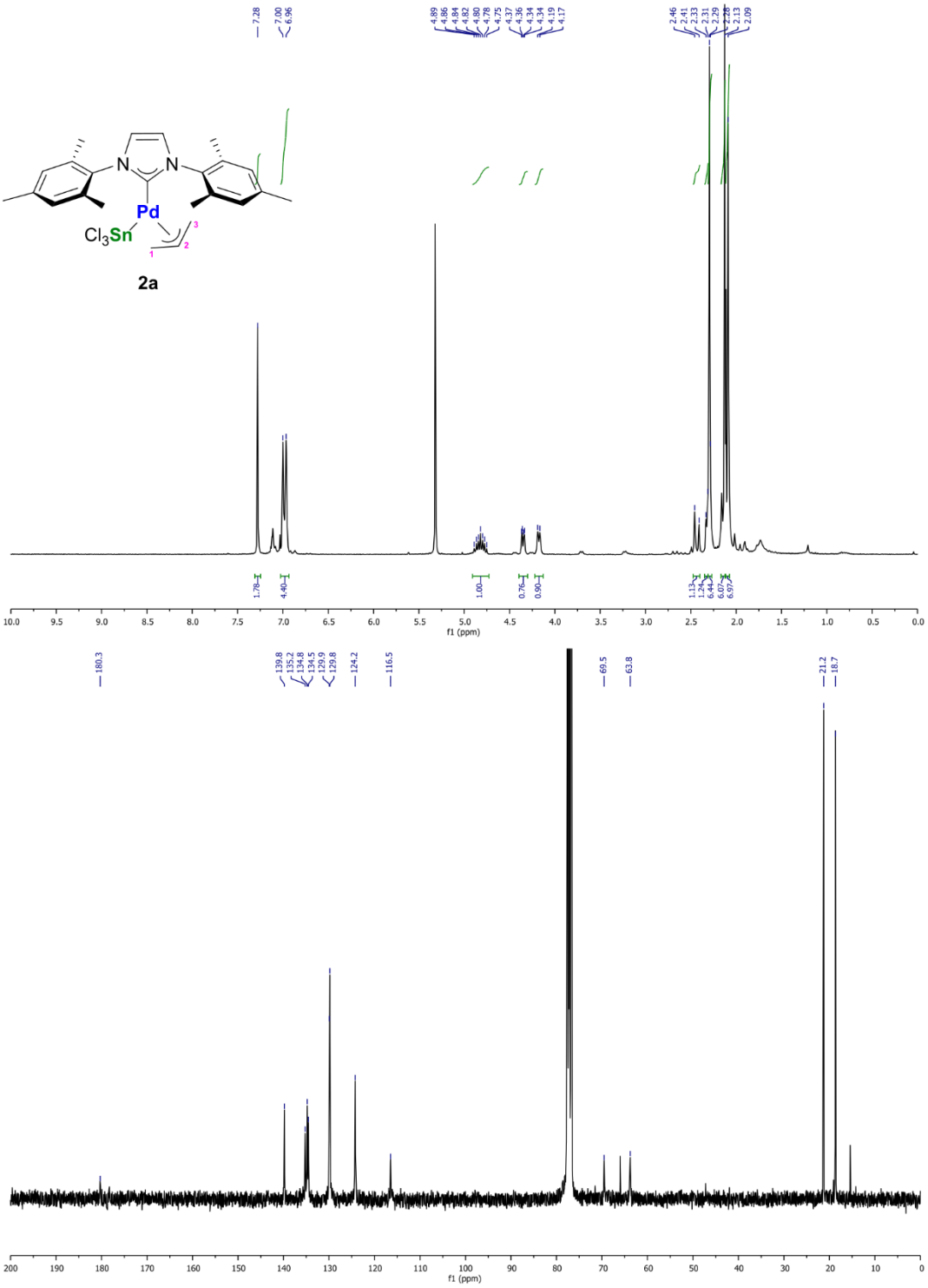


*^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of [Pd(allyl)(IMes)$SnCl_3$] (**2a**)*



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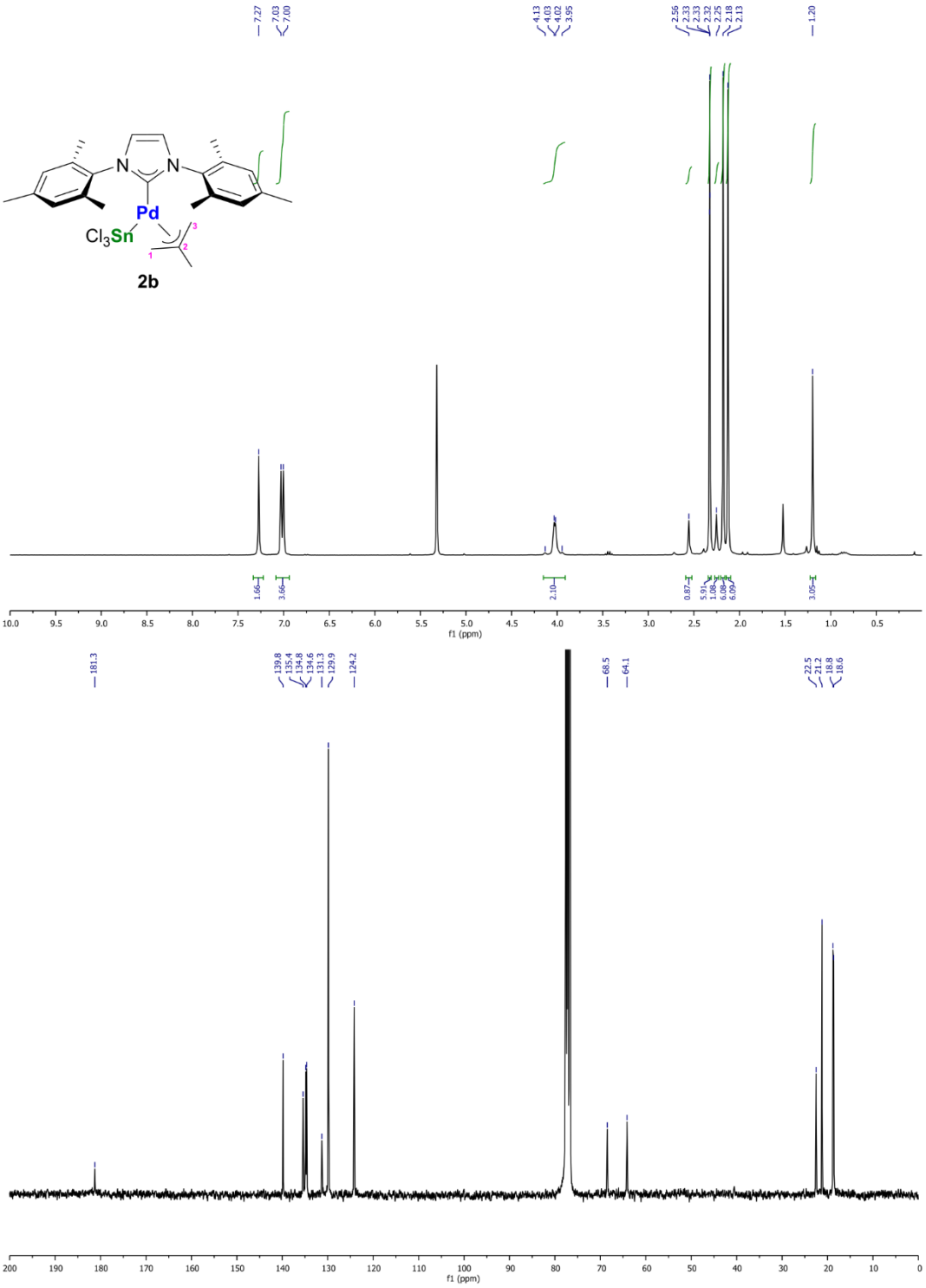

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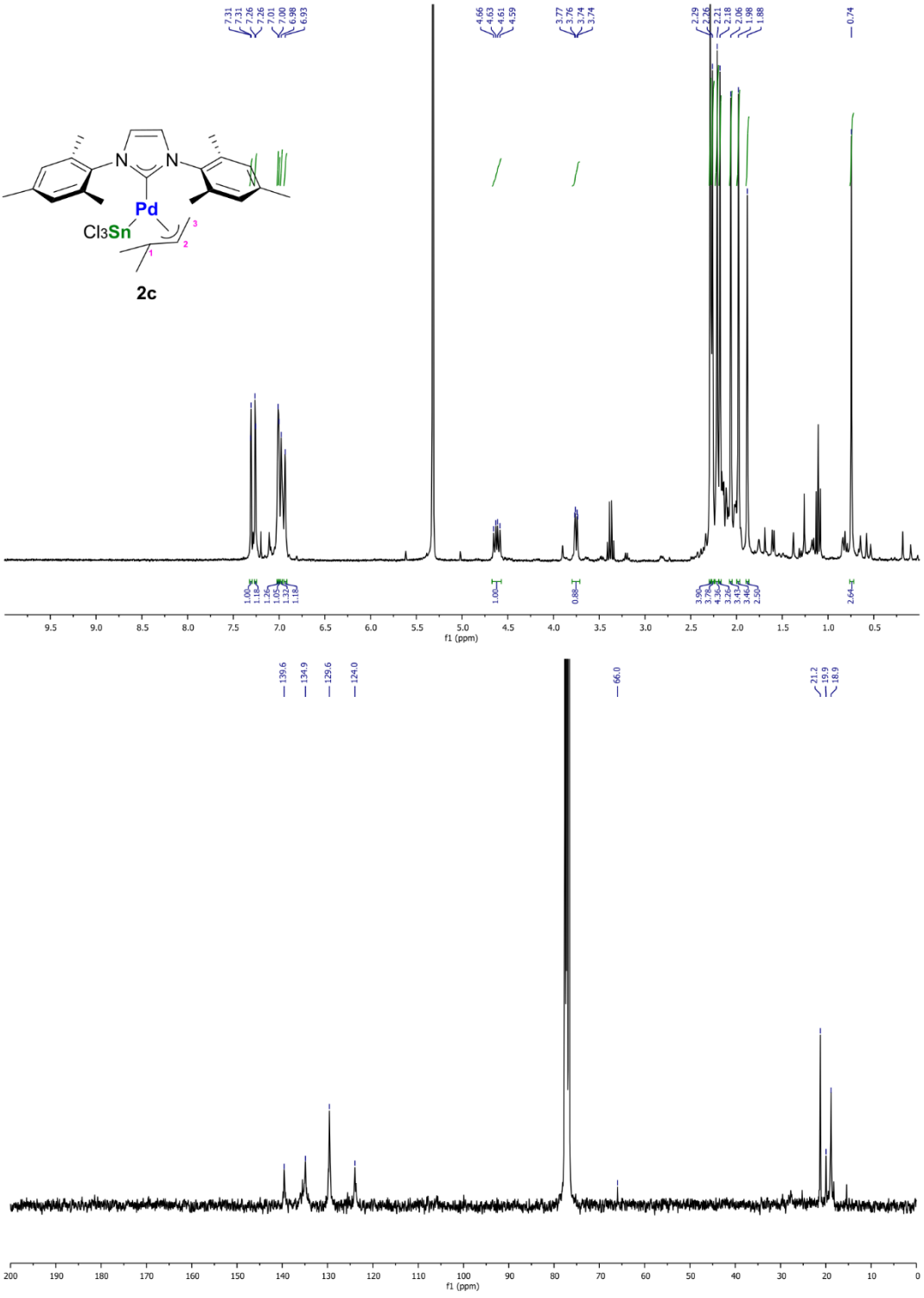

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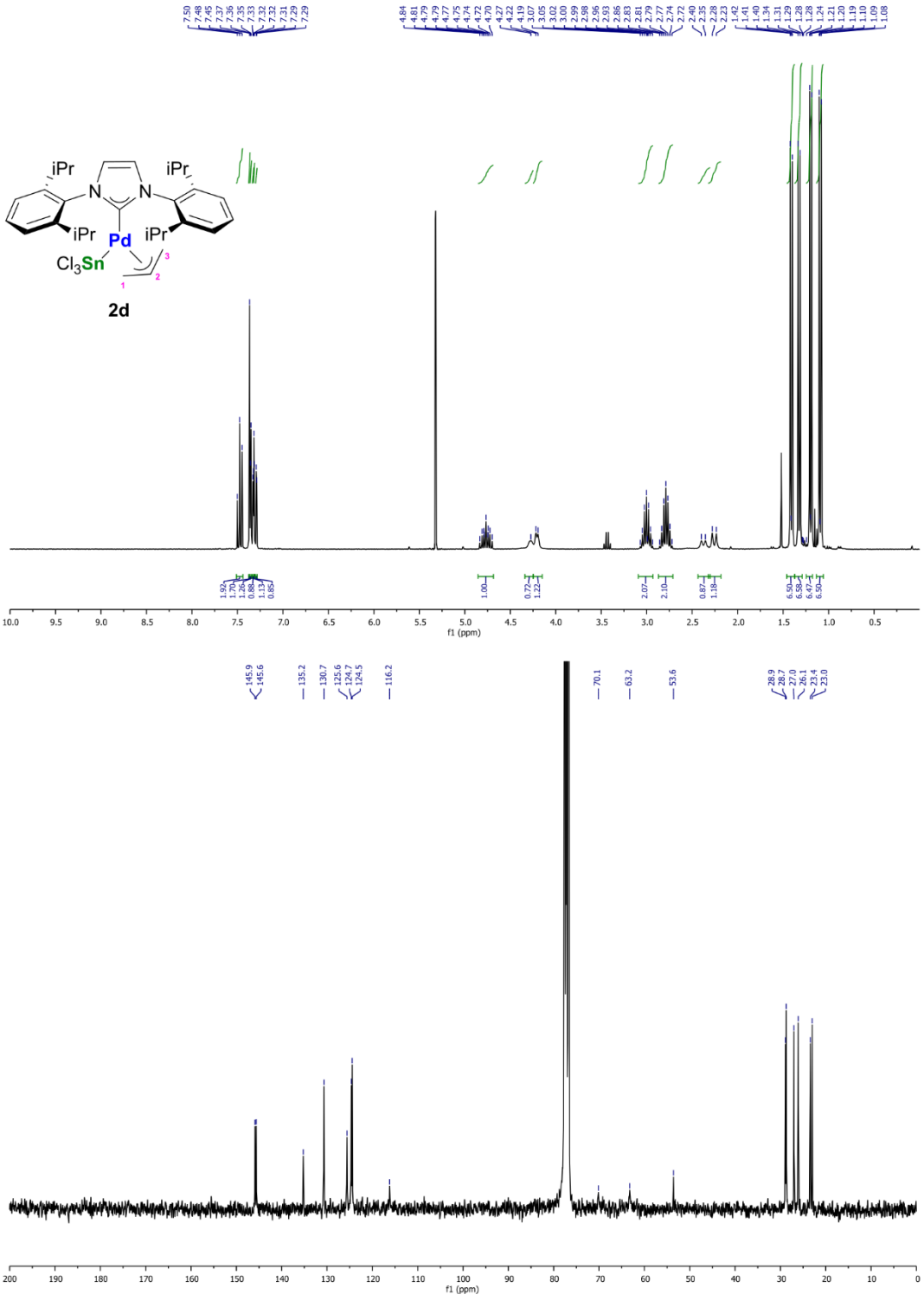

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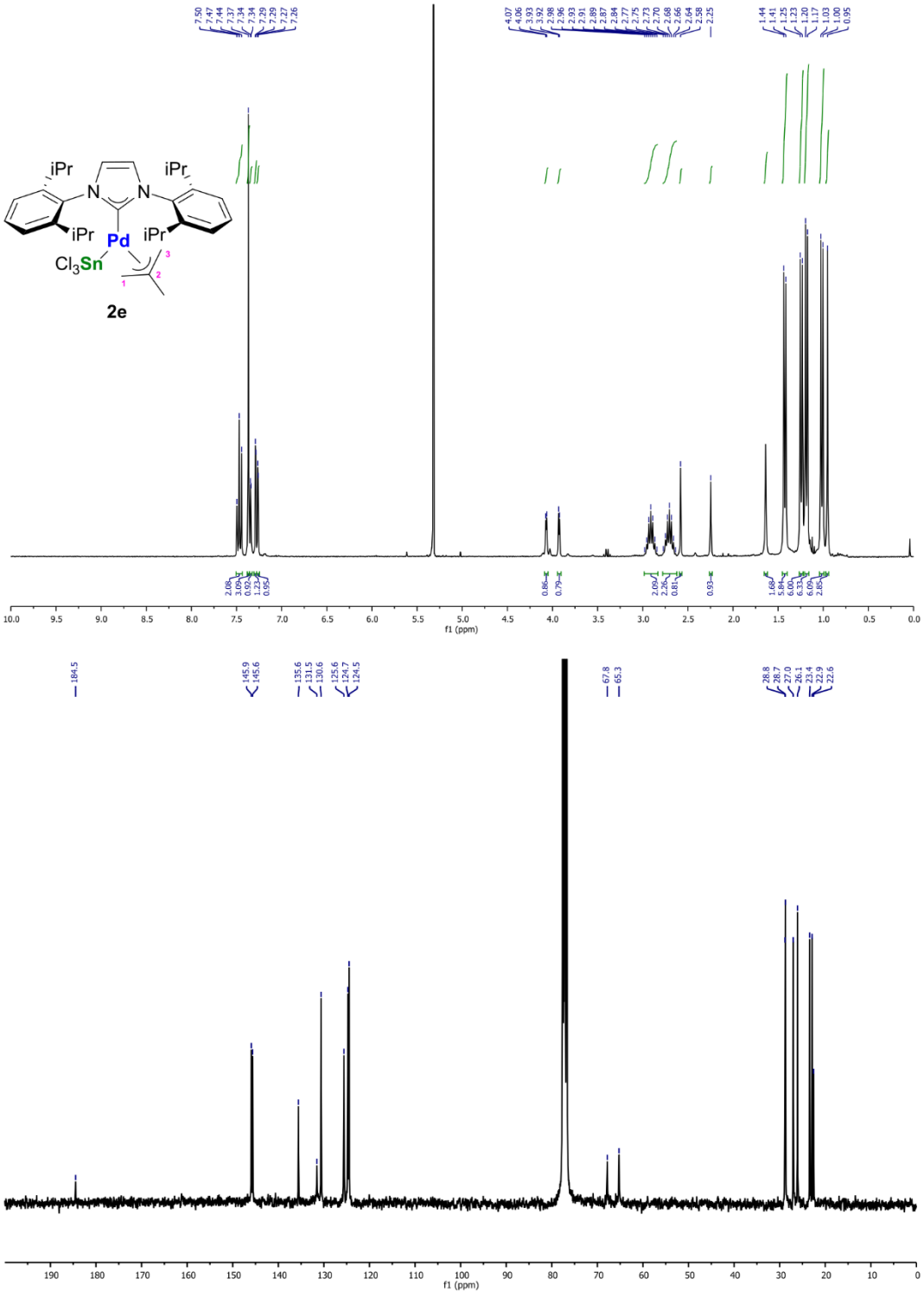

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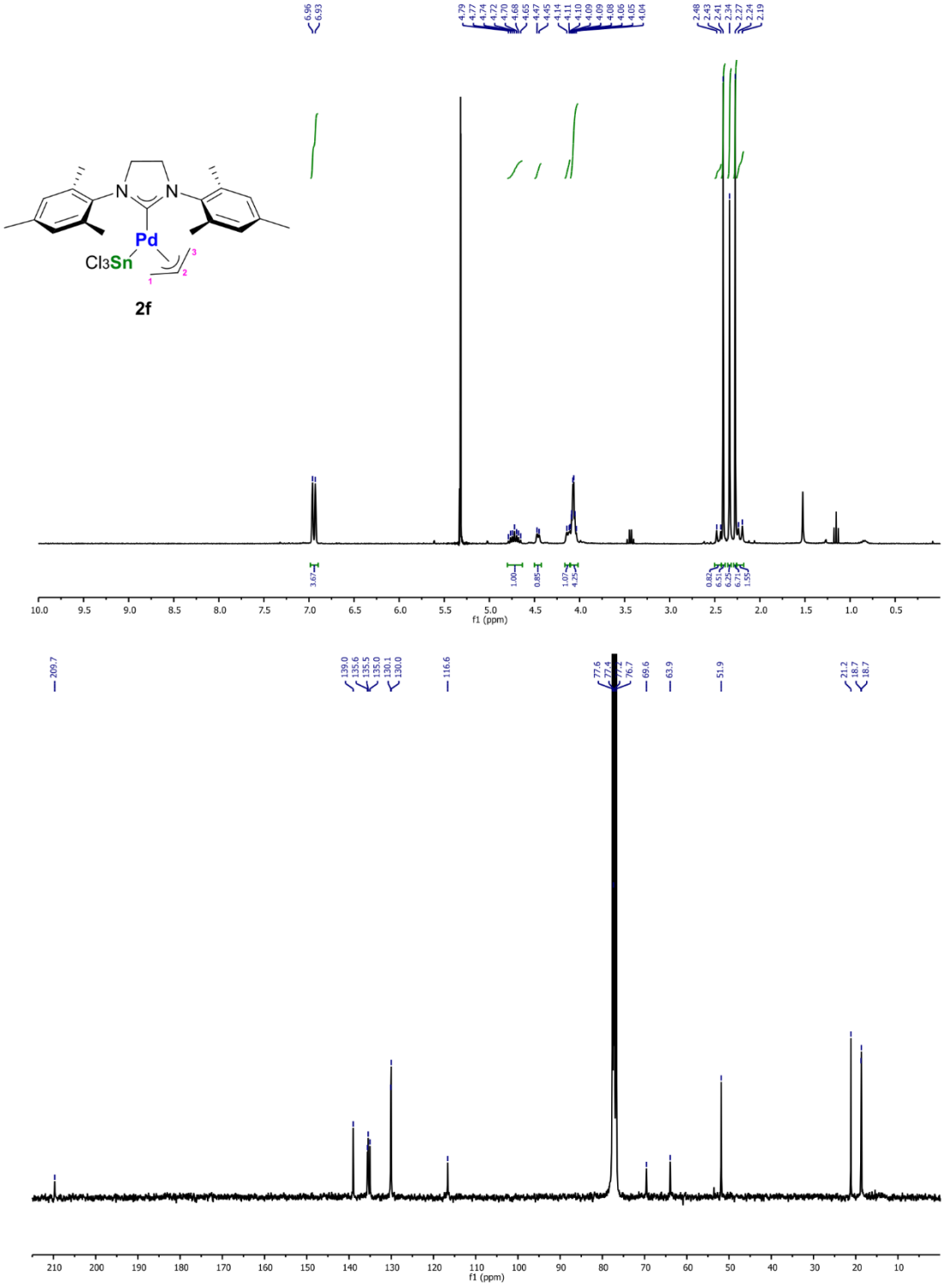

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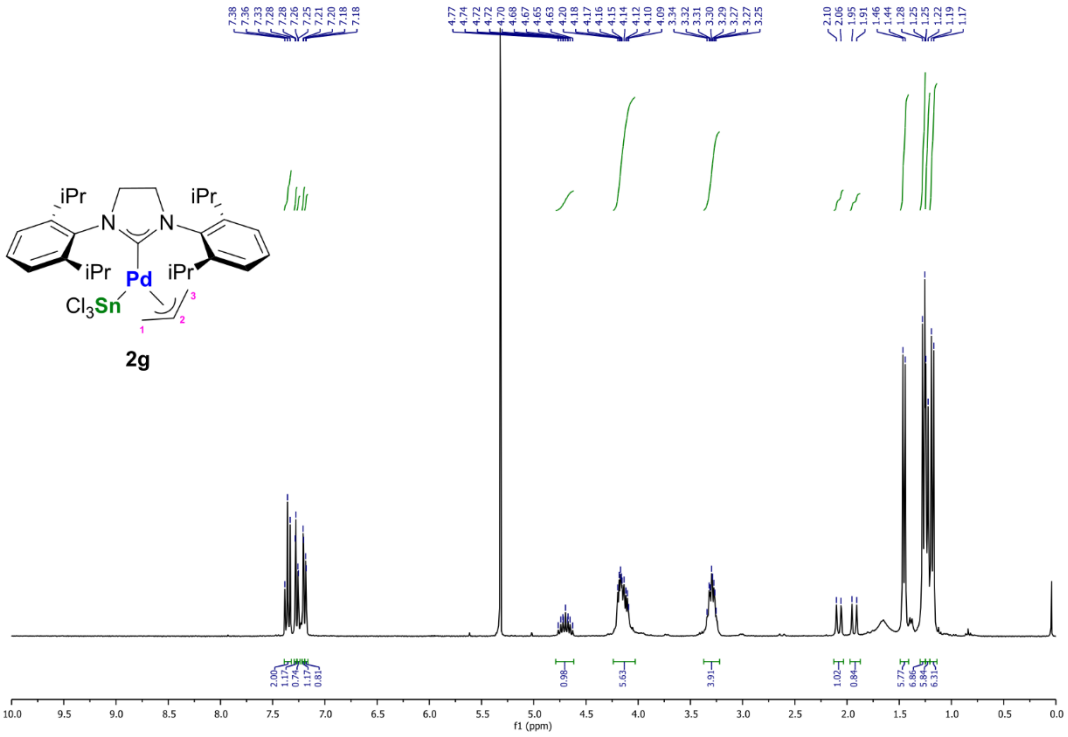
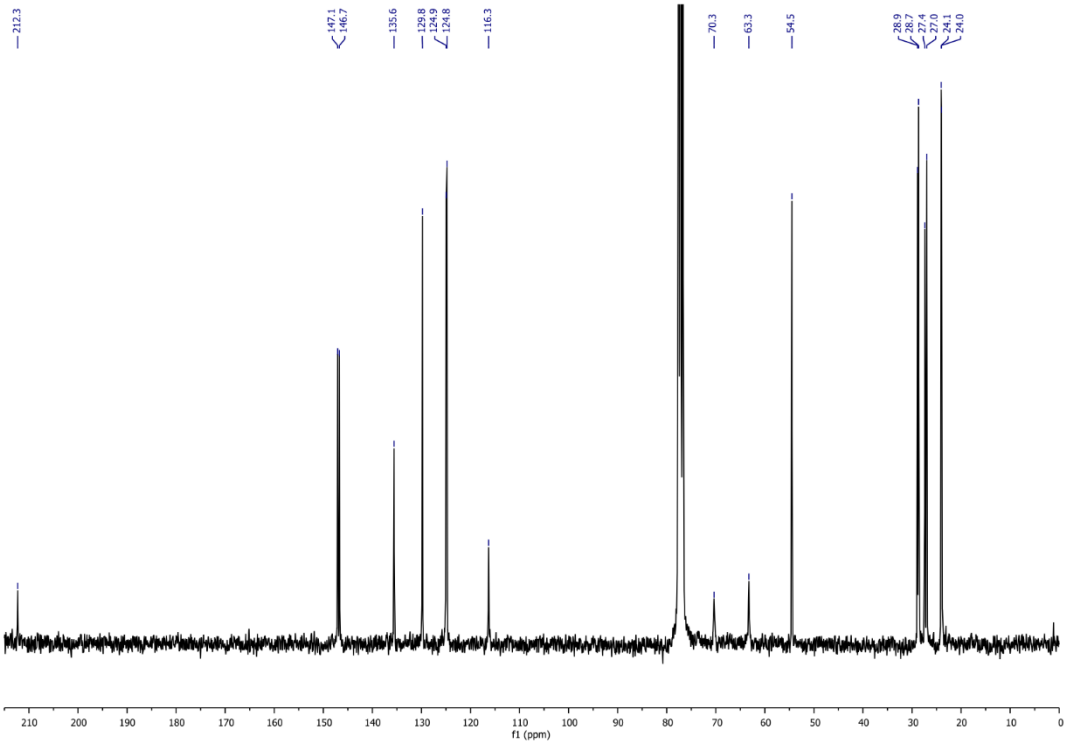
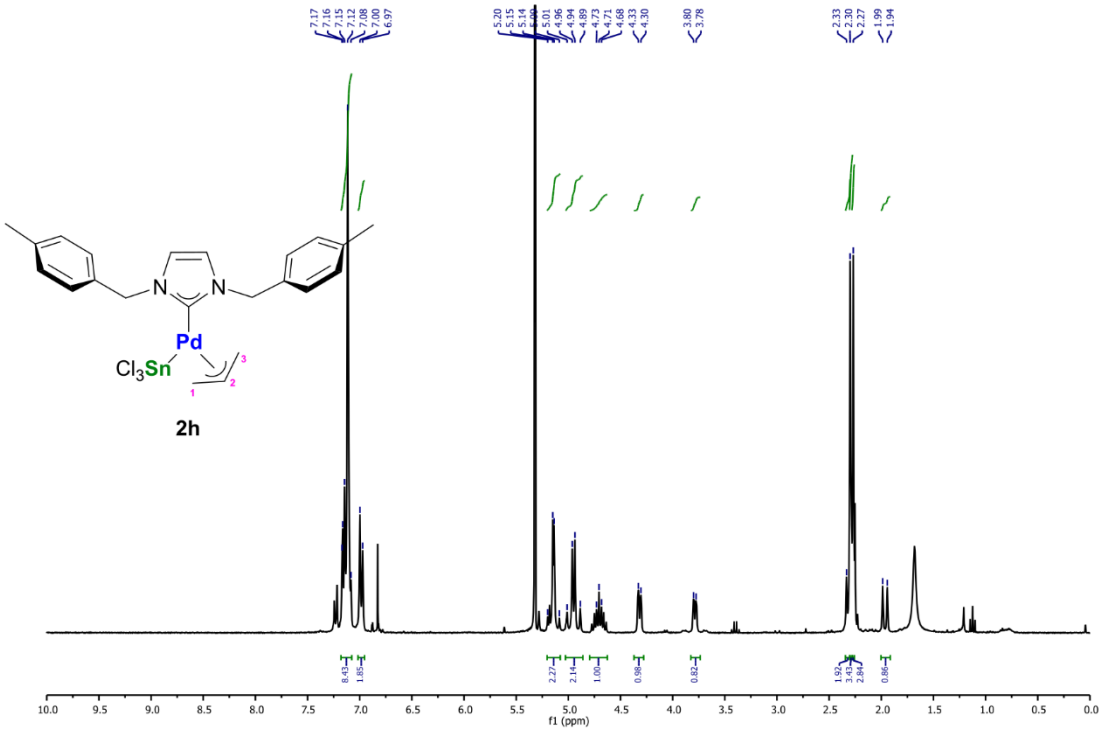
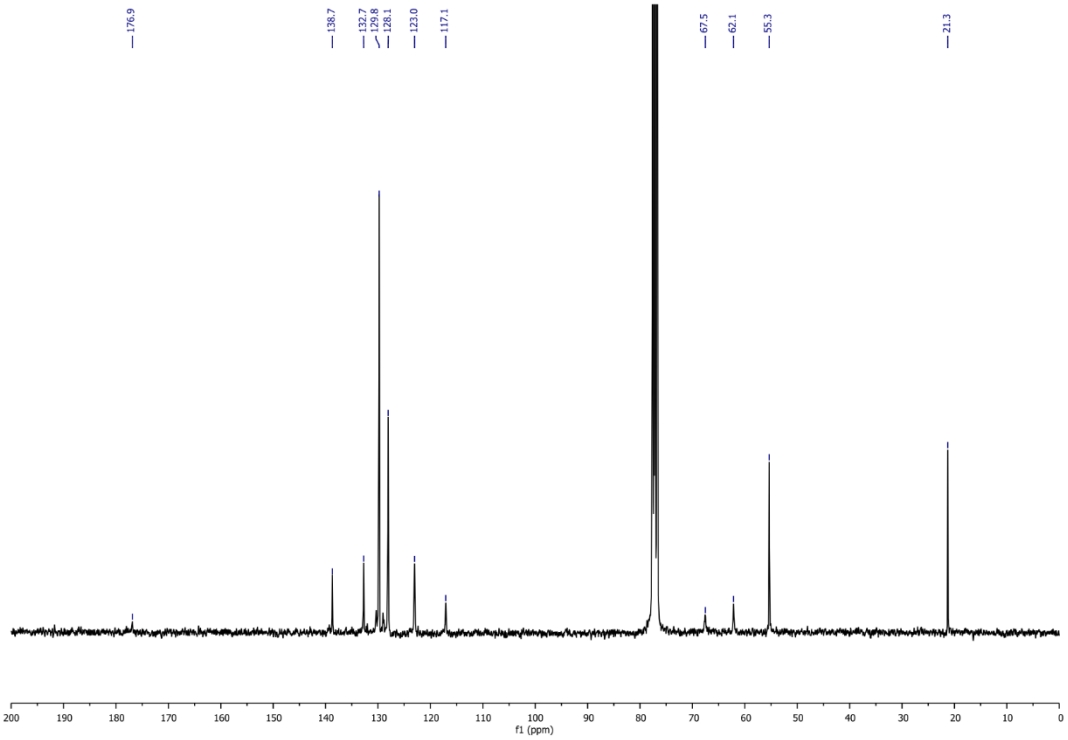


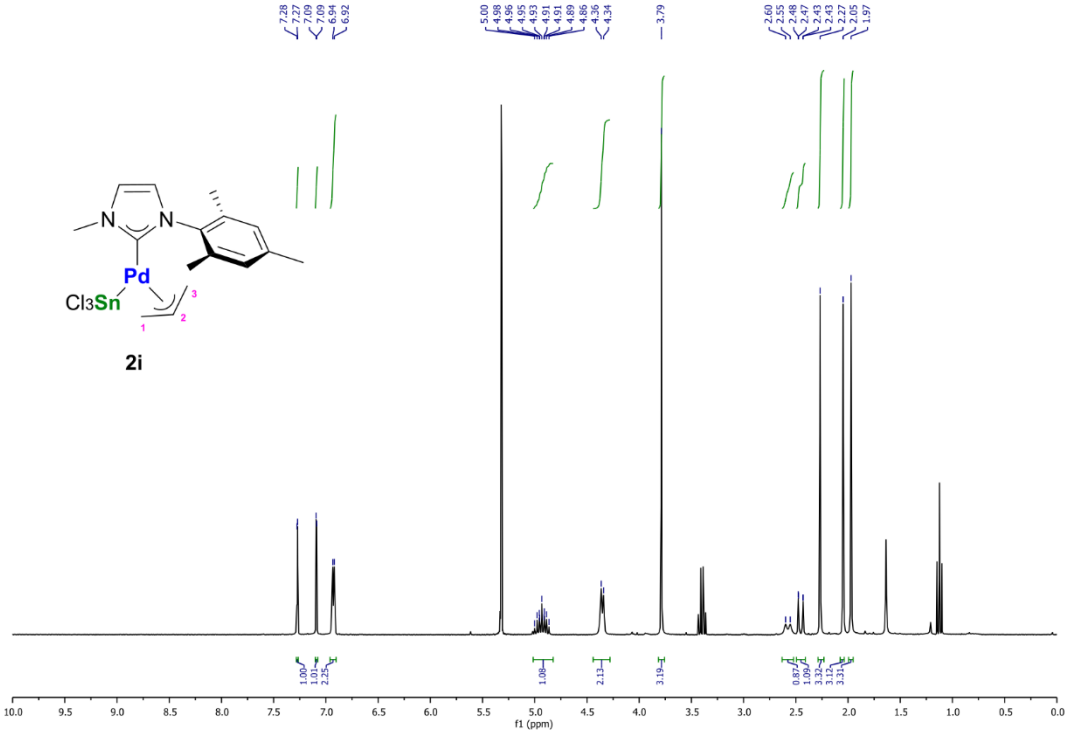


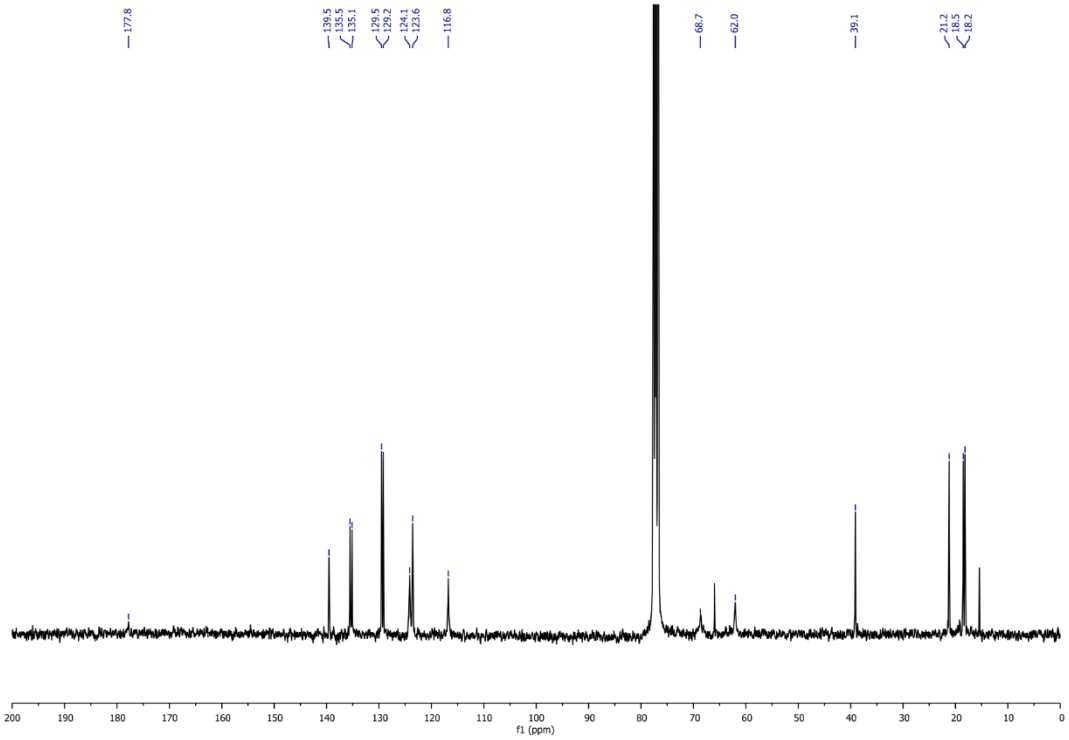
*^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of [Pd(allyl)(Tol-CH_2-Im-CH_2-Tol)$SnCl_3$] (**2h**)*



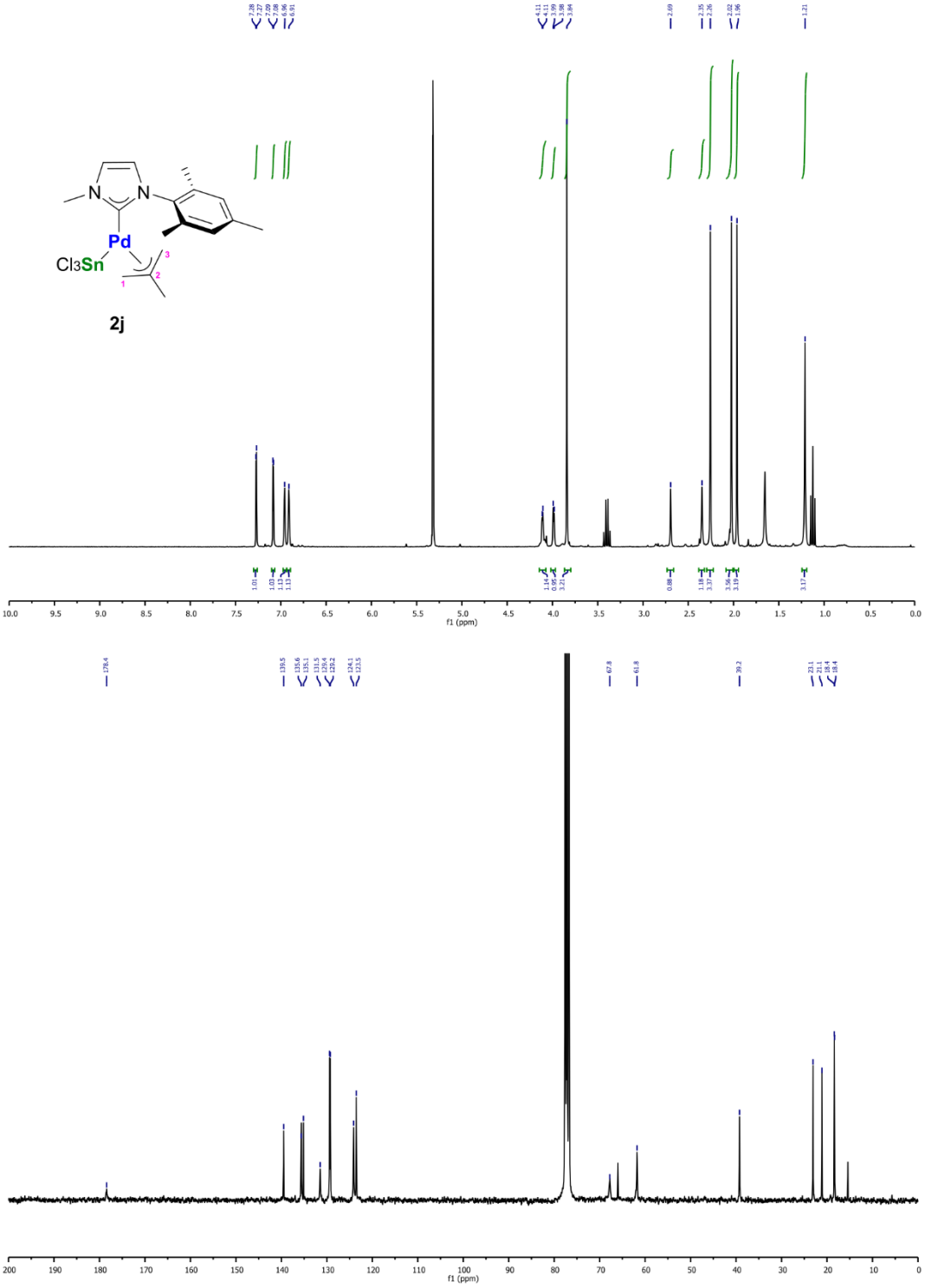


*^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of [Pd(allyl)(Me-Im-Mes)$SnCl_3$] (**2i**)*

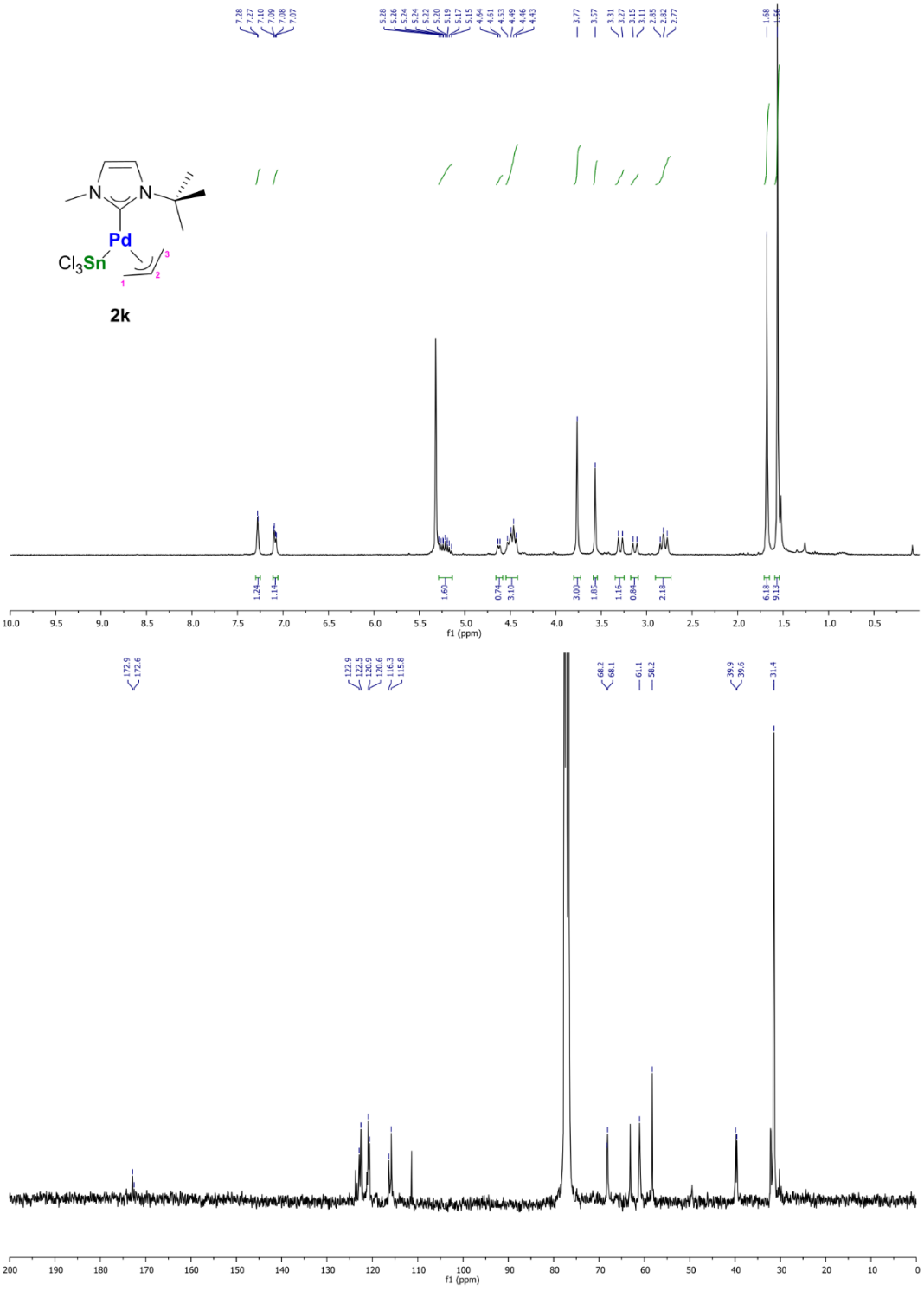




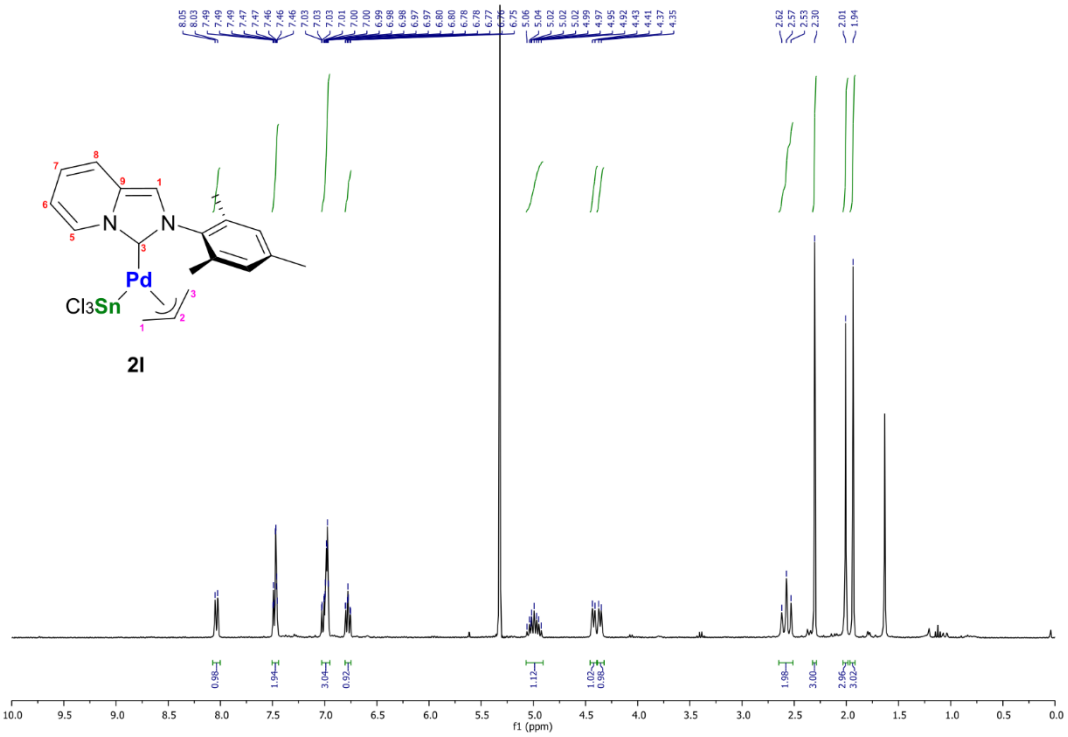
*^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of [Pd(2-methyl-allyl)(Me-Im-Mes)$SnCl_3$] (**2j**)*

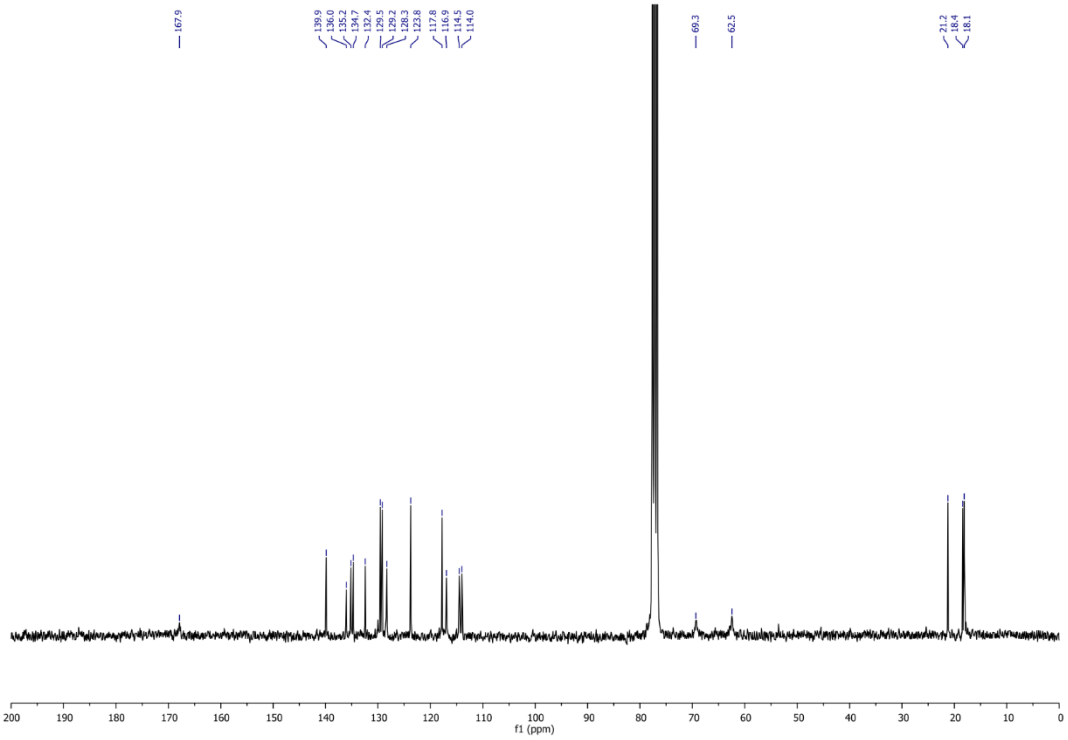


*^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of [Pd(allyl)(Me-Im-^{t}Bu)$SnCl_3$] (**2k**)*

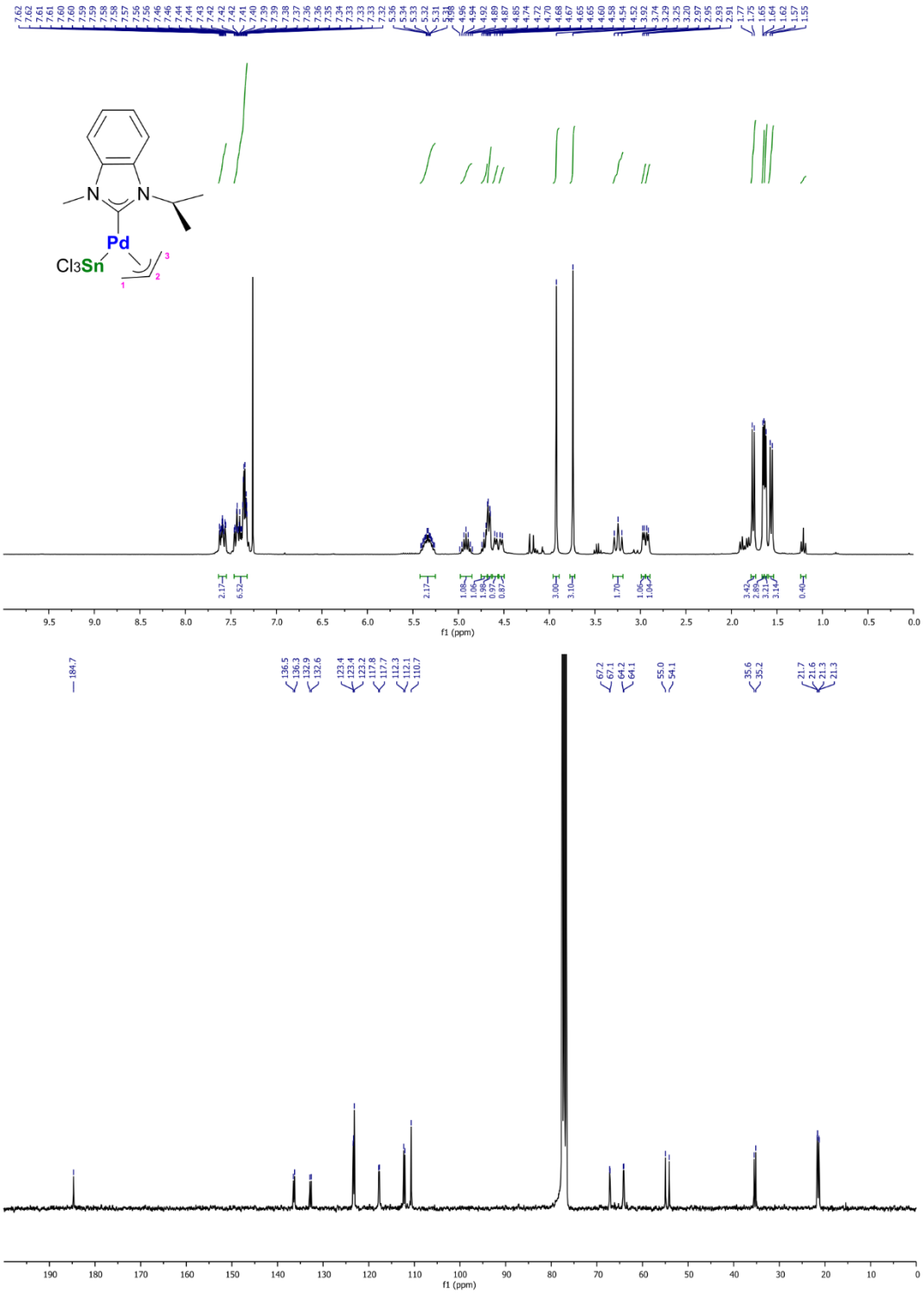


*^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of [Pd(allyl)((1,5-a)pirydin-Im-Mes)$SnCl_3$] (**2l**)*



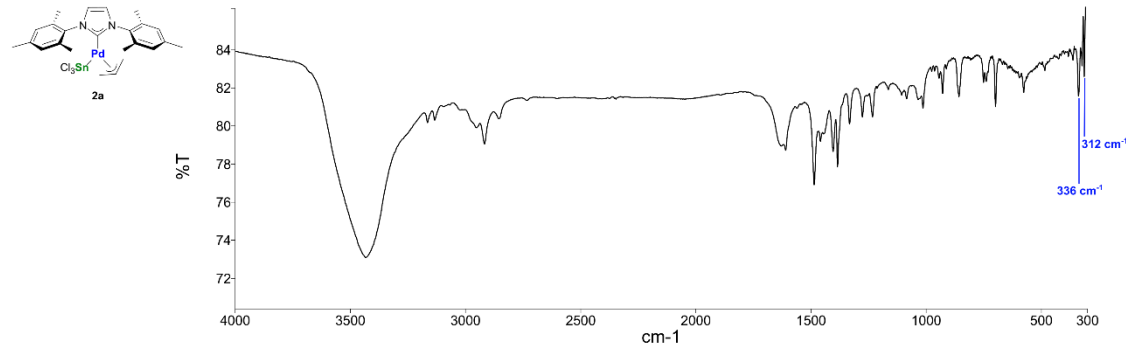


*^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra of [Pd(allyl)(iPr-BzIm-Me)$SnCl_3$] (***2m***)*

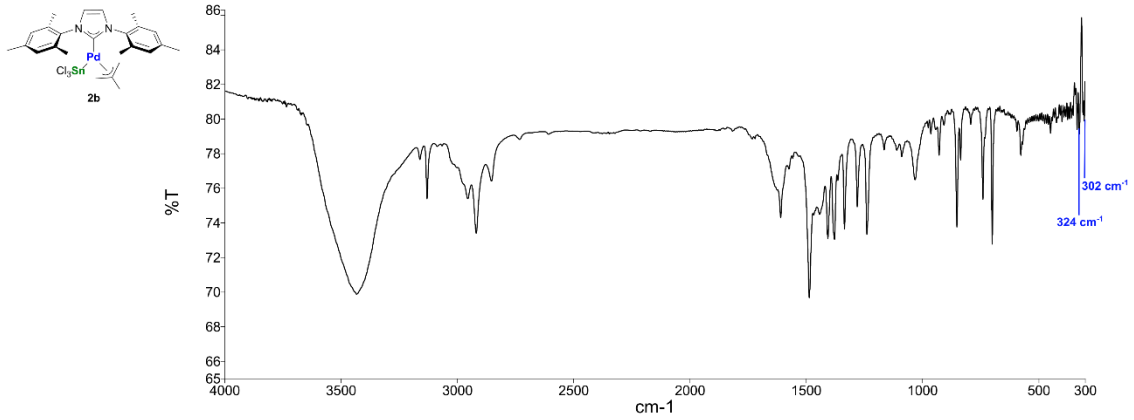


IR Spectra

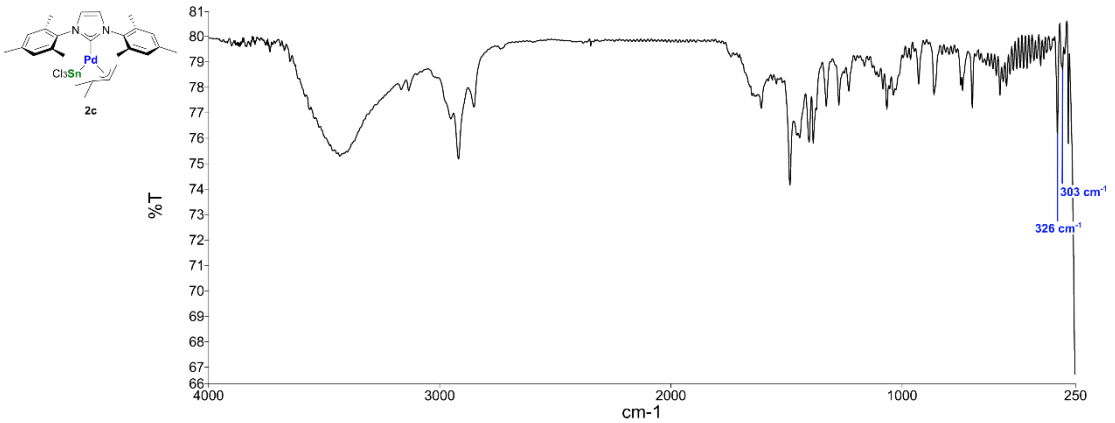
*IR spectra of [Pd(2-methyl-allyl)(IMes)SnCl$_3$] (**2a**)*



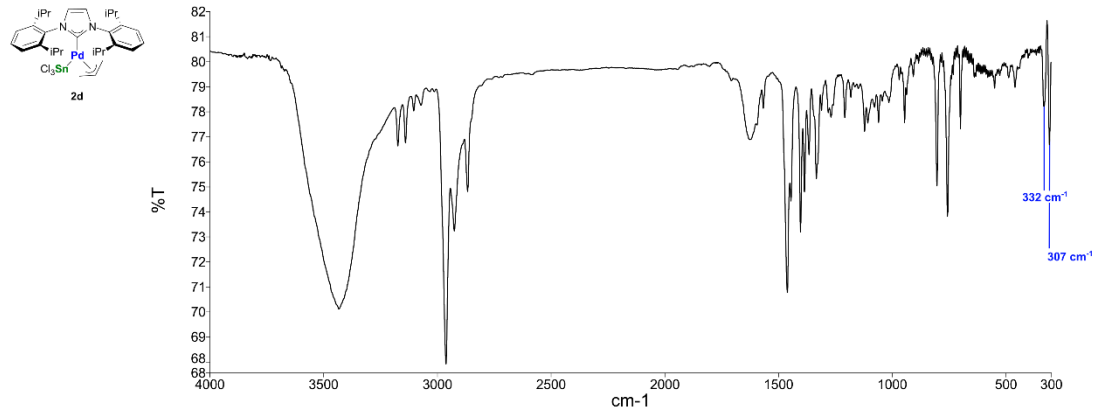
*IR spectra of [Pd(2-methyl-allyl)(IMes)SnCl$_3$] (**2b**)*



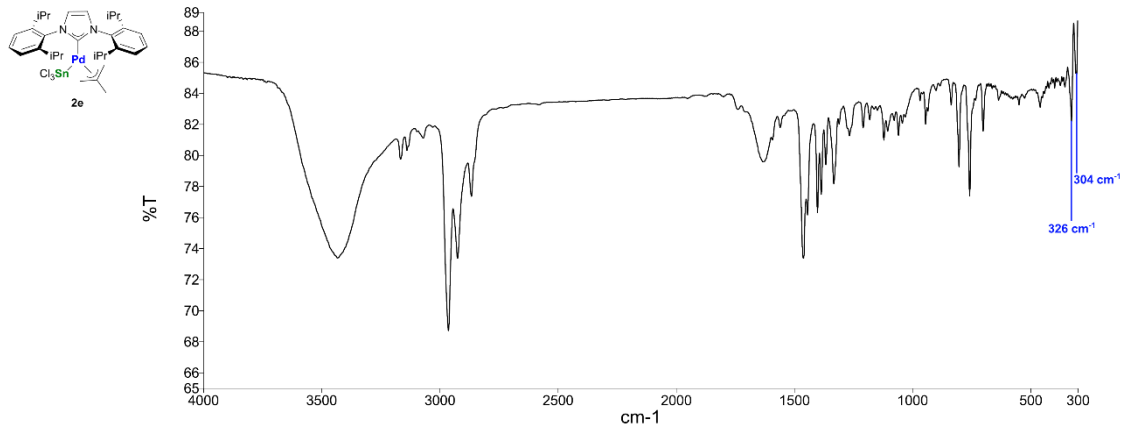
*IR spectra of [Pd(1,1-dimethyl-allyl)(IMes)SnCl$_3$] (**2c**)*



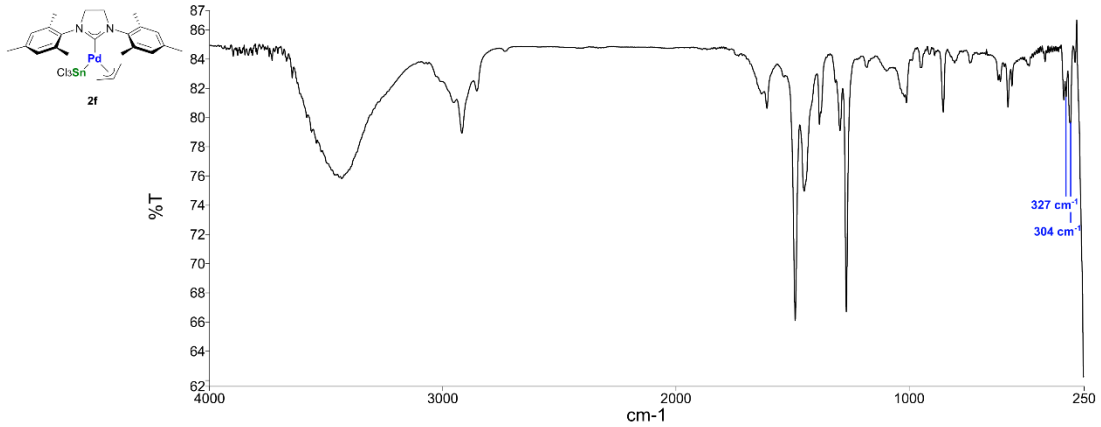
*IR spectra of [Pd(allyl)(IPr)SnCl$_3$] (**2d**)*



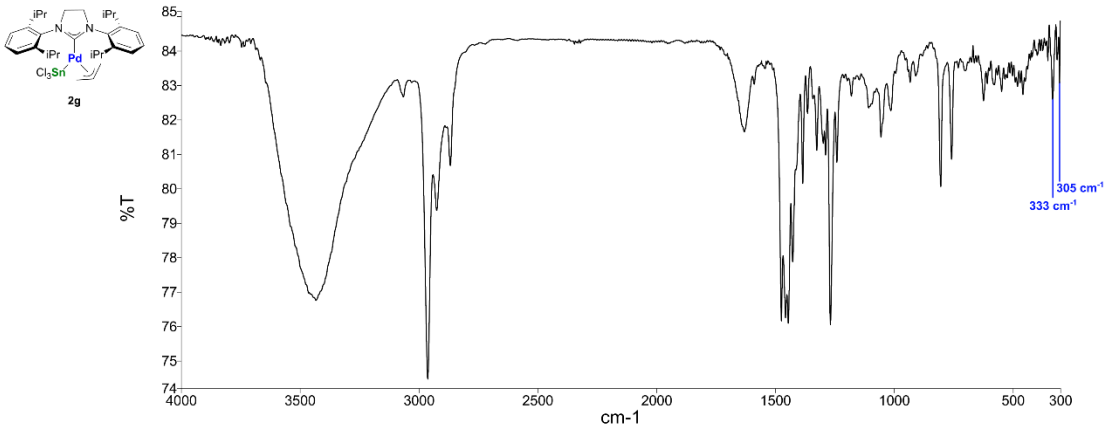
*IR spectra of [Pd(2-Me-allyl)(IPr)SnCl$_3$] (**2e**)*



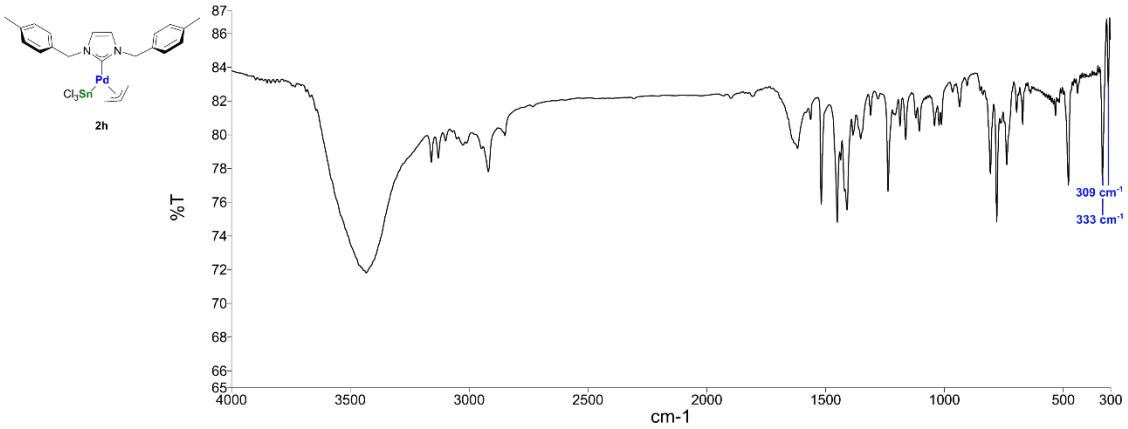
*IR spectra of [Pd(allyl)(SIMes)SnCl$_3$] (**2f**)*



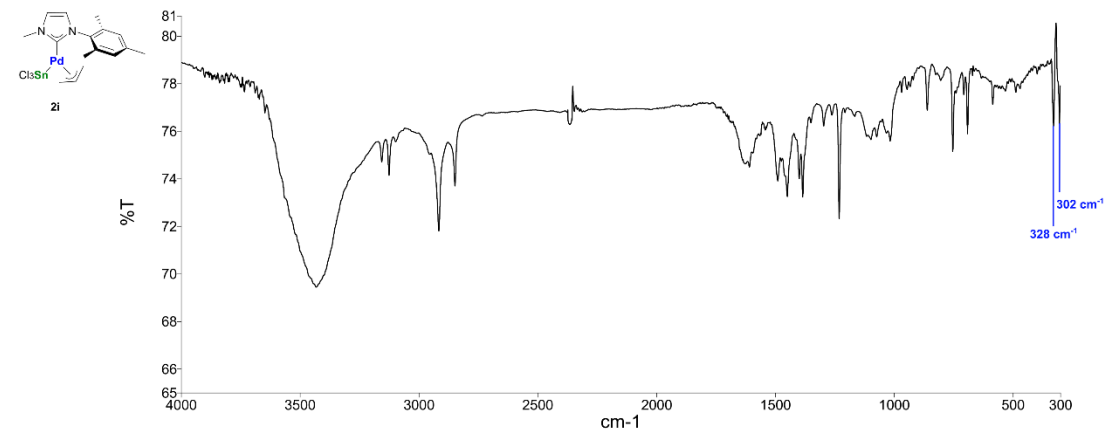
*IR spectra of [Pd(allyl)(SIPr)SnCl$_3$] (**2g**)*



*IR spectra of [Pd(allyl)(Tol-CH_2-Im-CH_2-Tol)$SnCl_3$] (**2h**)*



*IR spectra of [Pd(allyl)(Me-Im-Mes)$SnCl_3$] (**2i**)*



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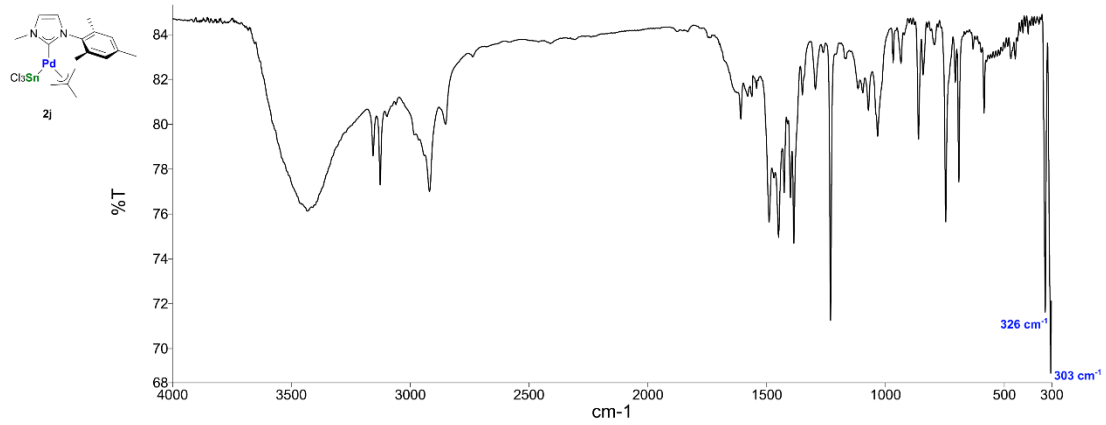
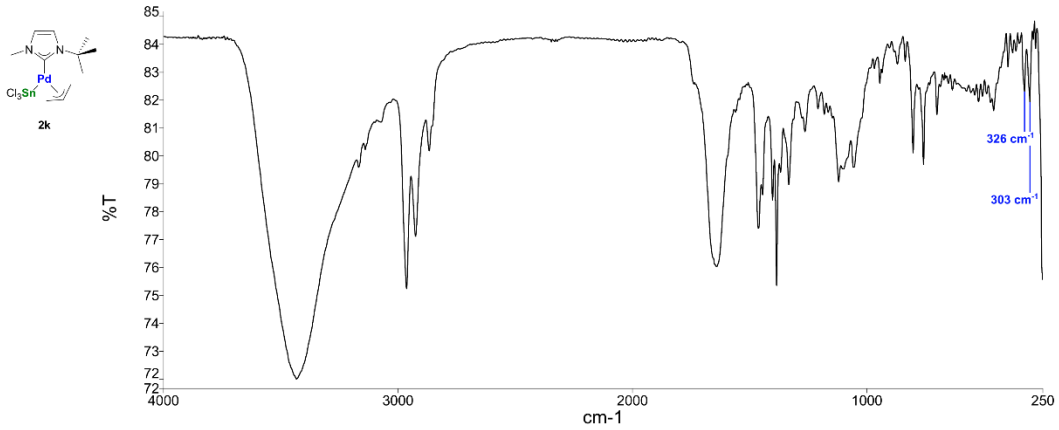
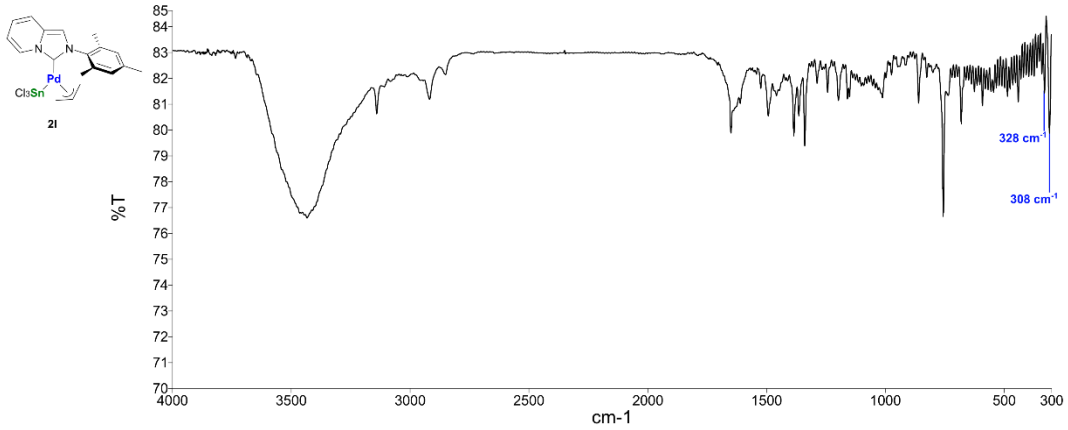


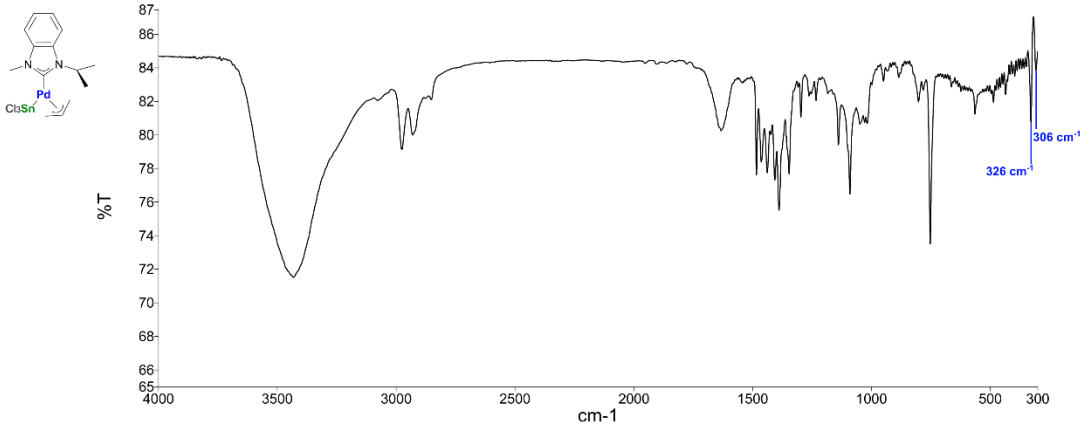
*IR spectra of [Pd(allyl)(Me-Im-^{t}Bu)$SnCl_3$] (**2k**)*



*IR spectra of [Pd(allyl)((1,5-a)pirydin-Im-Mes)$SnCl_3$] (**2l**)*



*^{1}H NMR and $^{13}C\{^1H\}$ NMR spectra of [Pd(allyl)(iPr-BzIm-Me)$SnCl_3$] (**2m**)*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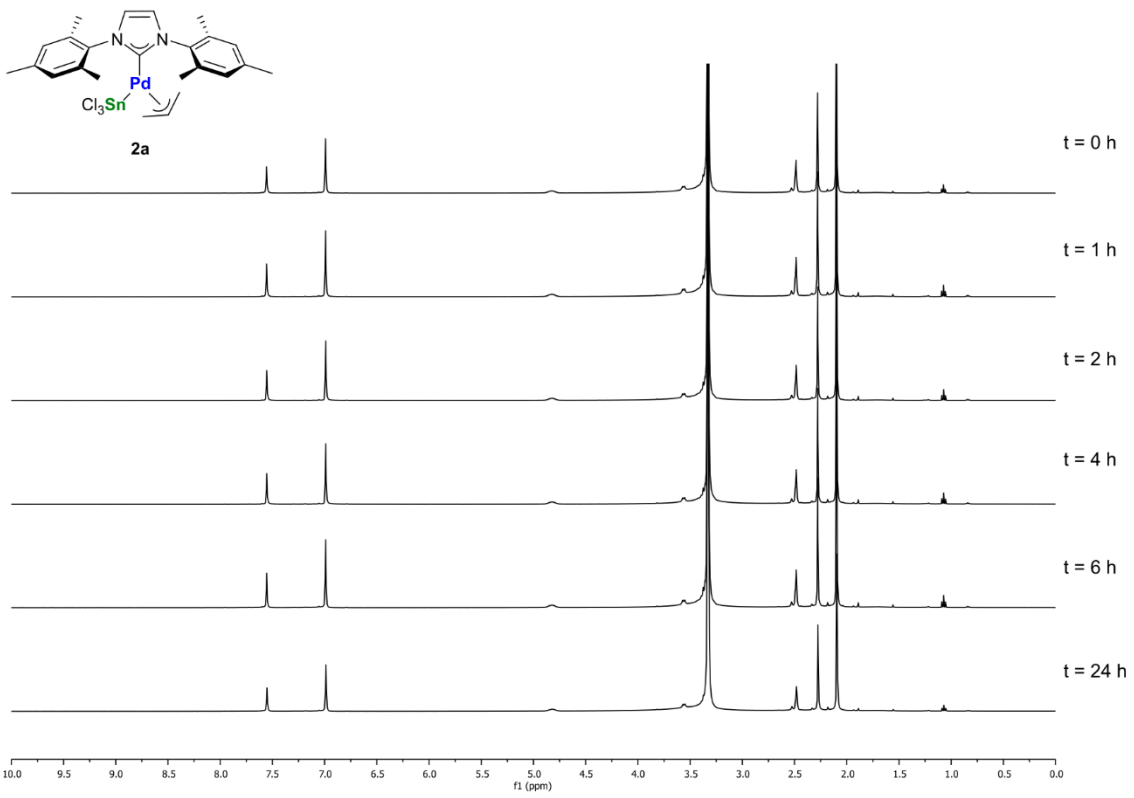
82
80
78
76
74
72
70
68
66
65
4000
3500
3000
2500
2000
1500
1000
500
300
cm-1
306 cm-1
326 cm-1

Stability in DMSO-d^6/D_2O

Stability of complexes **2a-m** in a mixture DMSO-d^6:D_2O, 3:1 was performed comparing ^1H NMR spectra registered within 24 hours. Registered spectra are reported below.

*Stability of complex **2a***



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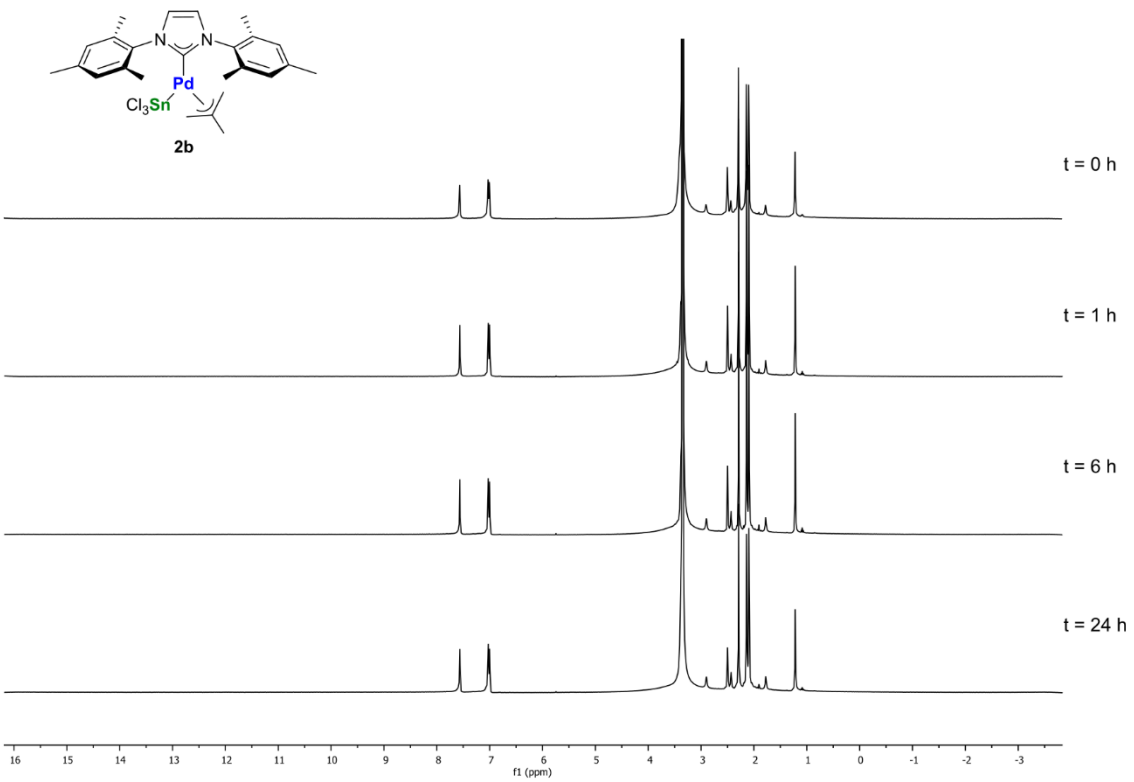

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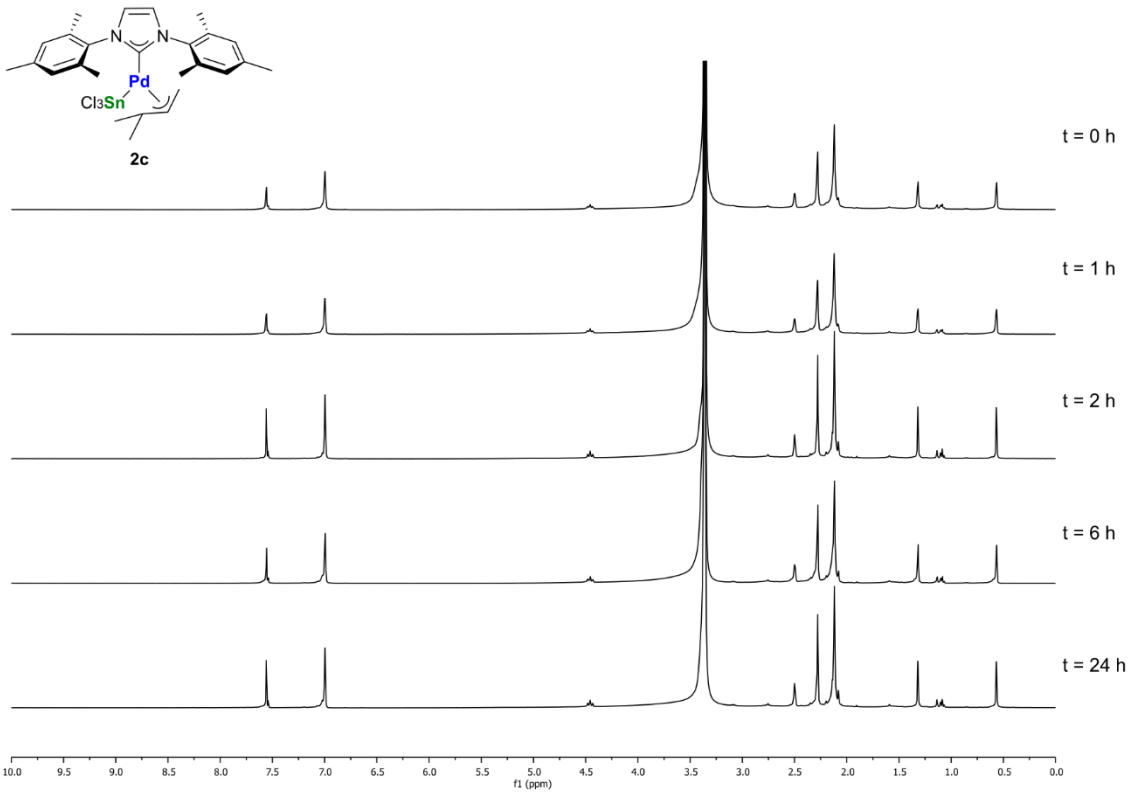
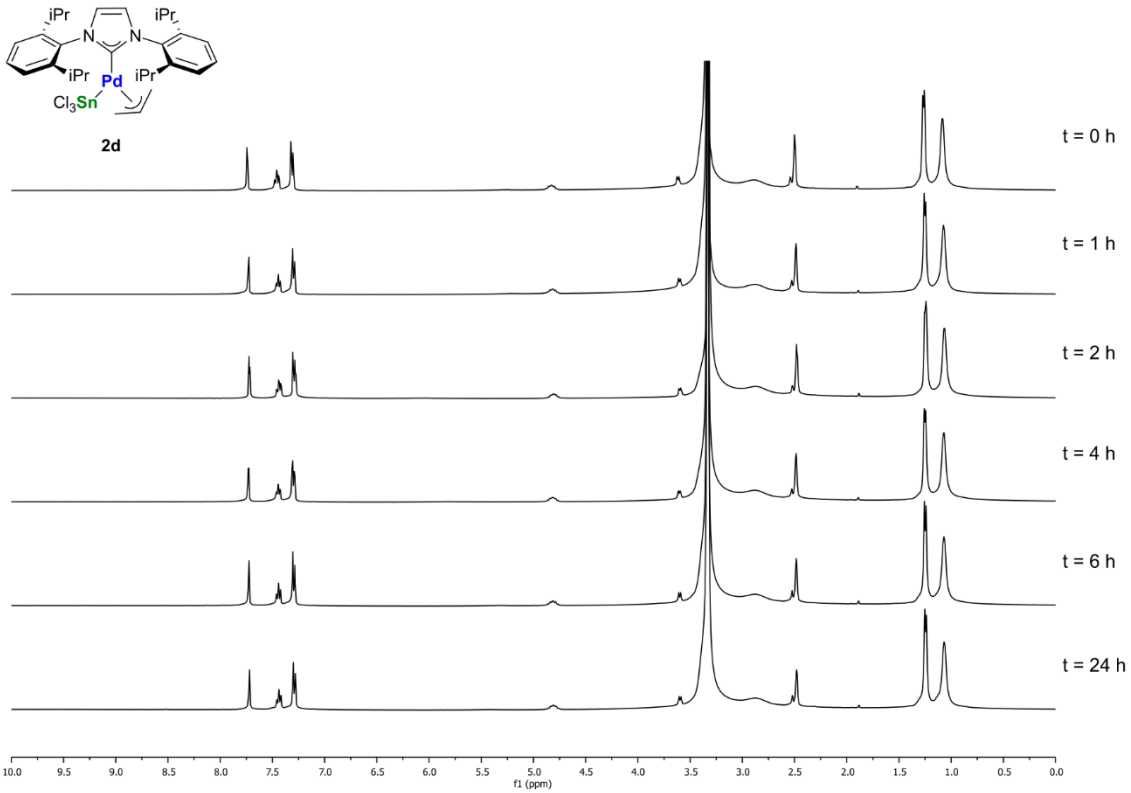


*Stability of complex **2d***



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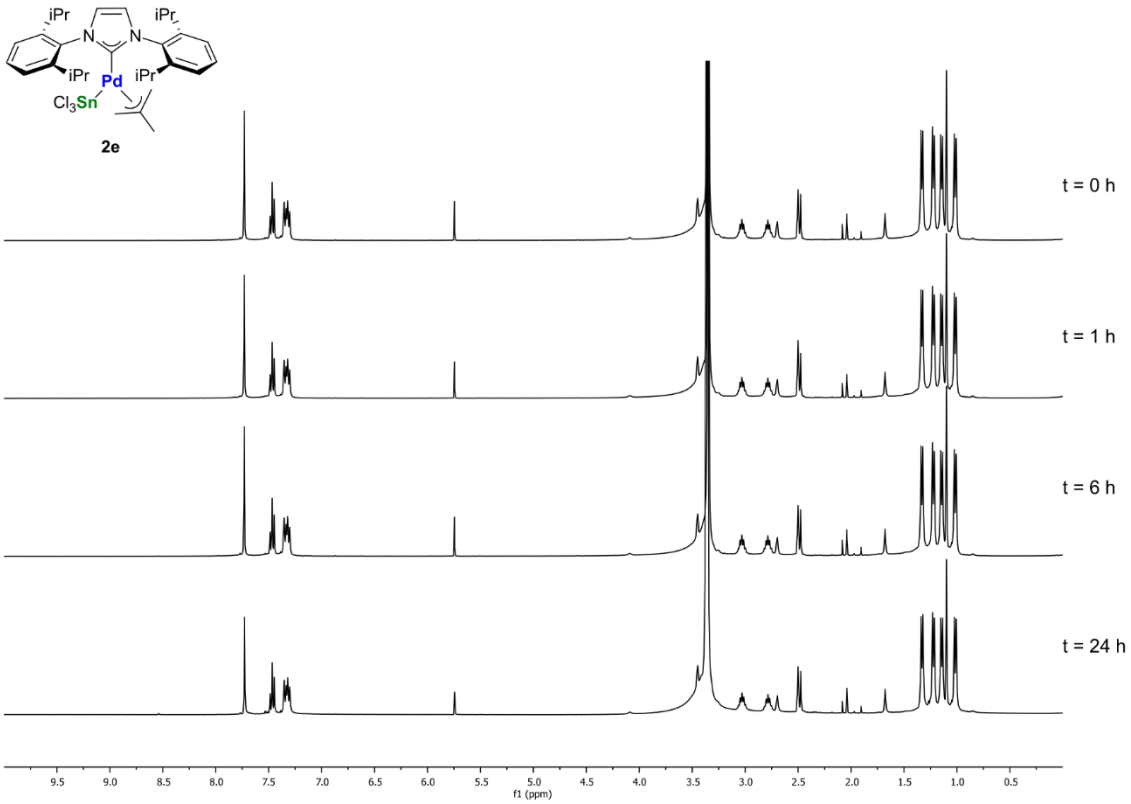

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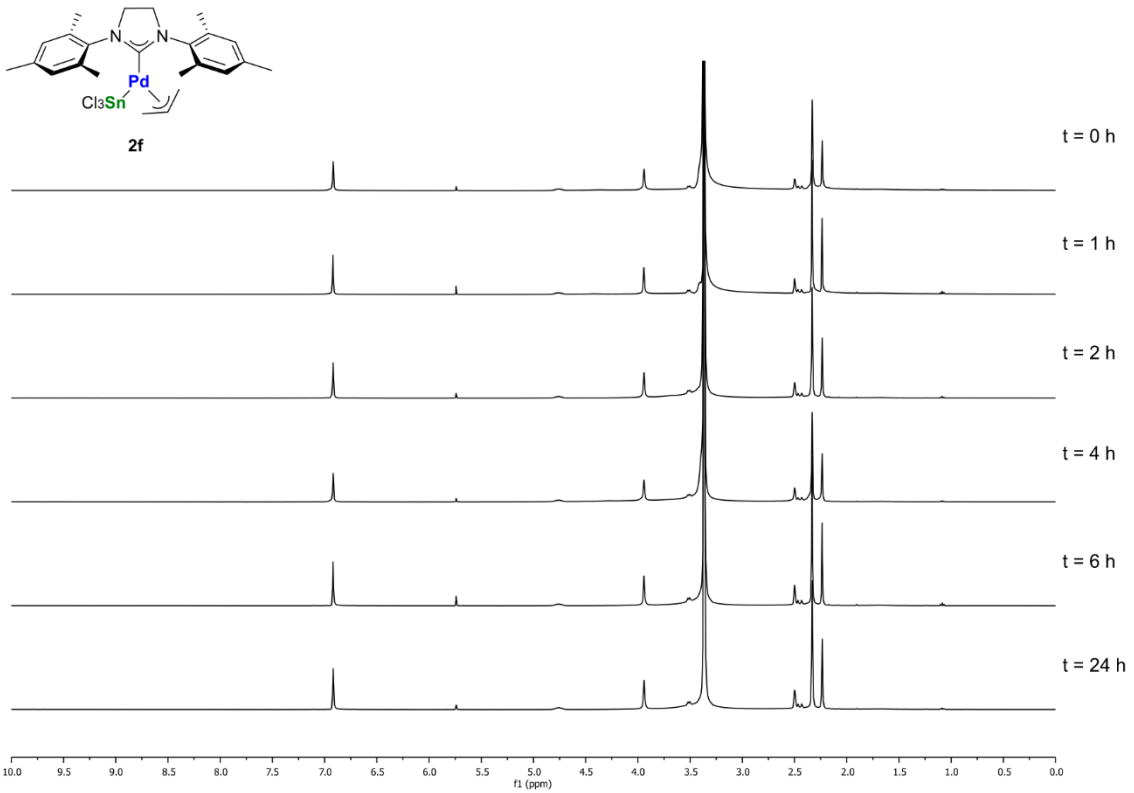
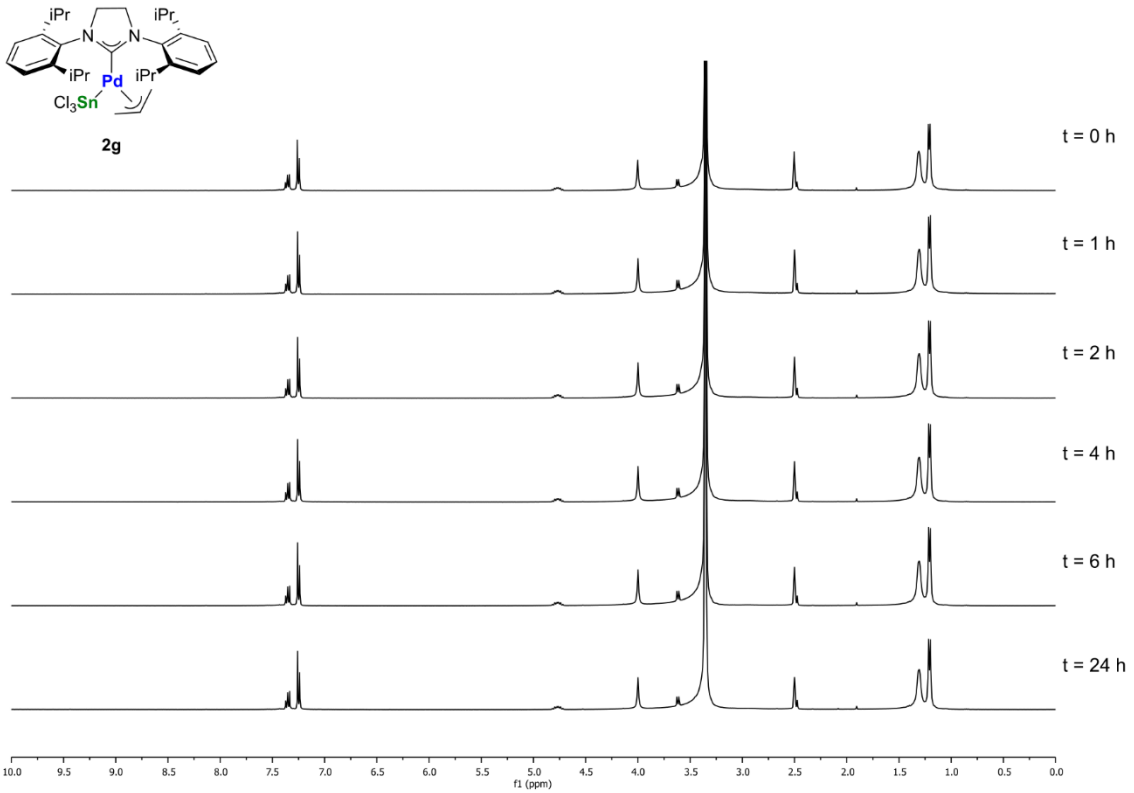
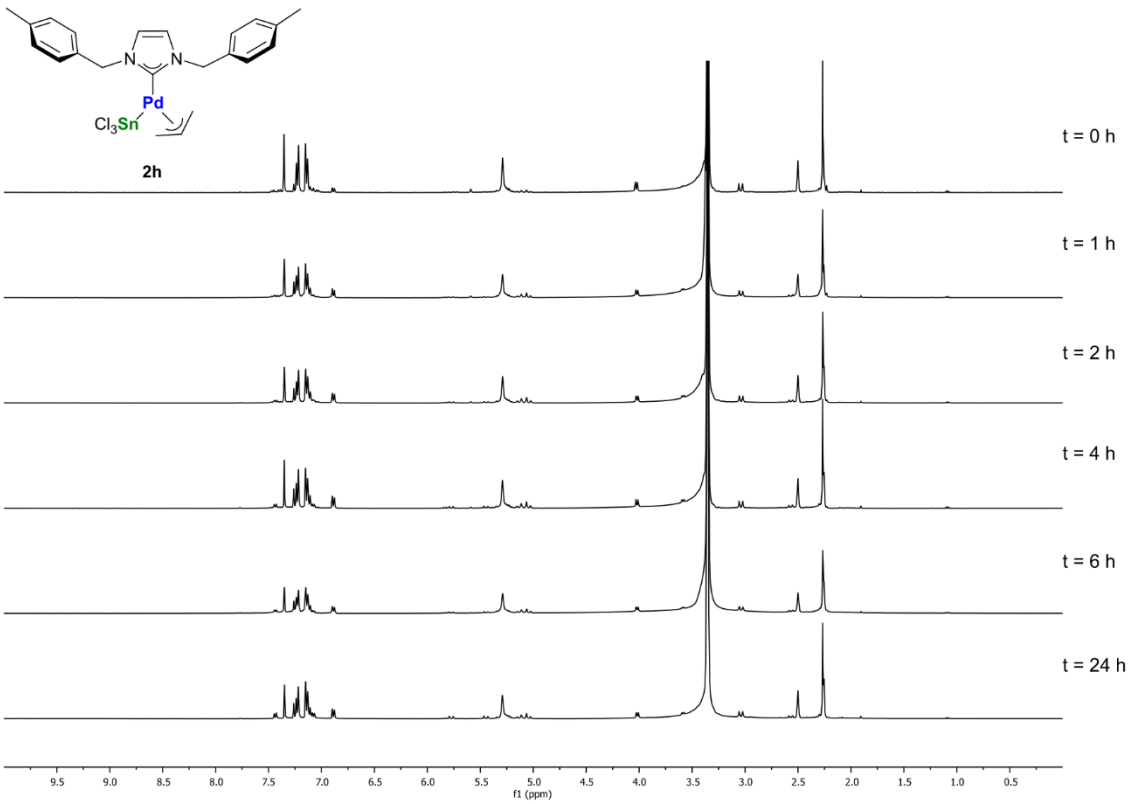


*Stability of complex **2g***



*Stability of complex **2h***



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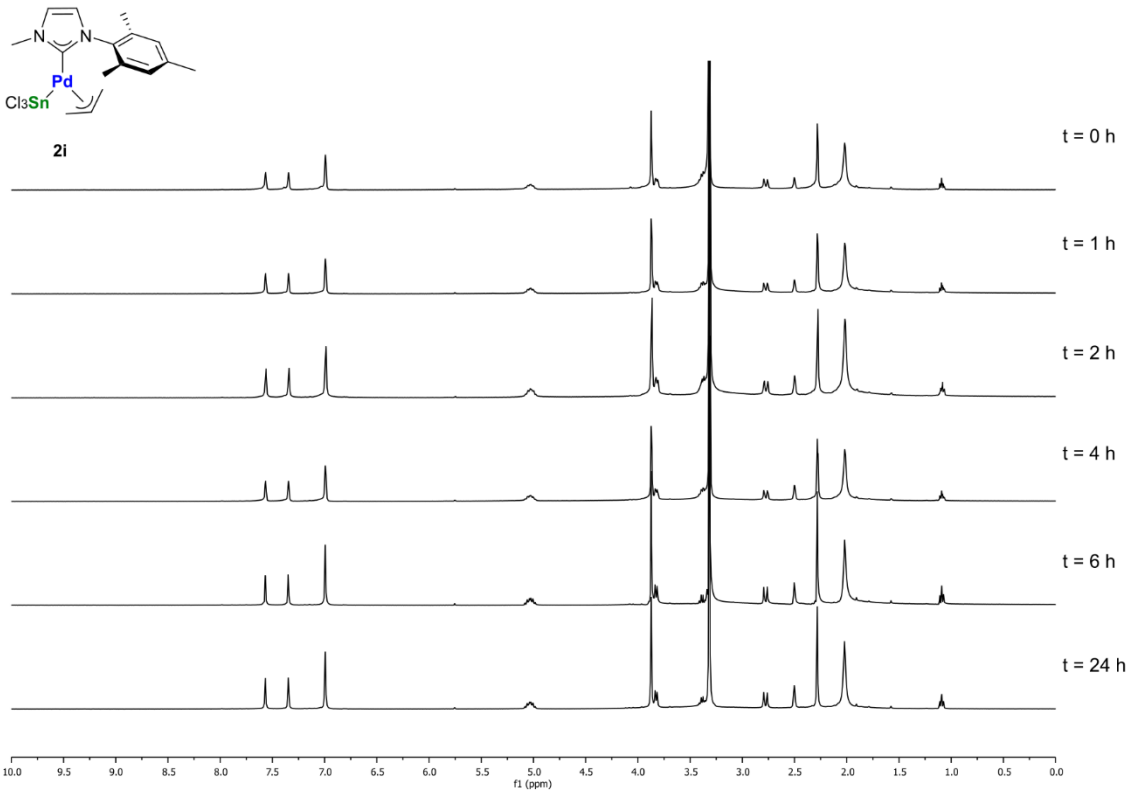

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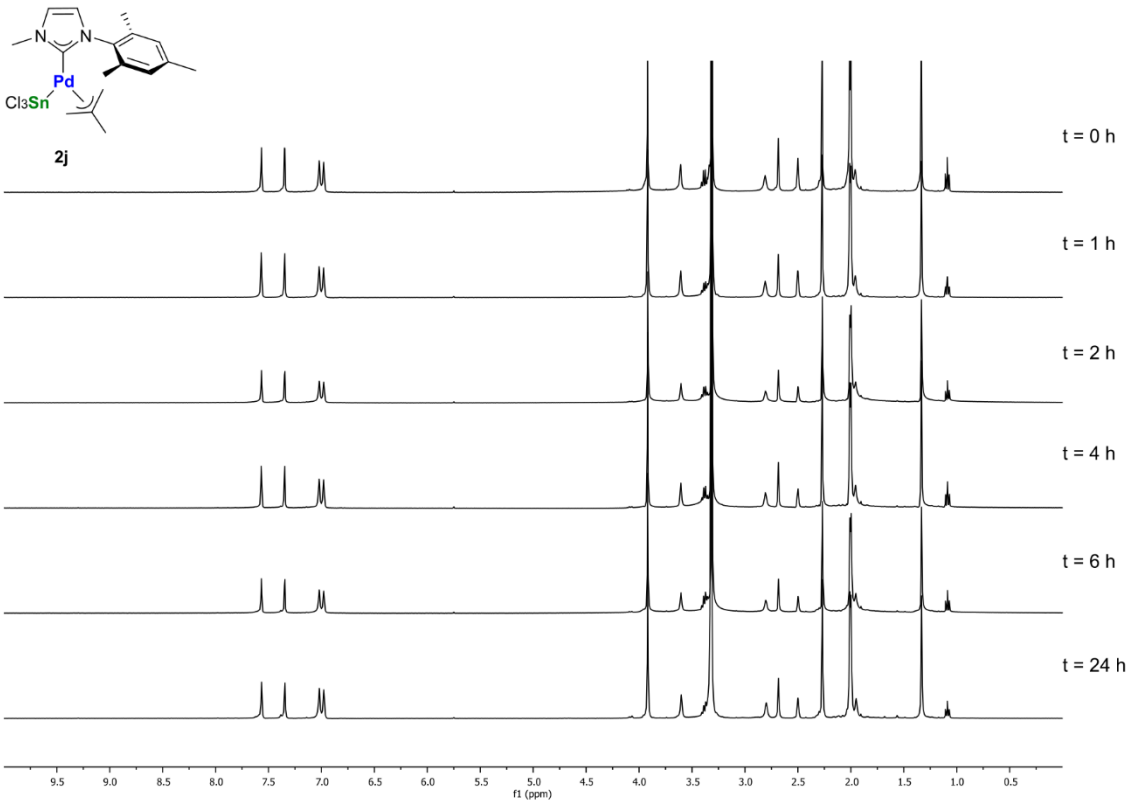

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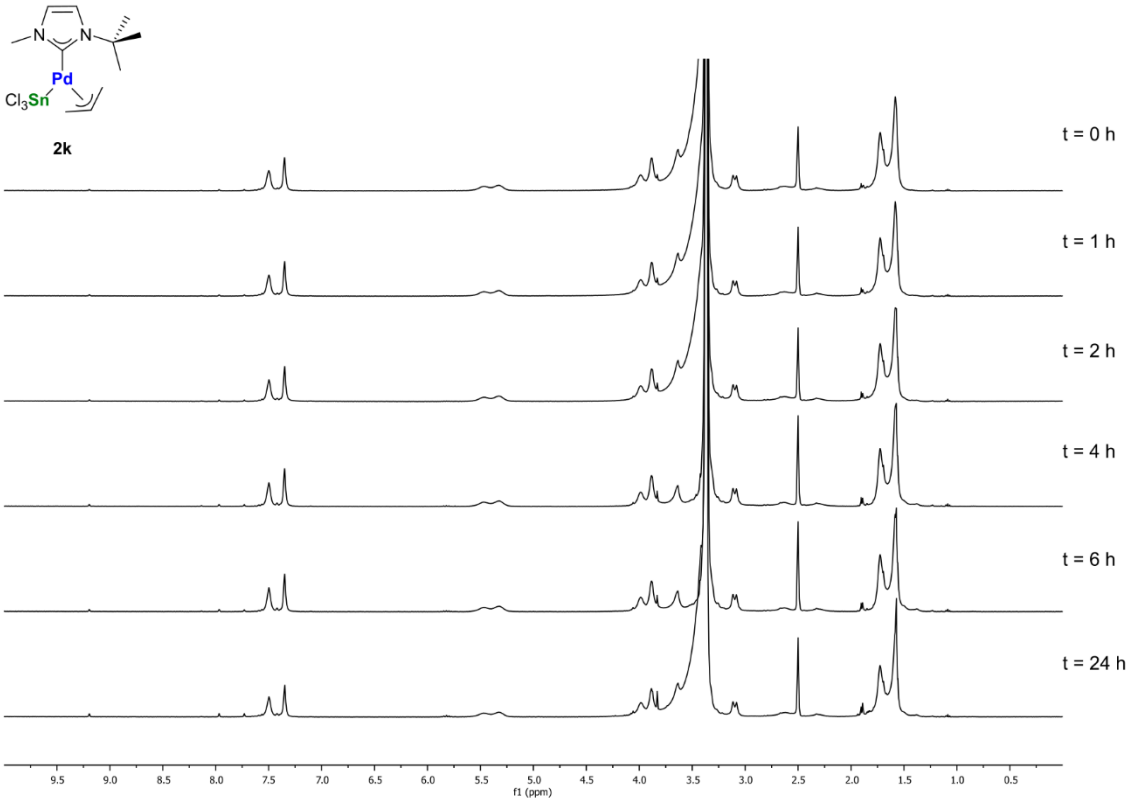
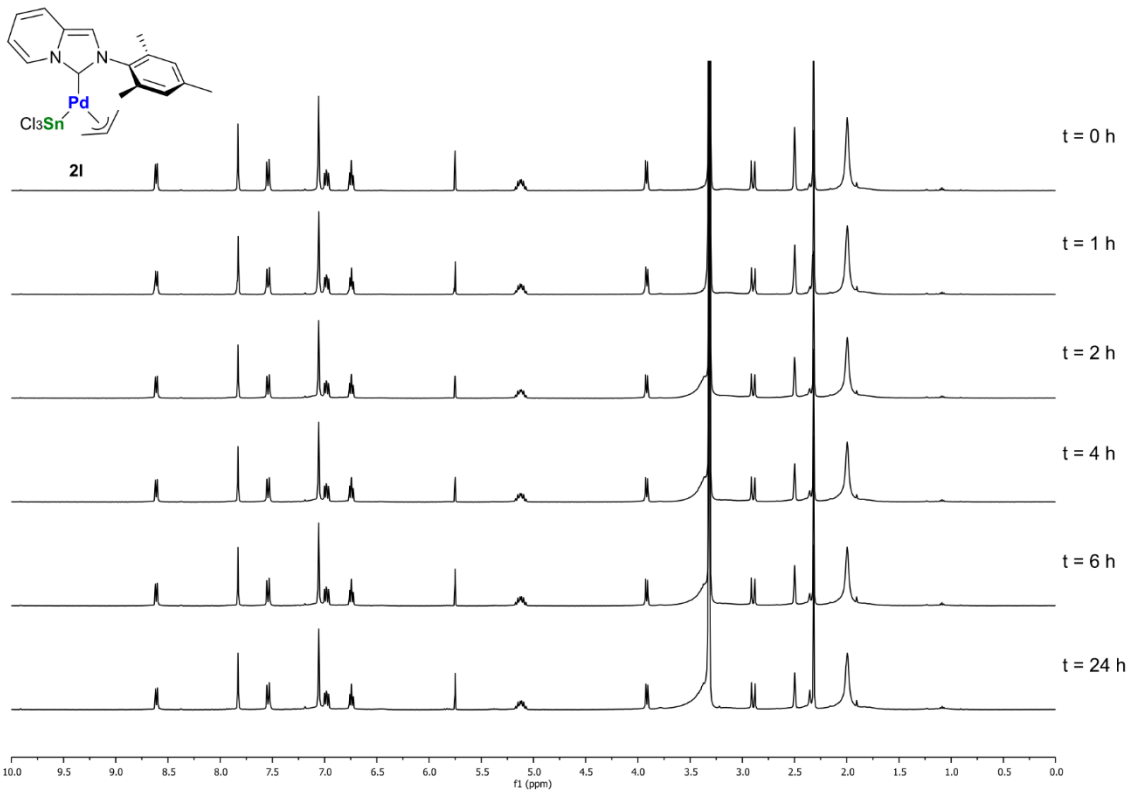
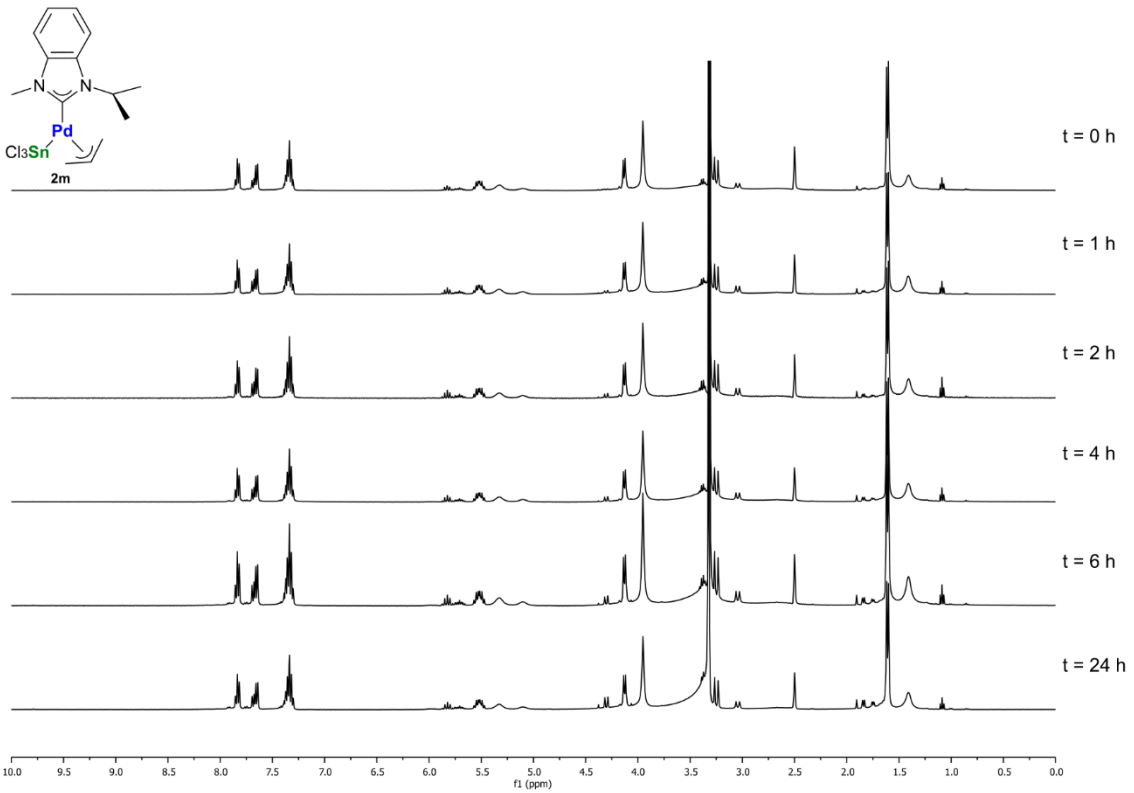


*Stability of complex **2l***



*Stability of complex **2m***



Crystallographic data

Table S1. Crystallographic data

Compound	**2d@100K**	**2d@200K**	**2d@298K**	**2b@100K**	**2f@100K**	**2f@298K**
Formula	$PdSnCl_3C_{30}H_{41}N_2 \times CH_2Cl_2$	$PdSnCl_3C_{30}H_{41}N_2 \times CH_2Cl_2$	$PdSnCl_3C_{30}H_{41}N_2 \times CH_2Cl_2$	$PdSnCl_3C_{25}H_{31}N_2$	$PdSnCl_3C_{25}H_{31}N_2$	$PdSnCl_3C_{24}H_{31}N_2$
M/g·mol^{-1}	846.01	846.01	846.01	690.96	678.95	678.95
Space group	*P bcm*	*P bcm*	*P bcm*	*P* $2_1/c$	*P* -1	*P* -1
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Monoclinic	Triclinic	Triclinic
a/Å	9.486(2)	9.541(2)	9.612(2)	10.700(2)	10.459(2)	10.564(2)
b/Å	19.360(4)	19.387(4)	19.423(4)	12.404(3)	11.488(2)	11.587(2)
c/Å	19.735(4)	19.905(4)	20.112(4)	20.971(4)	12.712(3)	13.012(3)
a/°	90	90	90	90	91.66(3)	92.01(3)
β/°	90	90	90	97.49(3)	95.76(3)	95.75(3)
g/°	90	90	90	90	116.71(3)	116.82(3)
V/Å^3	3624.3(13)	3681.9(13)	3754.8(13)	2759.6(10)	1352.8(6)	1408.4(6)
Z	4	4	4	4	2	2
T/K	100(2)	200(2)	298(2)	100(2)	100(2)	100(2)
D_c/g·cm^{-3}	1.550	1.526	1.497	1.663	1.667	1.601
F(000)	1696	1696	1696	1368	672	672
μ/mm^{-1}	1.072	1.056	1.035	1.269	1.293	1.242
Measured Reflections	78923	85993	85302	65230	62992	62302
Unique Reflections	8605	8717	8692	12012	11743	12291
R_{int}	0.0386	0.0503	0.0864	0.0253	0.0438	0.0838
Obs. Refl.ns [I³2σ(I)]	8284	8245	6451	11616	11240	10152
θ_{min}-θ_{max}/°	1.84 – 31.10	1.83 – 31.10	1.80 – 31.10	1.67 – 31.10	1.41 – 31.10	1.38 – 31.11
Hkl ranges	-15,15; -30,29; -31,31	-15,15; -30,30; -31,31	-16,16; -31,31; -31,31	-17,17; -20,20; -34,34	-17,17; -18,18; -21,21	-16,16; -19,19; -21,21
R(F^2)(Obs.Refl.ns)	0.0273	0.0276	0.0458	0.0215	0.0220	0.0613
wR(F^2)(All Refl.ns)	0.0761	0.0806	0.1511	0.0541	0.0570	0.1644
No. Variables	206	206	206	296	315	315
Goodness of fit	1.026	1.022	1.050	1.057	1.054	1.134
$\Delta\rho_{max}$;$\Delta\rho_{min}$/e·Å^{-3}	1.84; -1.24	0.82; -0.84	1.05; -0.88	2.46; -1.35	0.92; -1.06	1.93; -2.25
CCDC Deposition N.	2512443	2512444	2512445	2512446	2512447	2512448

Table S2. Selected metal distances and angles for **2d** at 100 K, 200 K and 298 K. Corresponding naming scheme in use is reported (hydrogens omitted for clarity).

2d – $PdSnCl_3C_{30}H_{41}N_2$											
100 K				200 K				298 K			
Distances	**(Å)**	**Angles**	**(°)**	**Distances**	**(Å)**	**Angles**	**(°)**	**Distances**	**(Å)**	**Angles**	**(°)**
Pd_11-C1_12	2.032(2)	C19_13-Pd_11-C20_13	67.84(11)	Pd_11-C1_12	2.040(2)	C19_13-Pd_11-C20_13	67.64(11)	Pd_11-C1_12	2.048(2)	C19_13-Pd_11-C20_13	67.12(20)
Pd_11-C19_13	2.188(3)	C20_13-Pd_11-C1_12	99.64(8)	Pd_11-C19_13	2.188(3)	C20_13-Pd_11-C1_12	99.84(9)	Pd_11-C19_13	2.181(6)	C20_13-Pd_11-C1_12	100.78(14)
Pd_11-C20_13	2.167(3)	C1_12-Pd_11-Sn_21	105.83(5)	Pd_11-C20_13	2.163(3)	C1_12-Pd_11-Sn_21	105.94(5)	Pd_11-C20_13	2.185(5)	C1_12-Pd_11-Sn_21	106.15(6)
Pd_11-C21_13	2.134(3)	Sn_21-Pd_11-C19_13	85.72(8)	Pd_11-C21_13	2.132(3)	Sn_21-Pd_11-C19_13	85.39(9)	Pd_11-C21_13	2.146(5)	Sn_21-Pd_11-C19_13	84.54(15)
Pd_11-Sn_21	2.538(1)	Cl_22-Sn_21-Cl_23	97.06(1)	Pd_11-Sn_21	2.542(1)	Cl_22-Sn_21-Cl_23	97.74(2)	Pd_11-Sn_21	2.546(1)	Cl_22-Sn_21-Cl_23	97.47(4)
Sn_21-Cl_22	2.370(1)	Cl_23-Sn_21-Cl_23[b]	97.88(1)	Sn_21-Cl_22	2.366(1)	Cl_23-Sn_21-Cl_23[b]	94.64(2)	Sn_21-Cl_22	2.361(1)	Cl_23-Sn_21-Cl_23[b]	96.75(3)
Sn_21-Cl_23	2.398(1)	Cl_23[b] -Sn_21-Cl_22	97.06(1)	Sn_21-Cl_23	2.394(1)	Cl_23[b] -Sn_21-Cl_22	97.74(2)	Sn_21-Cl_23	2.390(1)	Cl_23[b] -Sn_21-Cl_22	97.47(4)
Sn_21-Cl_23[b]	2.398(1)	Pd-NHC Ave Plane[a]	90	Sn_21-Cl_23[b]	2.394(1)	Pd-NHC Ave Plane[a]	90	Sn_21-Cl_23[b]	2.390(1)	Pd-NHC Ave Plane[a]	90

[a]Average angle between the mean metal coordination plane and the mean NHC plane; [b]Atom generated through crystallographic mirror plane (x, y,-z+1/2).

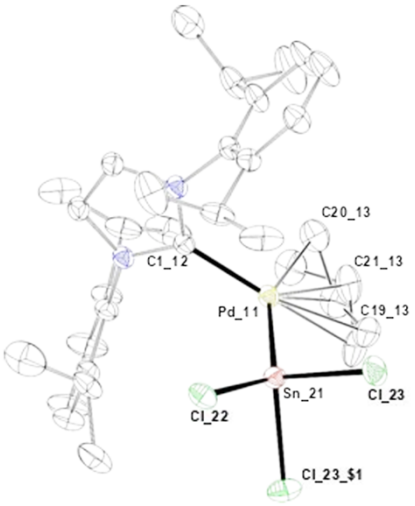


Table S3. Selected metal distances and angles for **2b** at 100 K. Corresponding naming scheme in use is reported (hydrogens omitted for clarity).

2b (100 K) – $PdSnCl_3C_{25}H_{31}N_2$			
Distances	**(Å)**	**Angles**	**(°)**
Pd_11-C1_12	2.044(1)	C19_13-Pd_11-C20_13	67.03(5)
Pd_11-C19_13	2.163(1)	C20_13-Pd_11-C1_12	100.78(5)
Pd_11-C20_13	2.179(1)	C1_12-Pd_11-Sn_21	102.60(3)
Pd_11-C21_13	2.169(1)	Sn_21-Pd_11-C19_13	89.68(4)
Pd_11-Sn_21	2.549(1)	Cl_22-Sn_21-Cl_23	96.10(2)
Sn_21-Cl_22	2.389(1)	Cl_23-Sn_21-Cl_24	94.64(2)
Sn_21-Cl_23	2.398(1)	Cl_24 -Sn_21-Cl_22	97.91(2)
Sn_21-Cl_24	2.380(1)	Pd-NHC Ave Plane[a]	59.06(3)

[a]Average angle between the mean metal coordination plane and the mean NHC plane

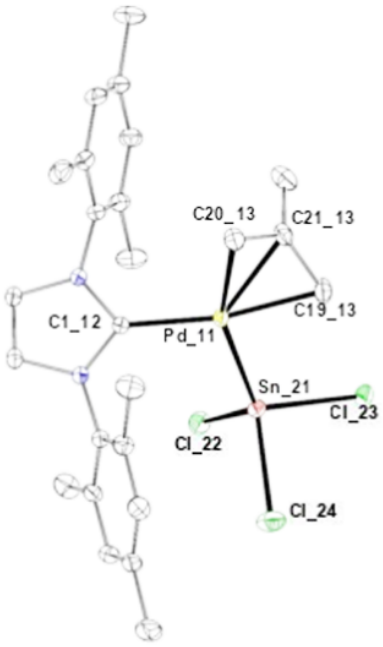


Table S4. Selected metal distances and angles for **2f** at 100 K and 298 K. Corresponding naming scheme in use is reported (hydrogens omitted for clarity).

2f – $PdSnCl_3C_{24}H_{31}N_2$							
100 K				298 K			
Distances	**(Å)**	**Angles**	**(°)**	**Distances**	**(Å)**	**Angles**	**(°)**
Pd_11-C1_12	2.029(1)	C19_13-Pd_11-C20_13[b]	67.6(3)	Pd_11-C1_12	2.031(2)	C19_13-Pd_11-C20_13[b]	67.1(6)
Pd_11-C19_13[b]	2.17(1)	C20_13-Pd_11-C1_12[b]	102.6(1)	Pd_11-C19_13[b]	2.18(2)	C20_13-Pd_11-C1_12[b]	102.6(4)
Pd_11-C20_13[b]	2.184(5)	C1_12-Pd_11-Sn_21	102.73(3)	Pd_11-C20_13[b]	2.18(1)	C1_12-Pd_11-Sn_21	103.48(6)
Pd_11-C21_13[b]	2.158(3)	Sn_21-Pd_11-C19_13[b]	86.7(3)	Pd_11-C21_13[b]	2.15(1)	Sn_21-Pd_11-C19_13[b]	86.2(4)
Pd_11-Sn_21	2.539(1)	Cl_22-Sn_21-Cl_23	94.92(2)	Pd_11-Sn_21	2.547(1)	Cl_22-Sn_21-Cl_23	95.04(6)
Sn_21-Cl_22	2.383(1)	Cl_23-Sn_21-Cl_24	99.56(2)	Sn_21-Cl_22	2.379(2)	Cl_23-Sn_21-Cl_24	99.26(5)
Sn_21-Cl_23	2.388(1)	Cl_24 -Sn_21-Cl_22	96.38(2)	Sn_21-Cl_23	2.378(1)	Cl_24 -Sn_21-Cl_22	96.47(5)
Sn_21-Cl_24	2.387(1)	Pd-NHC Ave Plane[a]	83.52(4)	Sn_21-Cl_24	2.381(2)	Pd-NHC Ave Plane[a]	85.36(8)

[a]Average angle between the mean metal coordination plane and the mean NHC plane; [b]Average angles and distances for disordered allyl ligand.

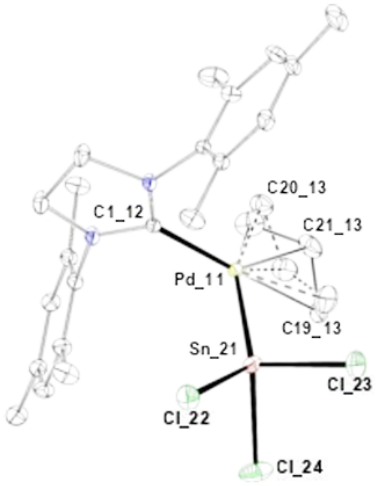


Figure S1. Ortep representations of molecular models for **2d** at 100 K (A), 200 K (B), 298 K (C), **2b** at 100 K (D), **2f** at 100 K (E) and VL9 at 298 K (F) crystals. Ellipsoids correspond to 50% probability.

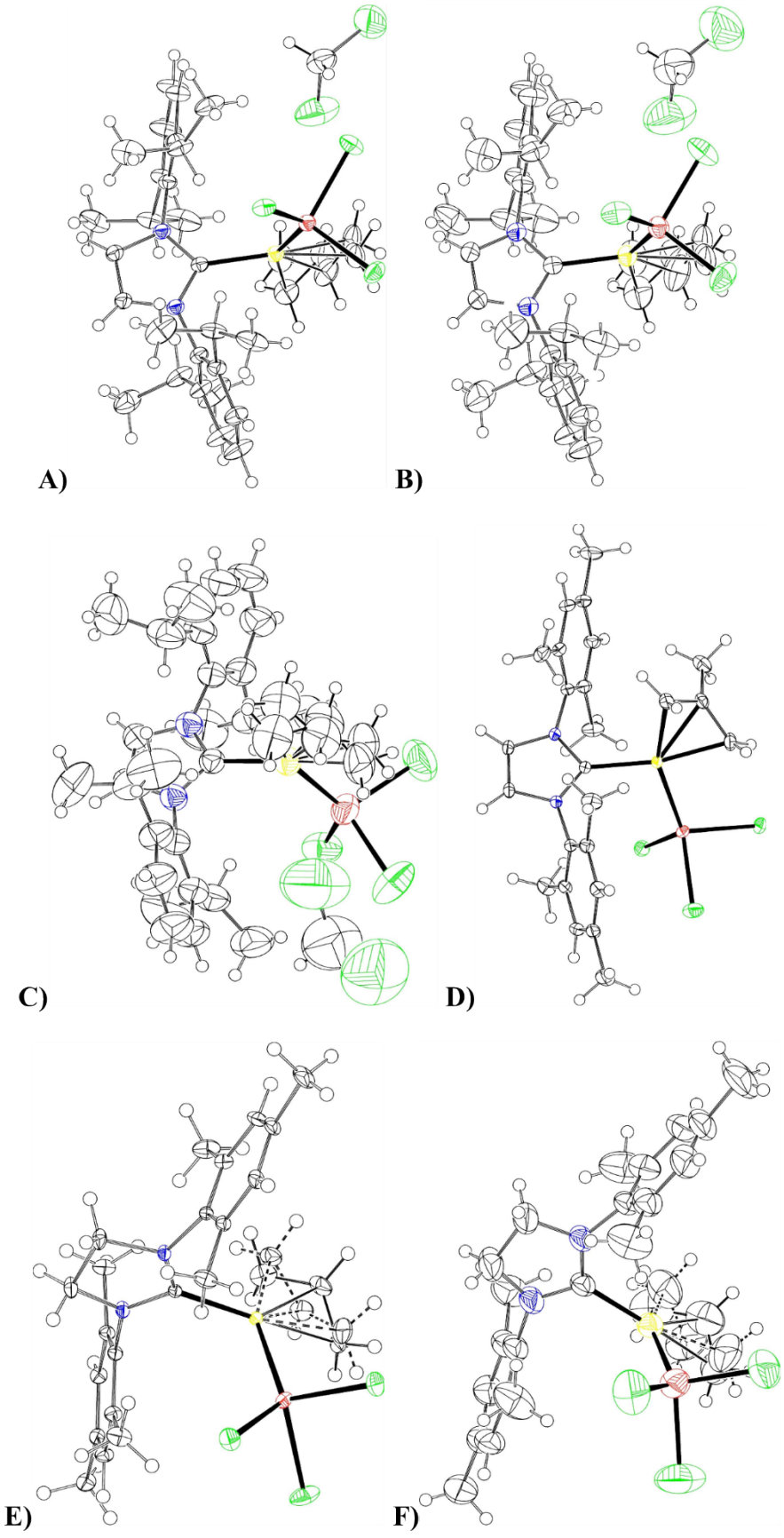


Figure S2. Superimposition of **2d** (shades of yellow sticks- A) and **2f** (sticks with different shades of pink- B) structures, obtained at different temperatures.

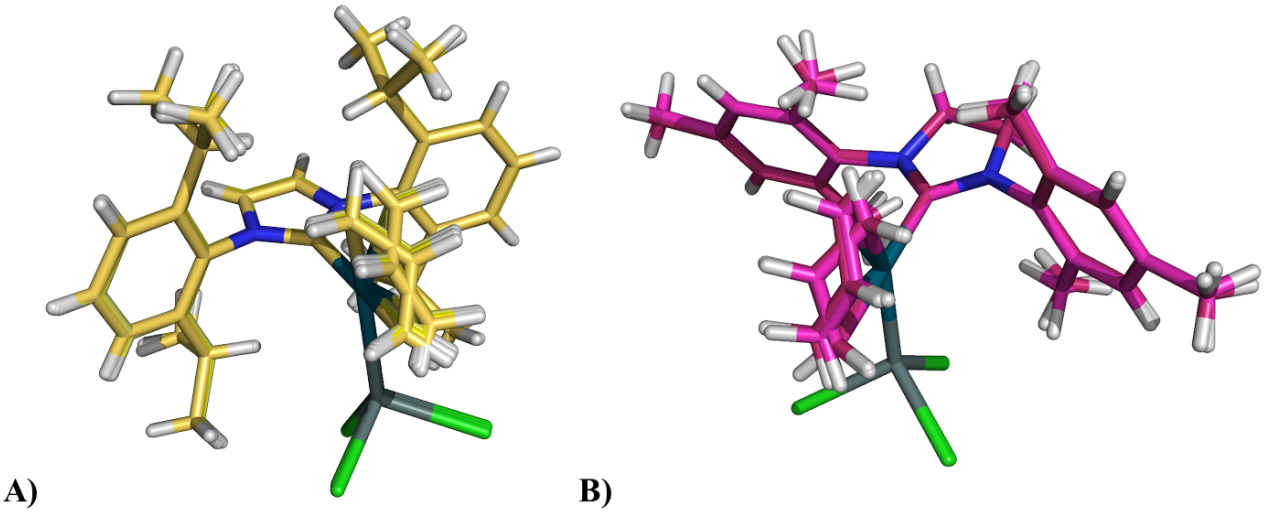
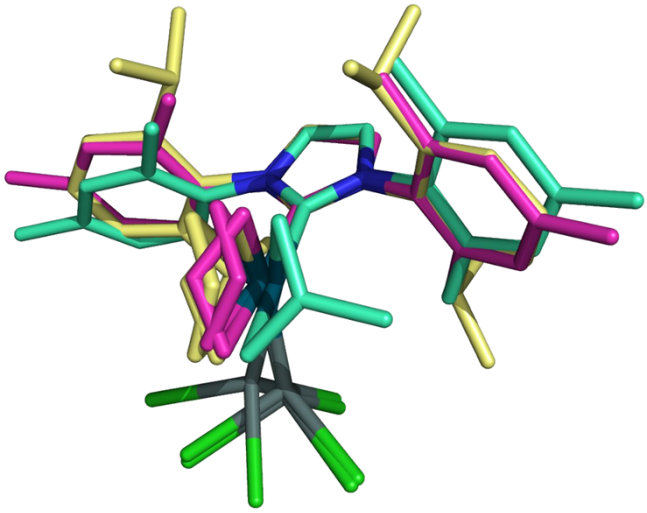


Figure S3. Superimposition of **2d** (yellow sticks), **2b** (cyan sticks) and **2f** (pink sticks) models, determined at 100 K. Hydrogens omitted for clarity



DFT Calculations

Cartesian coordinates

Energies (Hartree), imaginary frequencies (cm^{-1}) and cartesian coordinates (Å) of all stationary points. Level of theory: COSMO-ZORA-BLYP-D3(BJ)/TZP.

$SnCl_2$
-0.34496971 nimag=0

Sn	0.000000000	0.000000000	0.346036000
Cl	0.000000000	1.859457000	-1.339321000
Cl	0.000000000	-1.859457000	-1.339321000

1a
-12.15241974 nimag=0

Pd	1.212500000	-0.193300000	12.826900000
N	4.030500000	0.995500000	13.091700000
N	2.553500000	2.565100000	13.258900000
C	2.677700000	1.213700000	13.080900000
C	4.750600000	-0.930900000	11.747600000
C	3.808800000	3.179300000	13.377600000
H	3.911900000	4.244500000	13.524800000
C	4.738700000	2.191000000	13.271100000
H	5.818100000	2.218200000	13.304200000
C	4.621300000	-0.320900000	13.007800000
C	5.268800000	-2.233700000	11.707900000
H	5.369000000	-2.728300000	10.741900000
C	5.653600000	-2.914300000	12.874100000
C	0.569600000	3.197100000	14.556400000
C	1.289900000	3.262900000	13.351000000
C	-1.152500000	4.610300000	13.533100000
C	-0.654600000	3.879200000	14.622700000
H	-1.226200000	3.842700000	15.549900000
C	4.334500000	-0.213900000	10.483000000
H	3.249900000	-0.047100000	10.462300000
H	4.614700000	-0.799200000	9.601300000
H	4.811600000	0.772200000	10.412600000
C	1.087500000	2.415800000	15.743800000
H	1.037400000	1.338200000	15.546200000
H	0.493000000	2.632800000	16.636800000
H	2.137000000	2.655400000	15.955500000
C	-0.390800000	4.660700000	12.355100000
H	-0.761200000	5.228900000	11.502000000
C	0.837100000	3.993300000	12.238500000
C	5.517500000	-2.260800000	14.108600000
H	5.804200000	-2.778400000	15.023700000
C	-2.494600000	5.308200000	13.617800000
H	-3.297800000	4.644800000	13.265000000
H	-2.514900000	6.209300000	12.993400000
H	-2.731000000	5.592200000	14.650000000
C	6.229600000	-4.313300000	12.798200000
H	5.791900000	-4.878900000	11.967100000
H	6.054400000	-4.866200000	13.728500000
H	7.316600000	-4.276500000	12.634900000
C	1.635300000	4.040400000	10.955700000
H	2.610900000	4.521200000	11.104400000
H	1.091900000	4.599300000	10.187100000
H	1.814300000	3.022800000	10.588200000
C	5.004100000	-0.958700000	14.200600000
C	4.855800000	-0.273700000	15.541800000
H	5.623000000	0.500500000	15.677700000
H	4.958500000	-0.997200000	16.356700000
H	3.882600000	0.221200000	15.631900000
C	-0.116400000	-2.050500000	12.916500000
H	-1.139300000	-1.998800000	12.552400000
H	0.561500000	-2.716500000	12.383500000
C	1.563100000	-1.416300000	14.582000000
H	2.320600000	-2.113600000	14.224400000
H	1.787000000	-0.932000000	15.528800000
C	0.198100000	-1.583400000	14.199200000
Cl	0.511200000	0.568100000	10.602000000
H	-0.582200000	-1.118800000	14.803200000

1k
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Pd	2.931646000	-1.376073000	13.697383000
N	3.991068000	1.262386000	12.325505000
N	3.405008000	1.529079000	14.399886000
C	3.498869000	0.585969000	13.415091000
C	3.827640000	2.776366000	13.945887000
H	3.830049000	3.653611000	14.577179000
C	4.201218000	2.610100000	12.646616000
H	4.595301000	3.328117000	11.946748000
C	1.725811000	-3.292542000	14.059783000
H	2.165046000	-4.262288000	13.839779000
H	1.476968000	-3.091217000	15.101219000
C	0.823349000	-1.155578000	13.261354000
H	0.406750000	-0.863423000	14.225960000
H	0.534209000	-0.533423000	12.417850000
C	1.176432000	-2.520455000	13.027862000
Cl	5.092767000	-2.112410000	14.613497000
C	2.873698000	1.275322000	15.746850000
H	1.793837000	1.457655000	15.769212000
H	3.074588000	0.234780000	16.009614000
H	3.373002000	1.939626000	16.456639000
C	4.355187000	0.628080000	10.996738000
C	5.545365000	-0.323600000	11.229674000
H	6.411390000	0.232817000	11.607780000
H	5.288213000	-1.098644000	11.957146000
H	5.823147000	-0.800541000	10.282288000
C	4.753228000	1.729336000	9.996908000
H	5.650188000	2.270204000	10.318101000
H	4.978742000	1.252110000	9.037701000
H	3.938685000	2.445122000	9.836122000
C	3.133059000	-0.134464000	10.450200000
H	2.271118000	0.535216000	10.347799000
H	3.378173000	-0.546776000	9.464959000
H	2.861223000	-0.958560000	11.115870000
H	1.248272000	-2.879916000	12.000586000

1a-RC
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Pd	0.847706000	-0.096395000	13.053900000
N	0.941206000	-3.065930000	12.056982000
N	1.473638000	-1.653669000	10.509682000
C	1.111907000	-1.727815000	11.828645000
C	-0.755508000	-4.073352000	13.518204000

C	1.525222000	-2.923994000	9.922986000
H	1.790388000	-3.065554000	8.885541000
C	1.190616000	-3.814162000	10.896422000
H	1.105905000	-4.890832000	10.883300000
C	0.574067000	-3.648644000	13.328162000
C	-1.081073000	-4.654998000	14.752186000
H	-2.109033000	-4.965291000	14.928554000
C	-0.125760000	-4.817760000	15.770549000
C	3.169727000	-0.075297000	9.711085000
C	1.811312000	-0.409826000	9.852755000
C	2.475544000	2.054698000	8.716548000
C	3.477978000	1.168650000	9.141416000
H	4.524640000	1.451722000	9.033290000
C	-1.799198000	-3.904084000	12.438177000
H	-2.796022000	-4.113287000	12.837235000
H	-1.614374000	-4.587989000	11.599227000
H	-1.789937000	-2.882498000	12.043417000
C	4.265759000	-1.020261000	10.155663000
H	4.374509000	-1.856664000	9.452129000
H	4.049861000	-1.456606000	11.137781000
H	5.226313000	-0.498166000	10.207862000
C	1.133941000	1.664182000	8.849513000
H	0.345219000	2.332522000	8.505273000
C	0.773963000	0.432153000	9.415158000
C	1.187760000	-4.387146000	15.532758000
H	1.939038000	-4.504885000	16.312405000
C	2.832980000	3.413216000	8.150392000
H	2.081060000	3.753963000	7.429166000
H	3.810745000	3.394012000	7.655229000
H	2.883745000	4.163507000	8.952969000
C	-0.523532000	-5.431067000	17.095327000
H	-0.815336000	-6.482222000	16.966193000
H	-1.387947000	-4.905345000	17.521648000
H	0.299402000	-5.390124000	17.816638000
C	-0.678072000	0.031154000	9.550771000
H	-0.847061000	-0.986496000	9.177669000
H	-1.318996000	0.719119000	8.990724000
H	-0.994664000	0.044215000	10.600927000
C	1.565218000	-3.801871000	14.313190000
C	2.989165000	-3.354166000	14.071862000
H	3.393688000	-3.797734000	13.153164000
H	3.630723000	-3.643340000	14.909464000
H	3.041415000	-2.266056000	13.952805000
C	1.100060000	1.765931000	14.390870000
H	0.320920000	2.522847000	14.387103000
H	1.260777000	1.241976000	15.331115000
C	2.891998000	0.569848000	13.241805000
H	3.240396000	0.061373000	14.141128000
H	3.532072000	0.482517000	12.370444000
C	2.051315000	1.718774000	13.368646000
H	1.983010000	2.418553000	12.535295000
Sn	-0.978359000	-1.398139000	15.757453000
Cl	-3.394031000	-2.189316000	16.150169000
Cl	-1.623735000	-0.340321000	13.332106000
Cl	-1.324460000	0.847898000	16.990961000

1k-RC

-7.10890310 nimag=0

Pd	0.890787000	-0.364262000	12.614629000
N	3.174847000	1.766124000	12.263863000
N	3.085335000	0.942835000	14.275357000
C	2.466906000	0.892723000	13.054571000
C	4.165290000	1.821734000	14.255306000
H	4.793575000	1.988847000	15.118509000
C	4.216568000	2.344870000	12.998386000
H	4.902327000	3.062443000	12.579336000
C	-1.138750000	-1.429537000	12.518442000
H	-1.367213000	-2.092052000	11.687516000
H	-1.085308000	-1.881607000	13.508294000
C	-0.736857000	0.832757000	13.363615000
H	-0.786176000	0.548526000	14.415145000
H	-0.716574000	1.902242000	13.170186000
C	-1.271090000	-0.044671000	12.368113000
Sn	4.856927000	-1.562175000	12.575418000
Cl	2.324910000	-2.280889000	11.901353000
Cl	5.562268000	-0.934834000	10.194701000
Cl	5.643507000	-3.990348000	12.403835000
C	2.709507000	0.131645000	15.442099000
H	2.570417000	0.781957000	16.310251000
H	1.777260000	-0.386231000	15.209210000
H	3.492589000	-0.603670000	15.655227000
C	2.768559000	2.230983000	10.873875000
C	2.299239000	1.037172000	10.025809000
H	3.084604000	0.281495000	9.941703000
H	1.404336000	0.568078000	10.451331000
H	2.049511000	1.401849000	9.023247000
C	3.987204000	2.879002000	10.189612000
H	4.832213000	2.182644000	10.153349000
H	3.707823000	3.132733000	9.162033000
H	4.297947000	3.805714000	10.683495000
C	1.632753000	3.259476000	11.052394000
H	1.963389000	4.100095000	11.673677000
H	1.329035000	3.647508000	10.073408000
H	0.764319000	2.791265000	11.526445000
H	-1.549885000	0.362958000	11.396062000

1a-TS

-12.51572699 nimag=1 v=-84.2

Pd	1.308735000	-0.412206000	13.396924000
N	1.047717000	-3.189508000	12.095784000
N	1.417318000	-1.693965000	10.576071000
C	1.253219000	-1.845067000	11.925752000
C	-0.392041000	-3.854184000	13.975445000
C	1.314540000	-2.923837000	9.915097000
H	1.416589000	-3.004995000	8.842839000
C	1.081168000	-3.865332000	10.872453000
H	0.936968000	-4.933653000	10.804643000
C	0.885157000	-3.804177000	13.395100000
C	-0.493516000	-4.366408000	15.279705000
H	-1.473068000	-4.395813000	15.755920000
C	0.626967000	-4.831505000	15.980739000
C	2.988200000	0.092371000	9.969904000
C	1.684166000	-0.429047000	9.922793000
C	2.192974000	2.017939000	8.678690000
C	3.217574000	1.324883000	9.341149000
H	4.222176000	1.746496000	9.364443000
C	-1.632531000	-3.424281000	13.224771000
H	-2.387033000	-3.026872000	13.911621000
H	-2.080396000	-4.285039000	12.707969000
H	-1.419069000	-2.669262000	12.464167000
C	4.109181000	-0.638164000	10.676241000
H	4.128962000	-1.702044000	10.410349000

H	3.983692000	-0.579792000	11.764427000
H	5.077363000	-0.197028000	10.420120000
C	0.911183000	1.448826000	8.643997000
H	0.104616000	1.975509000	8.135182000
C	0.628797000	0.224890000	9.264799000
C	1.880199000	-4.796968000	15.344618000
H	2.760020000	-5.162000000	15.874091000
C	2.456340000	3.366817000	8.042361000
H	1.828338000	3.518659000	7.156536000
H	3.507432000	3.471165000	7.749107000
H	2.227524000	4.176697000	8.750430000
C	0.495964000	-5.381415000	17.385715000
H	0.611875000	-6.474555000	17.387123000
H	-0.483704000	-5.145850000	17.815480000
H	1.272936000	-4.971892000	18.043687000
C	-0.768955000	-0.348954000	9.255143000
H	-0.799545000	-1.343612000	8.793160000
H	-1.448177000	0.307476000	8.703134000
H	-1.158224000	-0.449307000	10.275188000
C	2.034092000	-4.291608000	14.048085000
C	3.386975000	-4.287381000	13.370063000
H	3.458984000	-5.109381000	12.644584000
H	4.187648000	-4.416763000	14.104864000
H	3.563099000	-3.358851000	12.817872000
C	1.671589000	0.832125000	15.305901000
H	1.425907000	1.890289000	15.289368000
H	1.128142000	0.210256000	16.014893000
C	3.060043000	-1.024604000	14.555983000
H	2.625089000	-1.733755000	15.258443000
H	3.921005000	-1.376508000	13.996233000
C	2.867809000	0.375734000	14.735531000
H	3.533279000	1.078718000	14.235630000
Sn	-1.385820000	0.262371000	13.686712000
Cl	-3.425148000	0.004192000	12.195367000
Cl	-0.154394000	1.973699000	12.172859000
Cl	-2.341025000	1.952725000	15.313129000

1k-TS

-7.09481395 nimag=1 v=-84.9

Pd	1.061395000	-0.473600000	12.552657000
N	3.725509000	0.629147000	11.274624000
N	3.317665000	1.441573000	13.250125000
C	2.809755000	0.598346000	12.296858000
C	4.546263000	1.957954000	12.857012000
H	5.113720000	2.637740000	13.476315000
C	4.804434000	1.448737000	11.621216000
H	5.649192000	1.610893000	10.971987000
C	-1.124226000	-1.137119000	12.903934000
H	-1.397762000	-2.170101000	12.707217000
H	-1.215802000	-0.787168000	13.930684000
C	-0.416981000	1.053831000	12.085968000
H	-0.572351000	1.551460000	13.042418000
H	-0.181318000	1.700185000	11.244792000
C	-1.006294000	-0.226273000	11.847469000
Sn	2.251847000	-2.094198000	14.521373000
Cl	2.020023000	-3.410698000	12.275504000
Cl	4.779055000	-1.867441000	14.464272000
Cl	2.099801000	-4.131071000	16.034816000
C	2.704542000	1.714848000	14.556413000
H	1.635528000	1.507591000	14.492822000
H	3.155732000	1.075604000	15.323383000
H	2.865152000	2.764544000	14.814476000
C	3.710519000	-0.181960000	9.991593000
C	4.540146000	-1.457136000	10.243968000
H	5.570103000	-1.199572000	10.516095000
H	4.098404000	-2.048955000	11.050306000
H	4.563813000	-2.066060000	9.332574000
C	4.340290000	0.668451000	8.867315000
H	5.405045000	0.859009000	9.033657000
H	4.250330000	0.117901000	7.925122000
H	3.818834000	1.626728000	8.759969000
C	2.269412000	-0.532710000	9.588984000
H	1.659512000	0.369750000	9.473567000
H	2.300462000	-1.056719000	8.627490000
H	1.792765000	-1.197463000	10.316640000
H	-1.144497000	-0.567930000	10.822065000

2a

-12.53159348 nimag=0

Pd	1.159200000	-0.155900000	13.046200000
N	4.018400000	0.999200000	13.178700000
N	2.564400000	2.589800000	13.383200000
C	2.669300000	1.237800000	13.186600000
C	4.558600000	-0.954100000	11.789100000
C	3.828700000	3.182200000	13.499500000
H	3.950500000	4.243100000	13.658500000
C	4.742900000	2.182800000	13.368200000
H	5.822500000	2.195300000	13.388800000
C	4.600600000	-0.316600000	13.042100000
C	5.073000000	-2.256300000	11.705600000
H	5.043000000	-2.769900000	10.745100000
C	5.620000000	-2.910400000	12.820400000
C	0.424800000	3.152300000	14.464200000
C	1.309500000	3.308600000	13.380700000
C	-1.154800000	4.626500000	13.305700000
C	-0.804000000	3.823300000	14.400700000
H	-1.504600000	3.710600000	15.227400000
C	3.958800000	-0.283200000	10.572800000
H	2.862000000	-0.324300000	10.608500000
H	4.285500000	-0.785200000	9.656900000
H	4.237800000	0.774900000	10.514800000
C	0.770700000	2.294400000	15.661800000
H	0.637600000	1.229600000	15.429300000
H	0.123200000	2.542300000	16.508700000
H	1.815600000	2.427900000	15.965400000
C	-0.229600000	4.779200000	12.263600000
H	-0.483300000	5.404500000	11.408600000
C	1.015700000	4.135300000	12.278700000
C	5.648200000	-2.231800000	14.048500000
H	6.056000000	-2.731000000	14.926900000
C	-2.517400000	5.278100000	13.230600000
H	-3.226600000	4.600300000	12.734400000
H	-2.484900000	6.208000000	12.651200000
H	-2.910700000	5.499000000	14.229800000
C	6.190200000	-4.307600000	12.694300000
H	5.658100000	-4.886600000	11.930400000
H	6.133600000	-4.847400000	13.646600000
H	7.248900000	-4.267100000	12.399200000
C	2.005400000	4.348300000	11.154200000
H	2.799900000	5.043200000	11.458500000
H	1.500700000	4.768600000	10.280600000
H	2.484200000	3.411400000	10.852000000

C	5.142300000	-0.931400000	14.185500000
C	5.150400000	-0.236100000	15.529700000
H	5.925500000	0.540500000	15.574200000
H	5.349100000	-0.954900000	16.330700000
H	4.192200000	0.257500000	15.731300000
C	-0.146500000	-2.006600000	13.164200000
H	-1.226400000	-1.931900000	13.072000000
H	0.363300000	-2.584500000	12.394200000
C	1.878800000	-1.679200000	14.502900000
H	2.515200000	-2.264100000	13.840800000
H	2.332800000	-1.339800000	15.428800000
C	0.467800000	-1.765600000	14.407100000
Sn	-0.356800000	0.746700000	11.091800000
Cl	-2.568600000	1.755500000	11.590000000
Cl	0.267200000	2.135000000	9.130100000
Cl	-1.211300000	-1.165900000	9.703800000
H	-0.141500000	-1.410000000	15.238300000

2k

-7.11026124 nimag=0

Pd	1.219246000	-0.363571000	12.438369000
N	3.182921000	2.041892000	11.948633000
N	3.273949000	1.273061000	13.979395000
C	2.622719000	1.114137000	12.789852000
C	4.236221000	2.274212000	13.892096000
H	4.866054000	2.546419000	14.726812000
C	4.175830000	2.762784000	12.621628000
H	4.746428000	3.550815000	12.159173000
C	-0.557017000	-1.771987000	12.392382000
H	-0.640580000	-2.526967000	11.615381000
H	-0.483913000	-2.135092000	13.417102000
C	-0.699366000	0.589601000	13.053761000
H	-0.672524000	0.379476000	14.122479000
H	-0.886368000	1.622163000	12.773058000
C	-0.968418000	-0.451631000	12.128273000
Sn	3.082240000	-2.165048000	12.038029000
Cl	3.522582000	-3.145490000	9.794117000
Cl	5.395577000	-1.373807000	12.534530000
Cl	3.137774000	-4.251718000	13.391787000
C	3.079731000	0.418544000	15.158492000
H	3.161445000	1.026787000	16.062653000
H	2.085460000	-0.029762000	15.103346000
H	3.838544000	-0.371153000	15.173035000
C	2.749565000	2.293515000	10.516915000
C	2.796773000	0.965646000	9.737585000
H	3.792590000	0.512601000	9.795940000
H	2.061436000	0.252654000	10.130085000
H	2.556846000	1.152904000	8.685342000
C	3.713224000	3.300052000	9.863104000
H	4.744354000	2.929184000	9.861816000
H	3.402977000	3.442441000	8.823098000
H	3.681403000	4.277218000	10.357239000
C	1.321634000	2.873893000	10.540125000
H	1.293254000	3.805127000	11.117670000
H	0.995336000	3.086299000	9.515773000
H	0.622872000	2.161807000	10.987052000
H	-1.274440000	-0.187805000	11.115420000