Supporting Information

for

Versatile coordinating abilities of acyclic N_4 and N_2P_2 ligand frameworks in conjunction with $Sn[N(SiMe_3)_2]_2$

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1. Plot of NMR Spectra

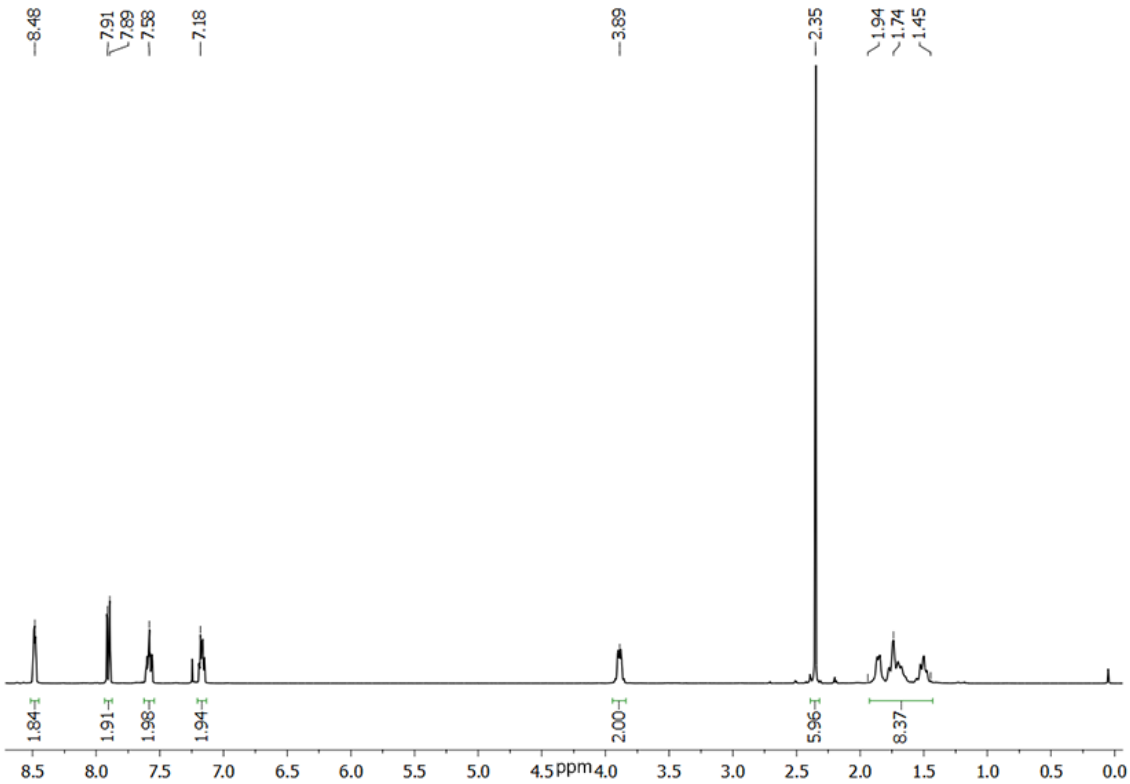

Figure S1. ^{1}H NMR of **L1** in $CDCl_3$

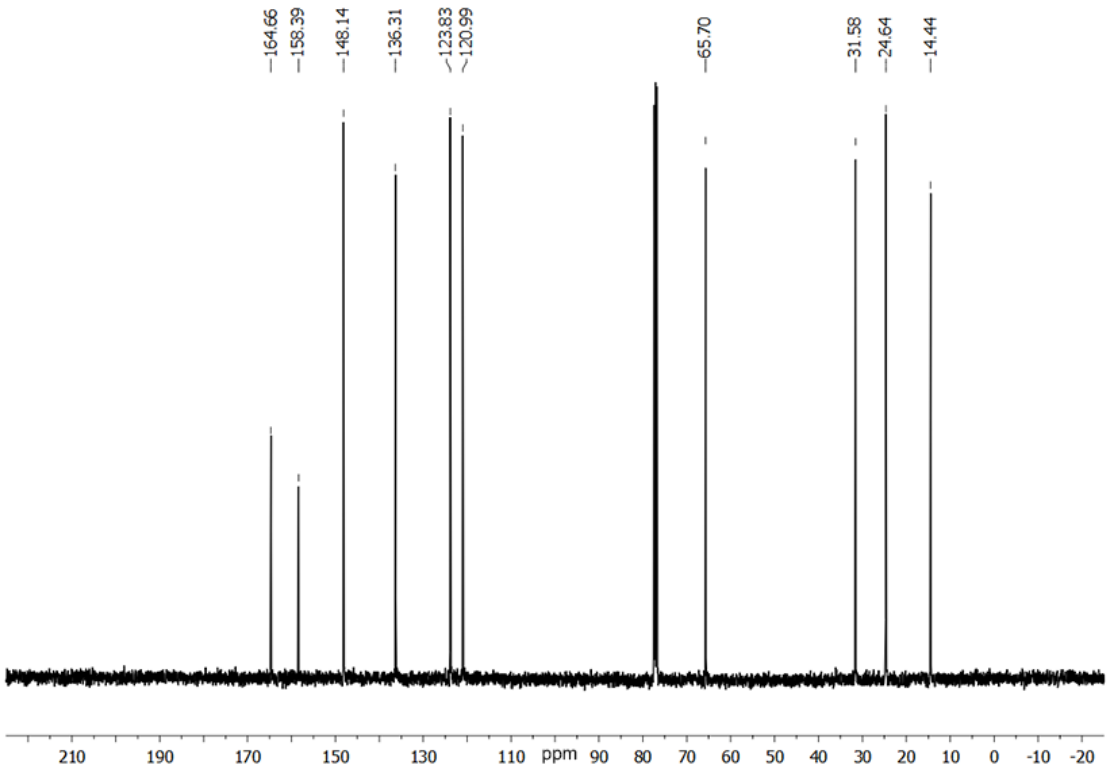

Figure S2. ^{13}C NMR of **L1** in $CDCl_3$

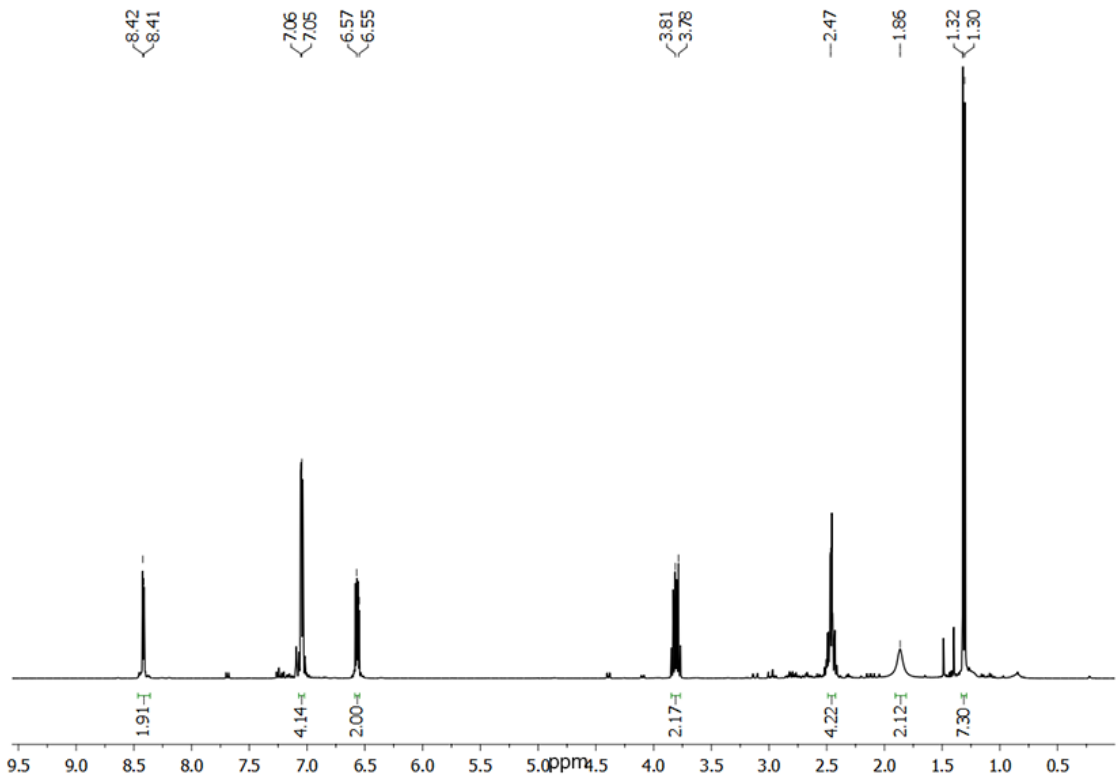

Figure S3. ^{1}H NMR of **L2** in C_6D_6

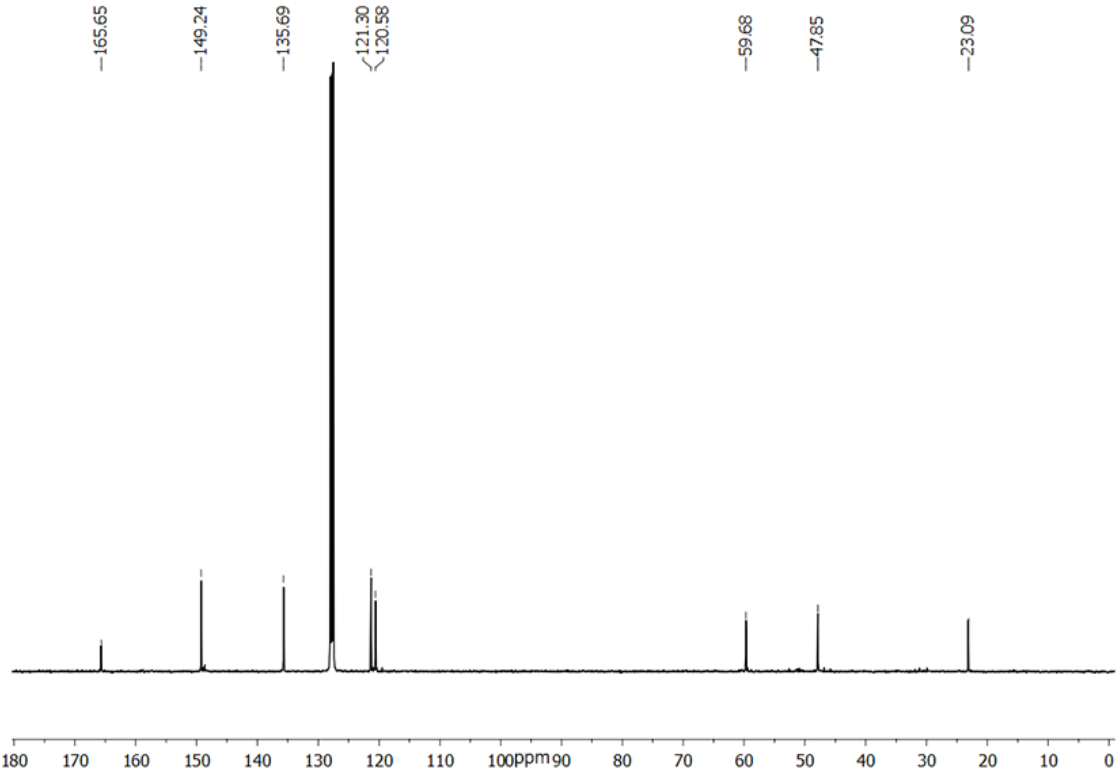

Figure S4. ^{13}C NMR of **L2** in C_6D_6

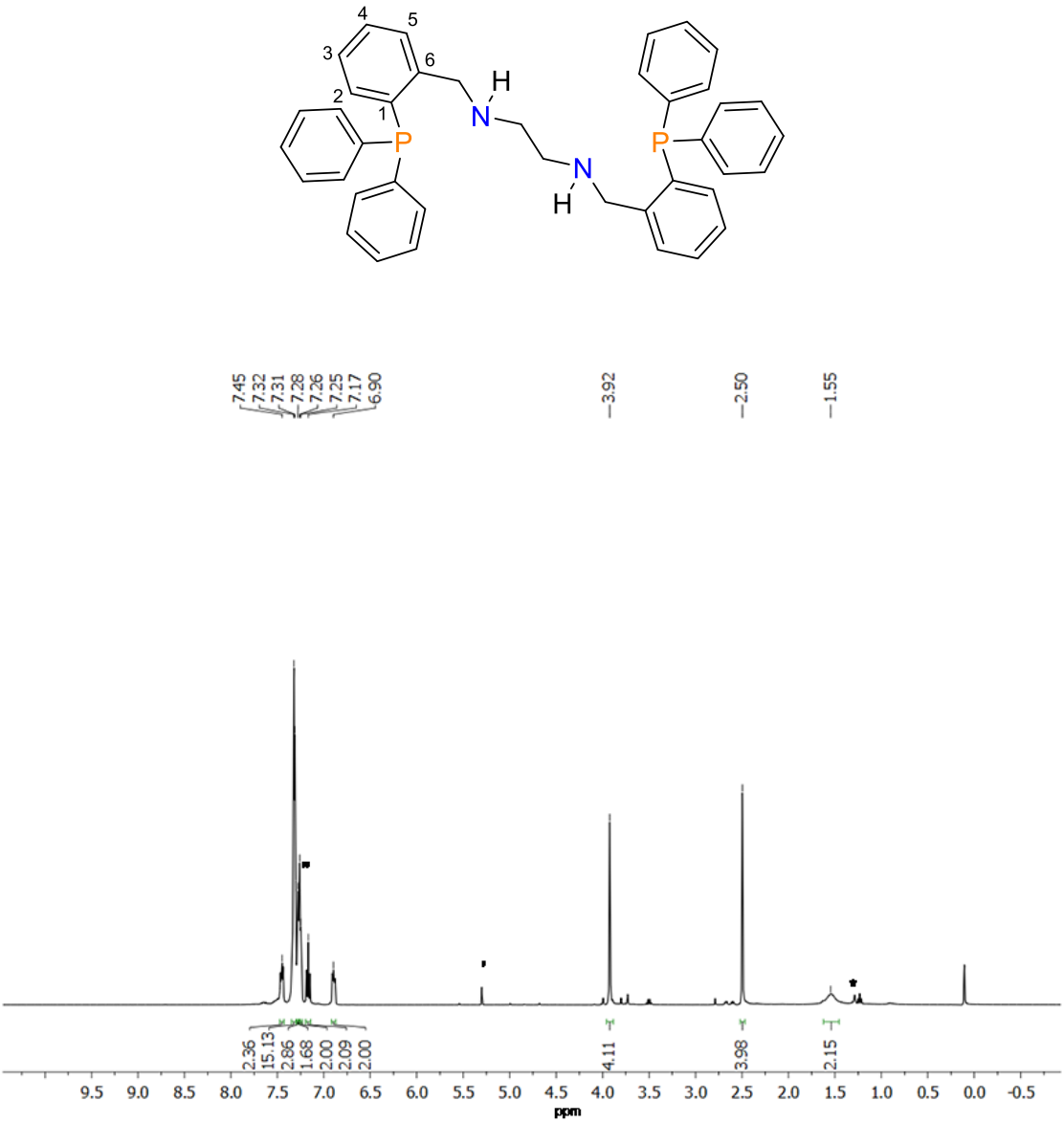

Figure S5. ^{1}H NMR of **L3** in $CDCl_3$ (’=DCM; *=impurity)

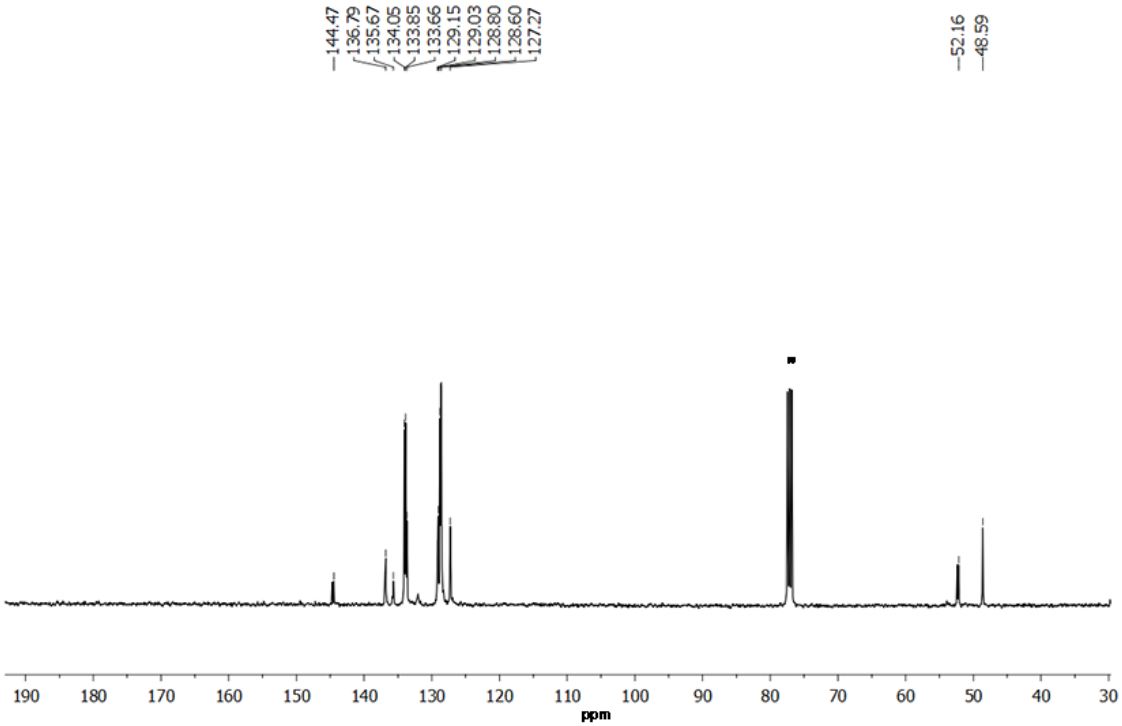

Figure S6. ^{13}C NMR of **L3** in $CDCl_3$

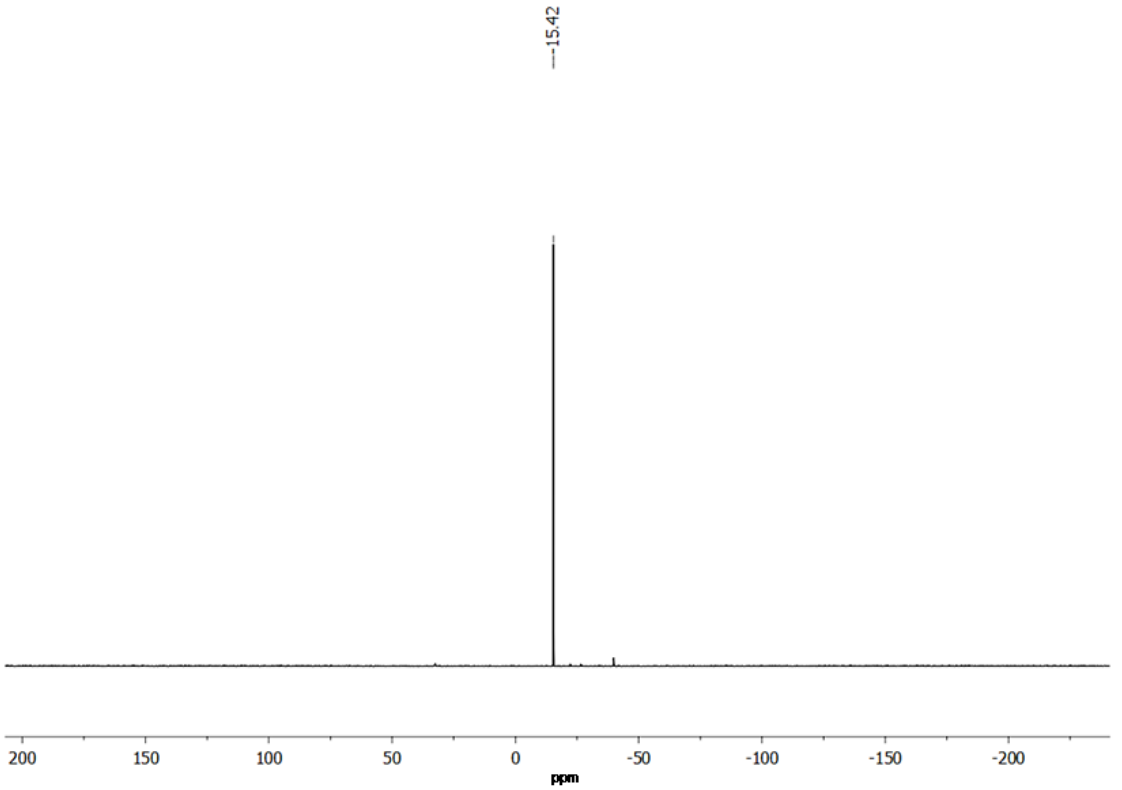

Figure S7. ^{31}P NMR of **L3** in $CDCl_3$

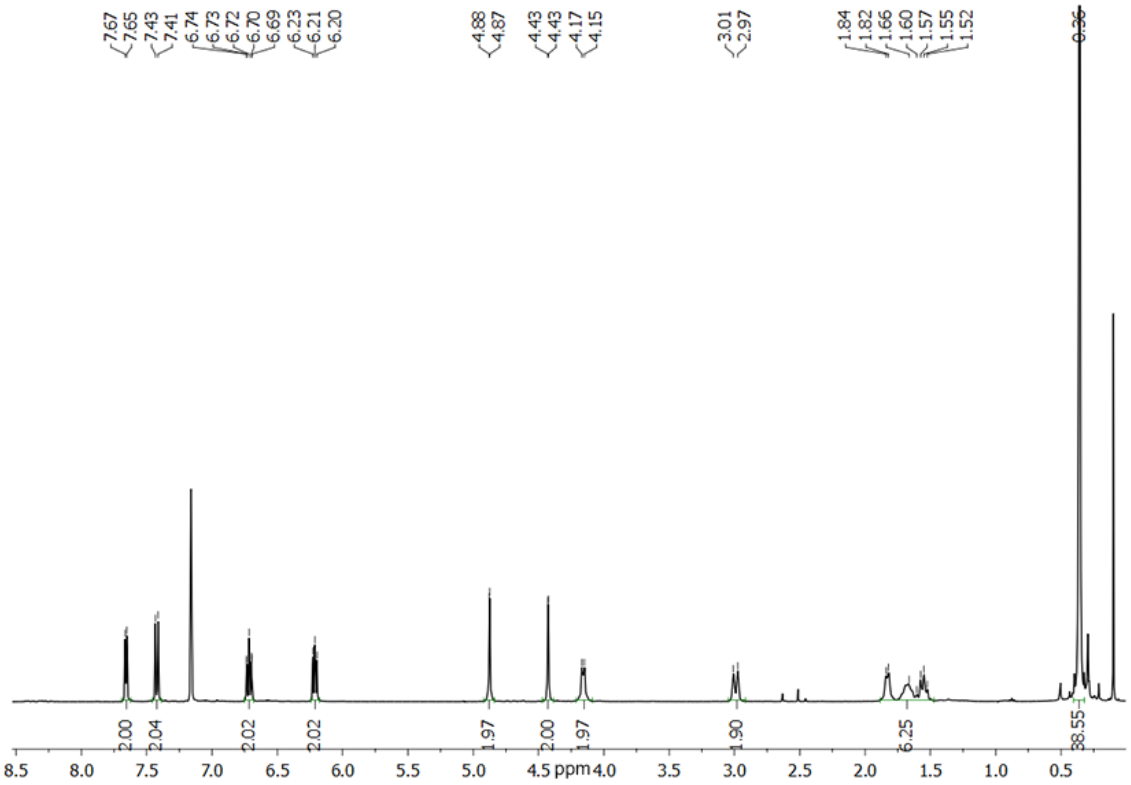

Figure S8. ^{1}H NMR of **1** in C_6D_6

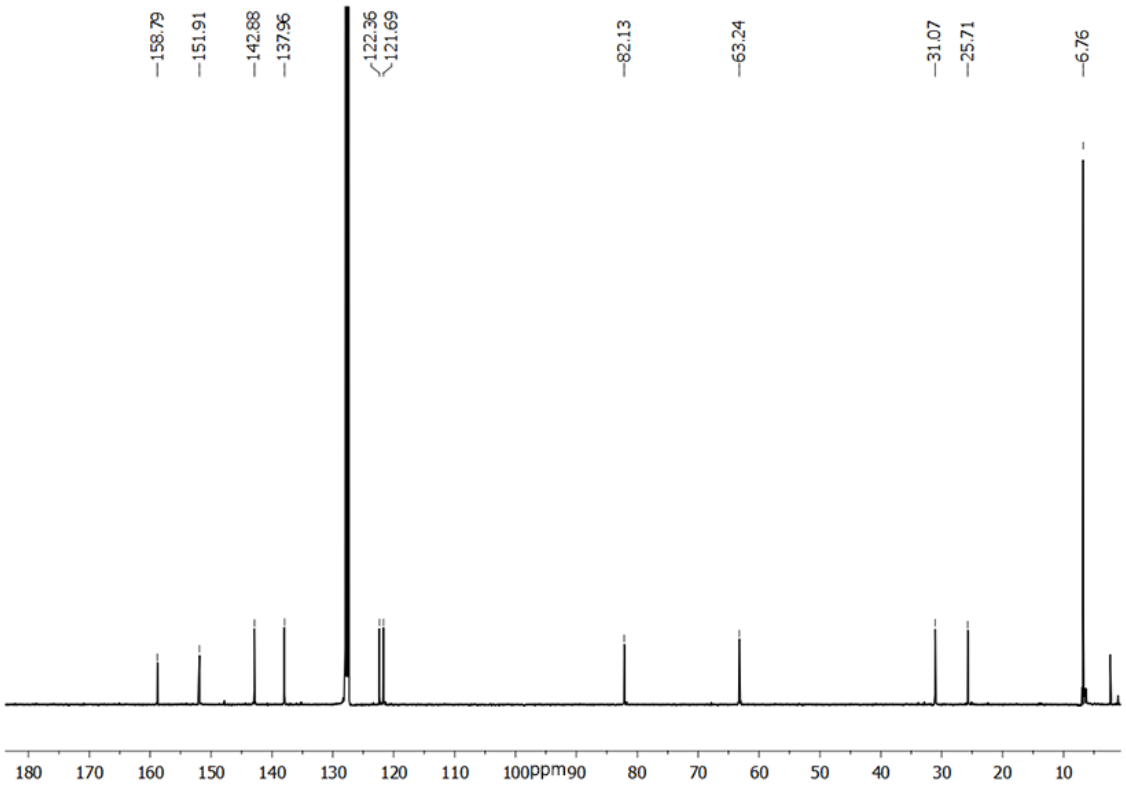

Figure S9. ^{13}C NMR of **1** in C_6D_6

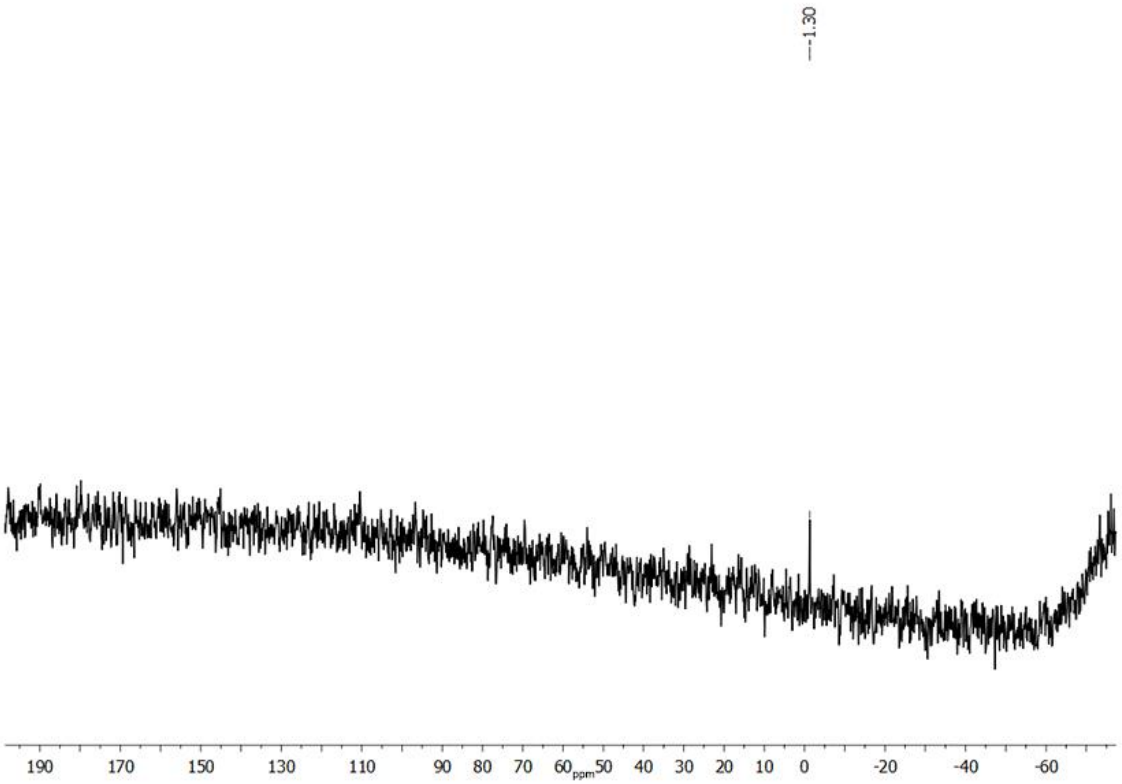

Figure S10. ^{29}Si NMR of **1** in C_6D_6

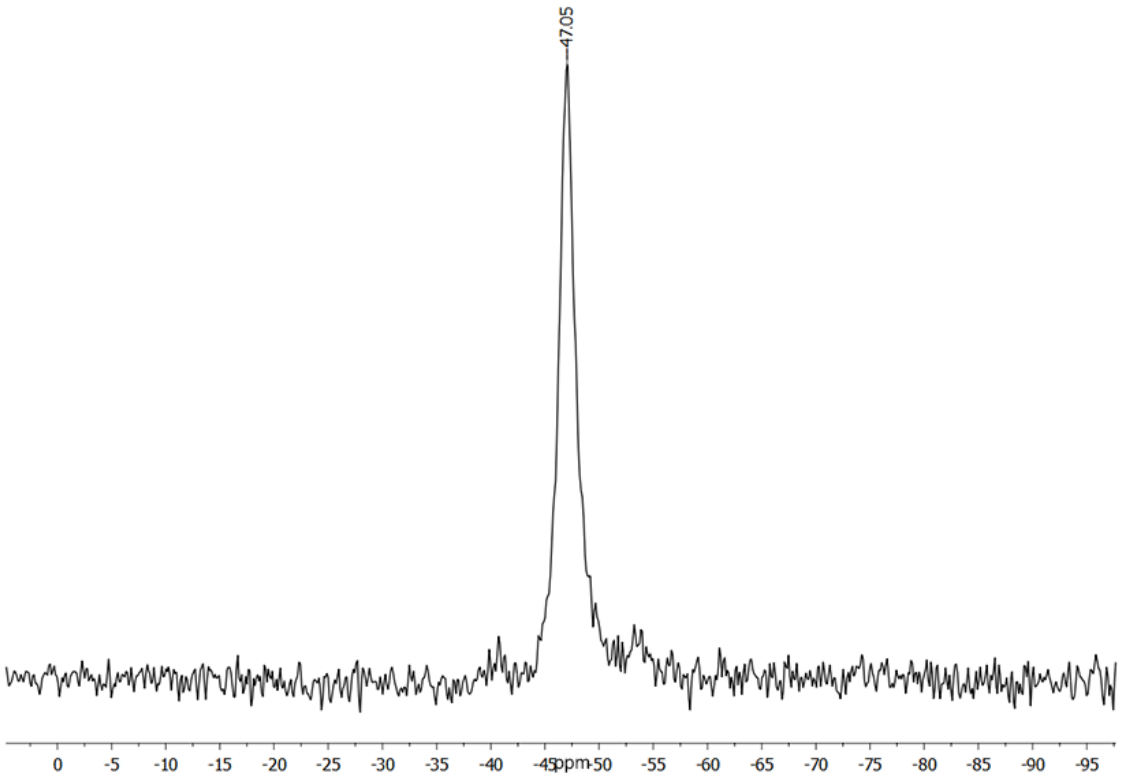

Figure S11. ^{119}Sn NMR of **1** in C_6D_6

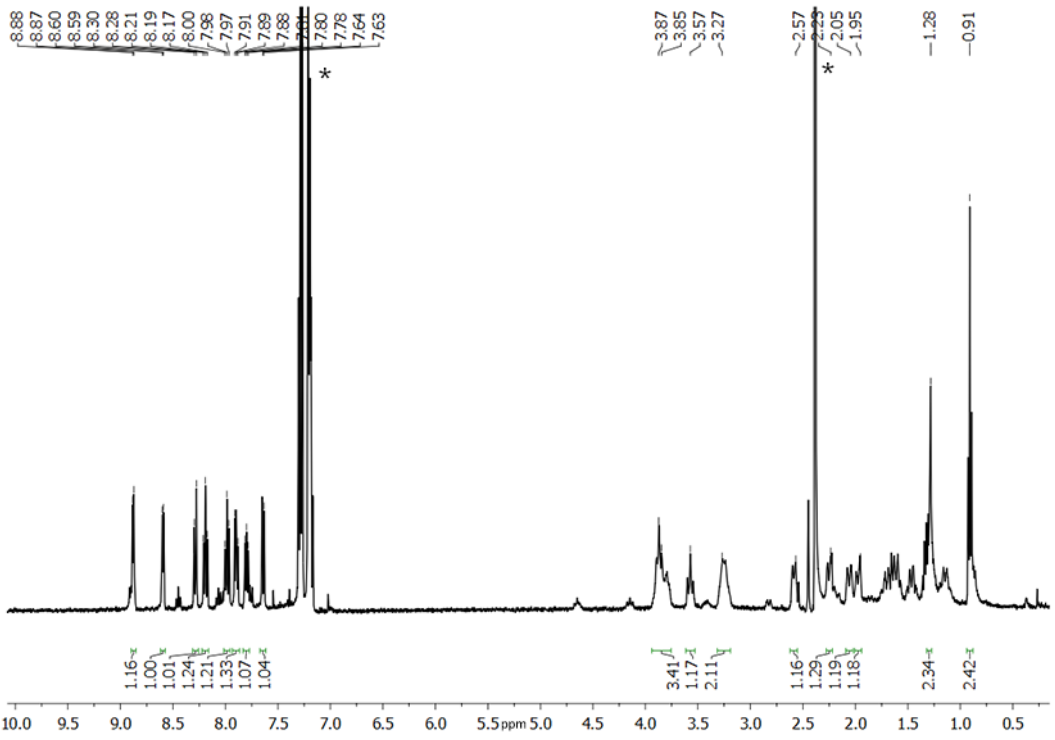

Figure S12. ^{1}H NMR of compound **2** in $CDCl_3$ (* = toluene)

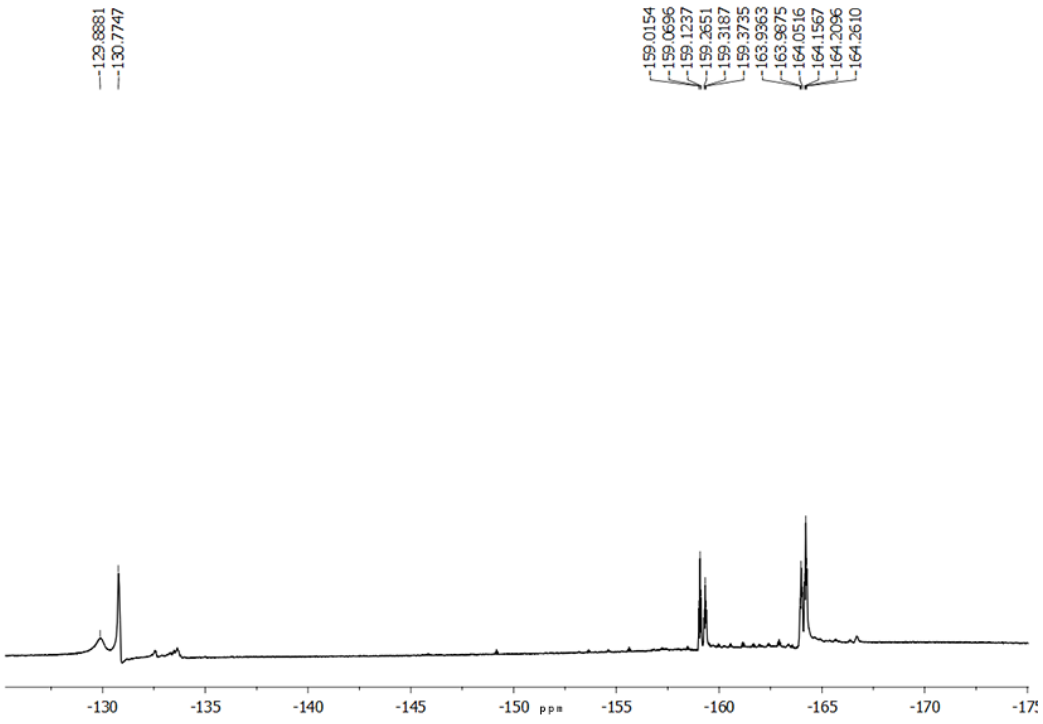

Figure S13. ^{19}F NMR of compound **2** in $CDCl_3$

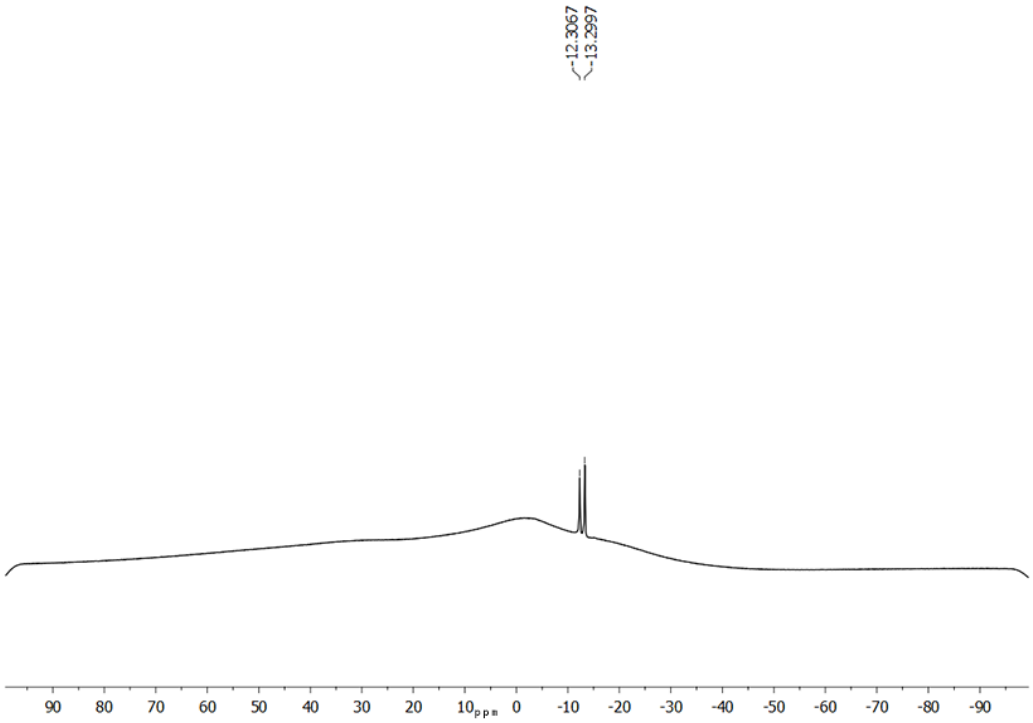

Figure S14. ^{11}B NMR of compound **2** in $CDCl_3$

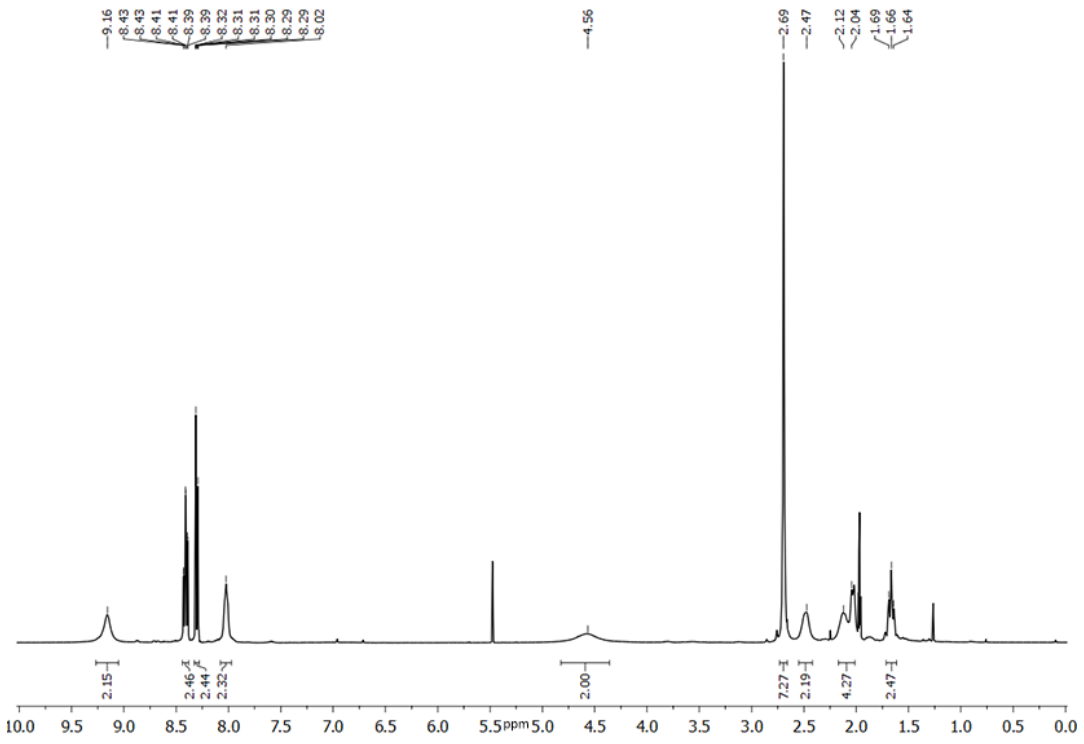

Figure S15. ^{1}H NMR of compound **3** in CD_3CN

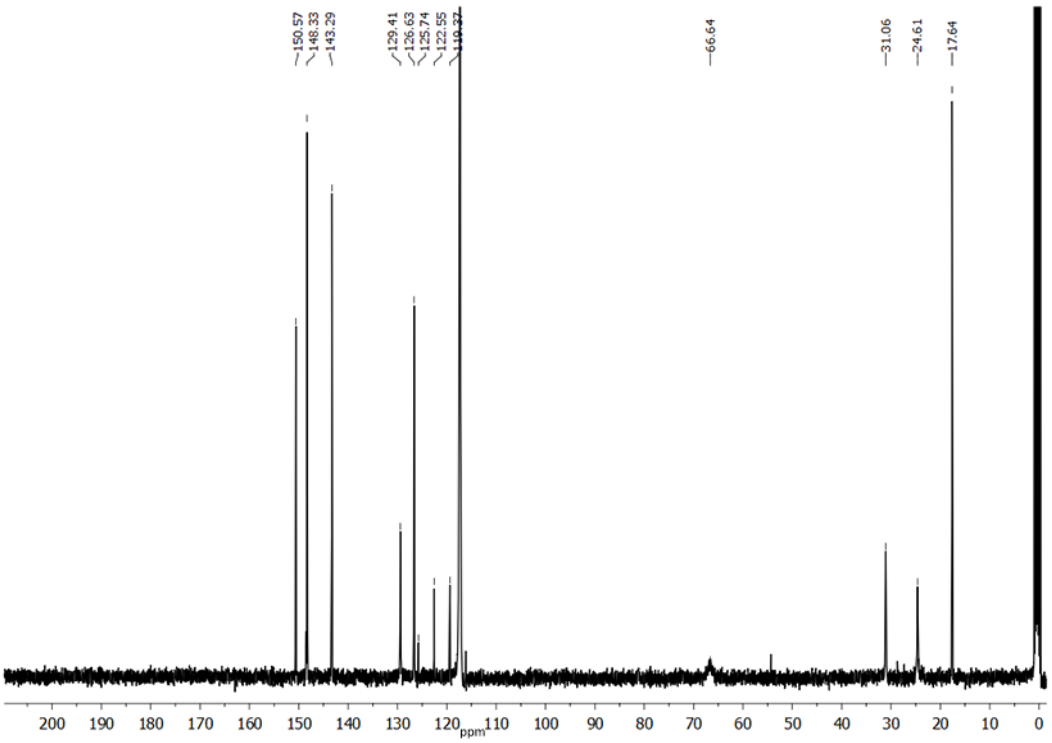

Figure S16. ^{13}C NMR of compound **3** in CD_3CN

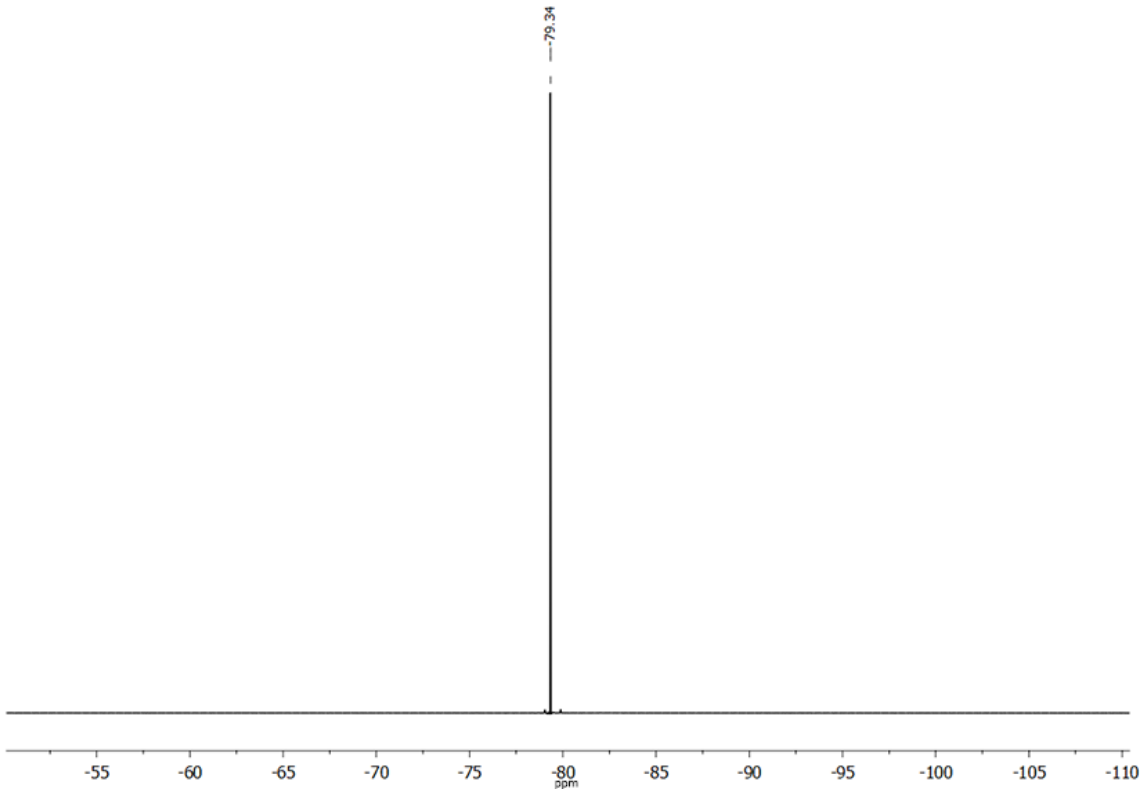

Figure S17. ^{19}F NMR of compound **3** in CD_3CN

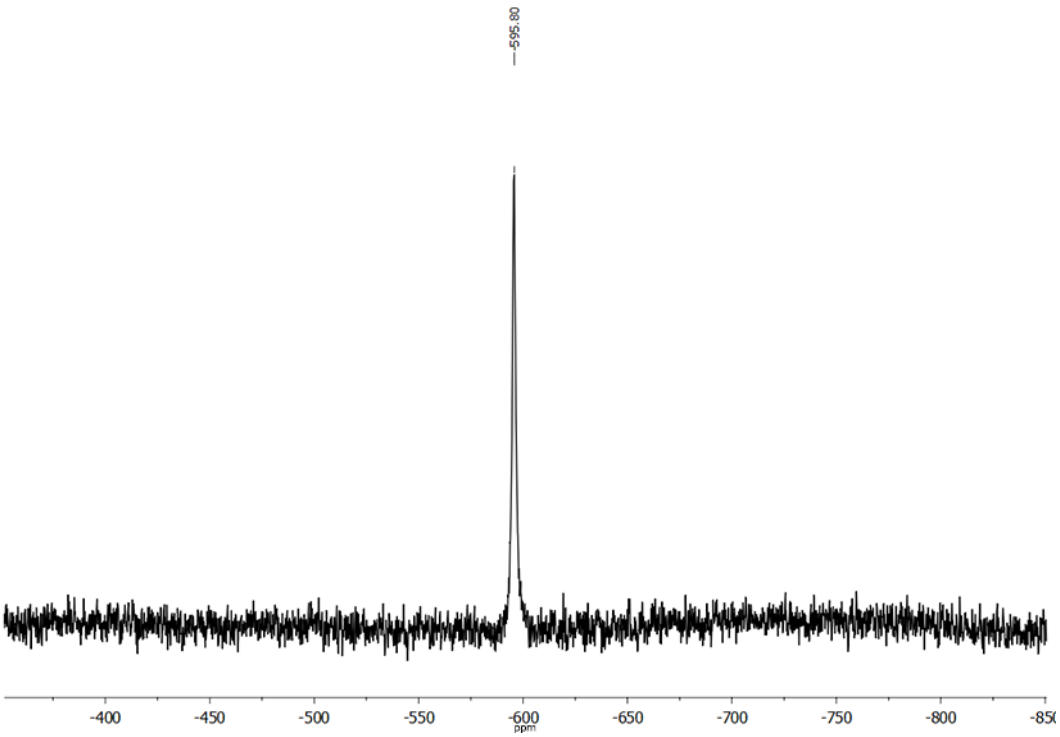

Figure S18. ^{119}Sn NMR of compound **3** in CD_3CN

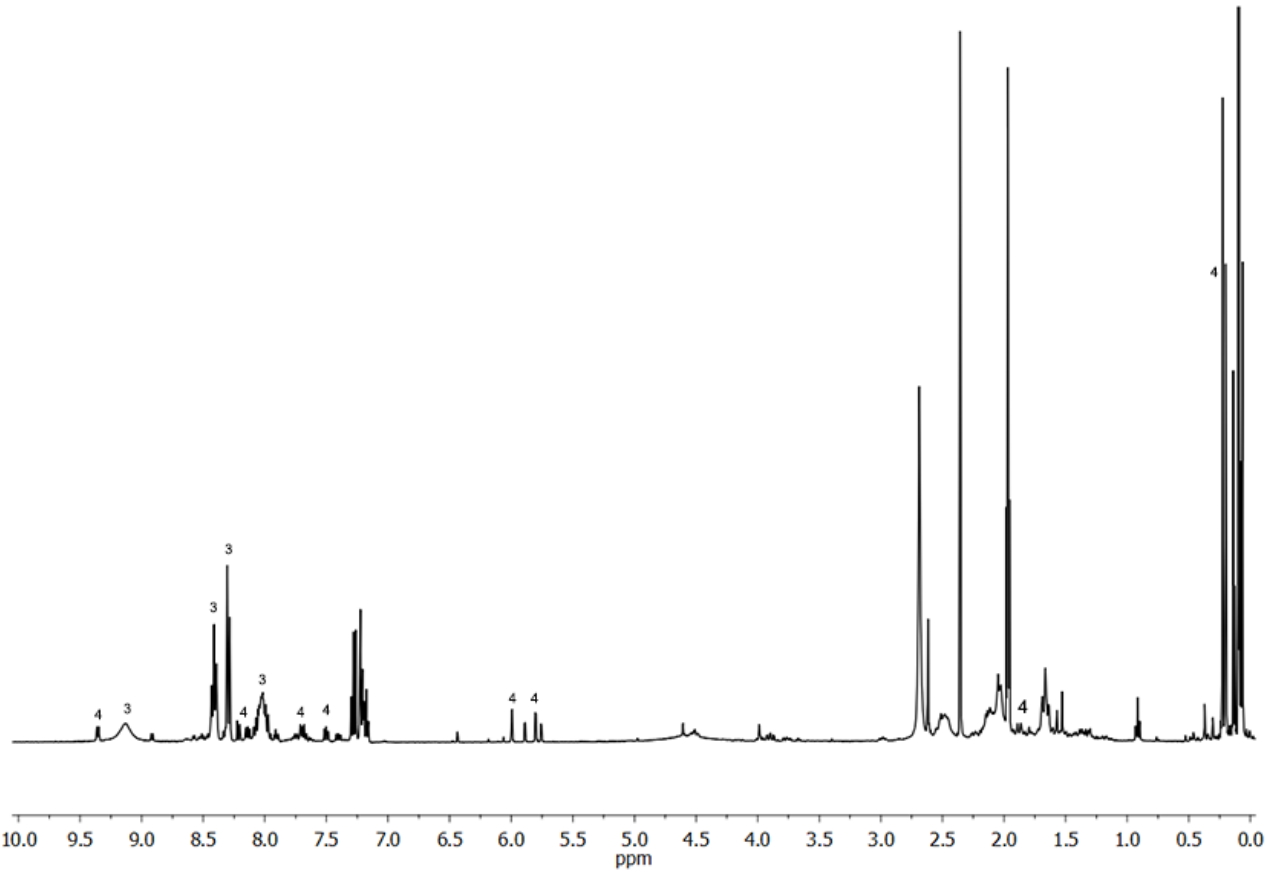

Figure S19. ^{1}H NMR of the mixture of **3** and **4** in CD_3CN

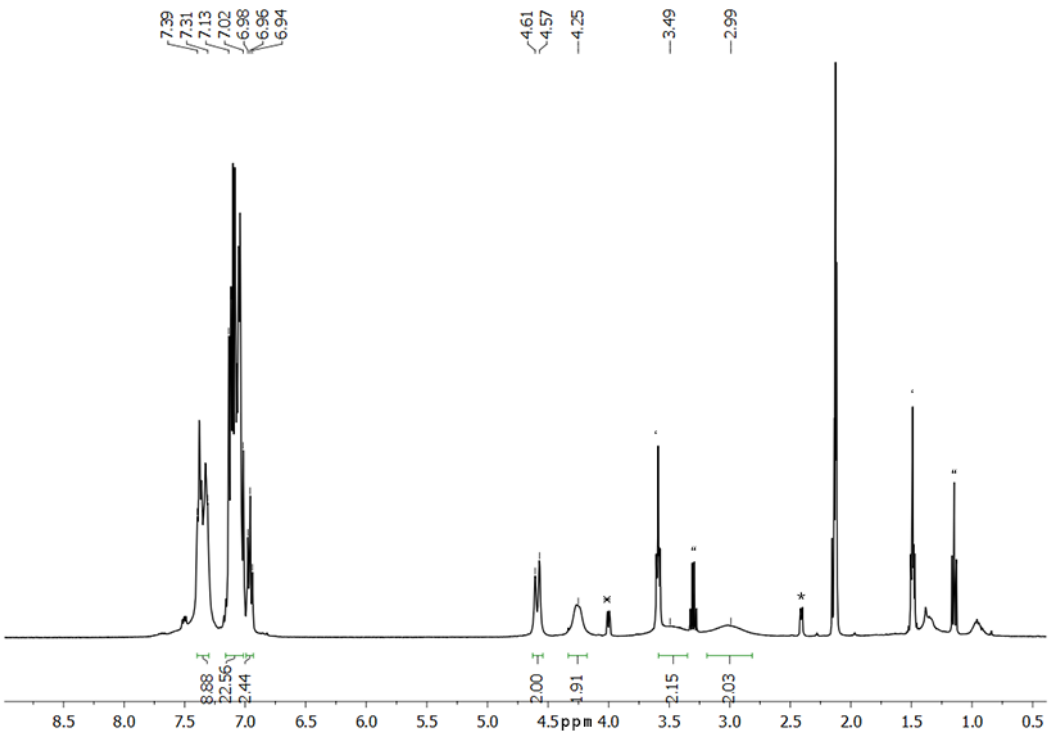

Figure S20. ^{1}H NMR of **5** in toluene-d_8 (* = L3, ‘ = Tetrahydrofuran, “ = Diethyl Ether)

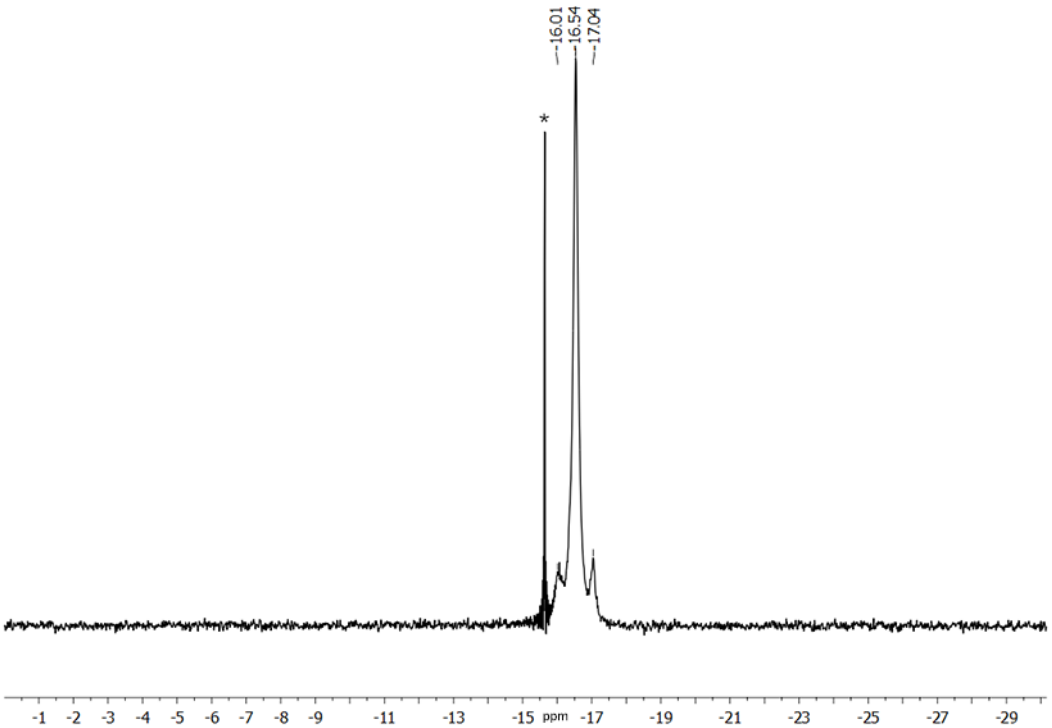

Figure S21. ^{31}P NMR of **5** in toluene-d_8 (* = L3)

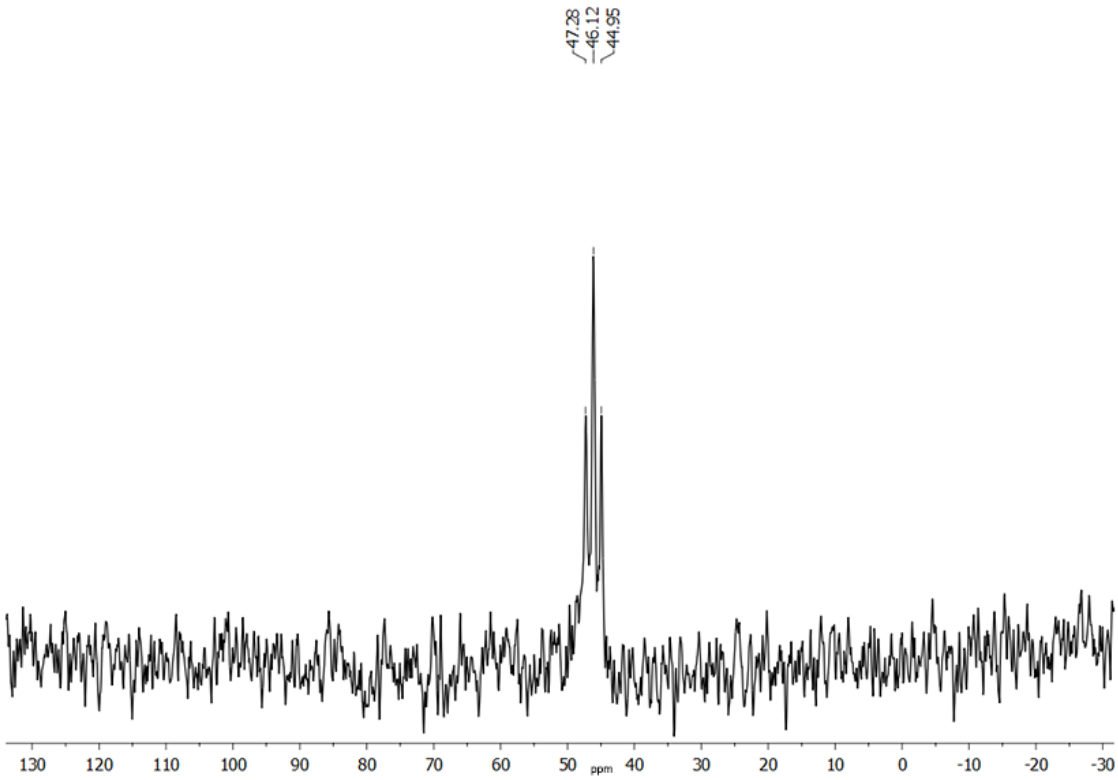

Figure S22. ^{119}Sn NMR of **5** in toluene-d_8

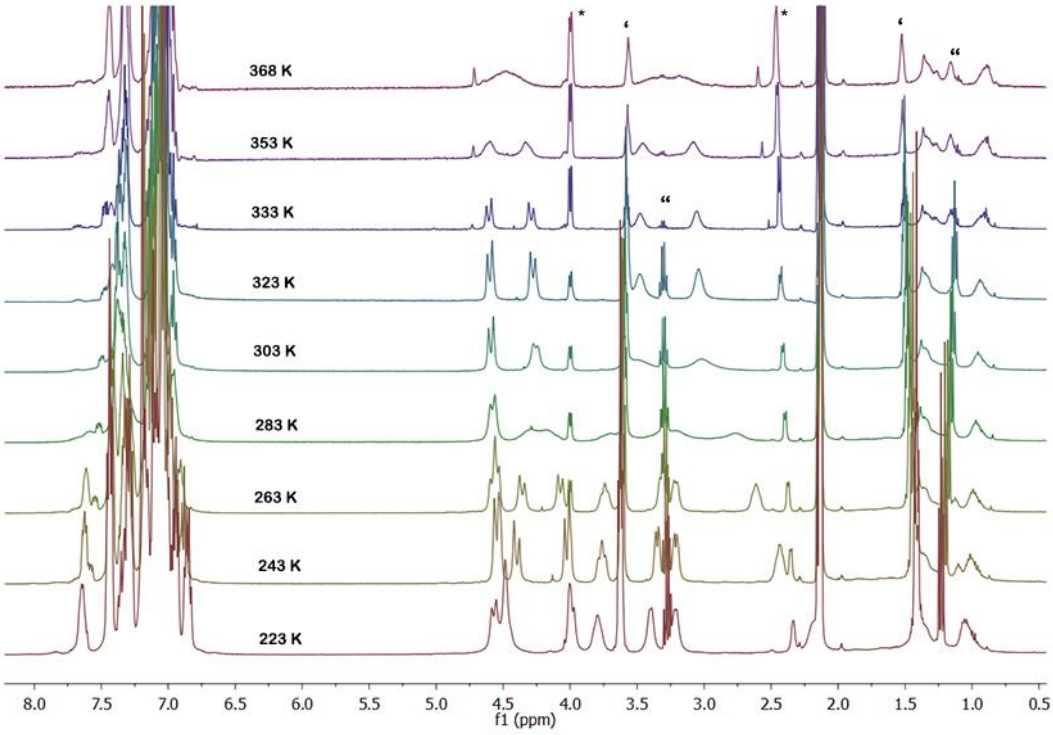

Figure S23. ^{1}H Variable Temperature NMR of **5** in toluene-d_8 (* = L3, ‘ = THF, “ = Diethyl Ether)

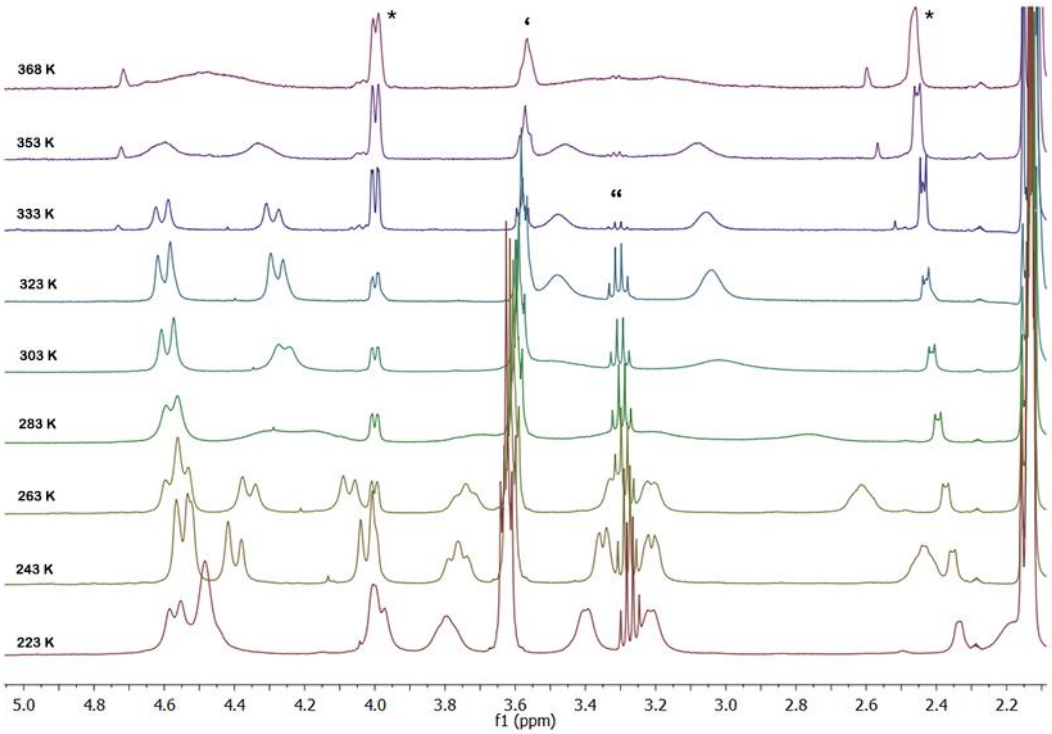

Figure S24. ^{1}H Variable Temperature NMR of **5** in toluene-d_8 (* = L3, ‘ = THF, “ = Diethyl Ether) (1.5 – 5 ppm scale has been zoomed)

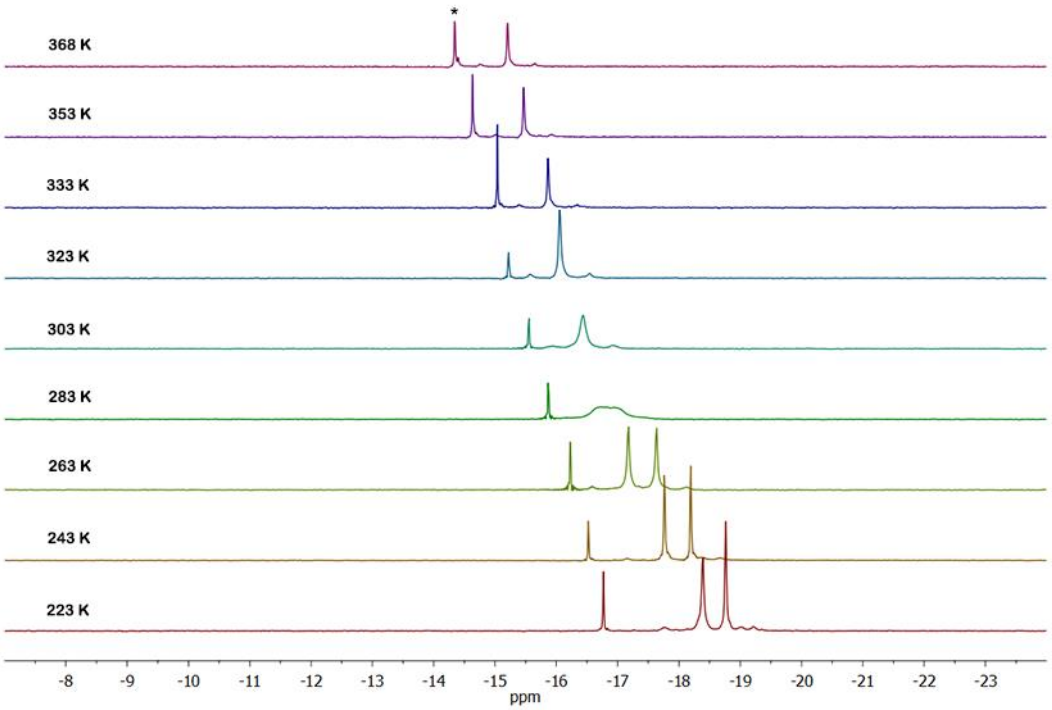

Figure S25 Variable Temperature ^{31}P NMR plots of **5** in toluene-d_8 (* = L3)

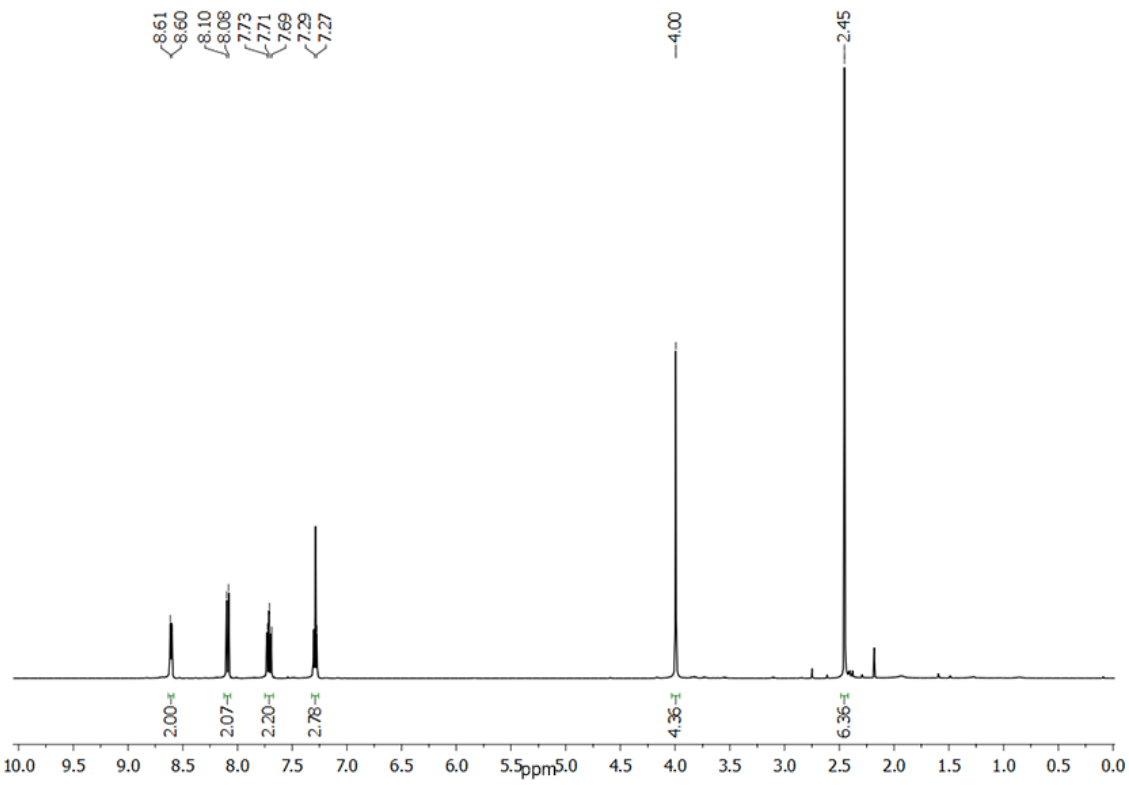

Figure S26. ^{1}H NMR in $CDCl_3$ of **L** obtained from the reaction between **L2** and $Sn[N(SiMe_3)_2]_2$

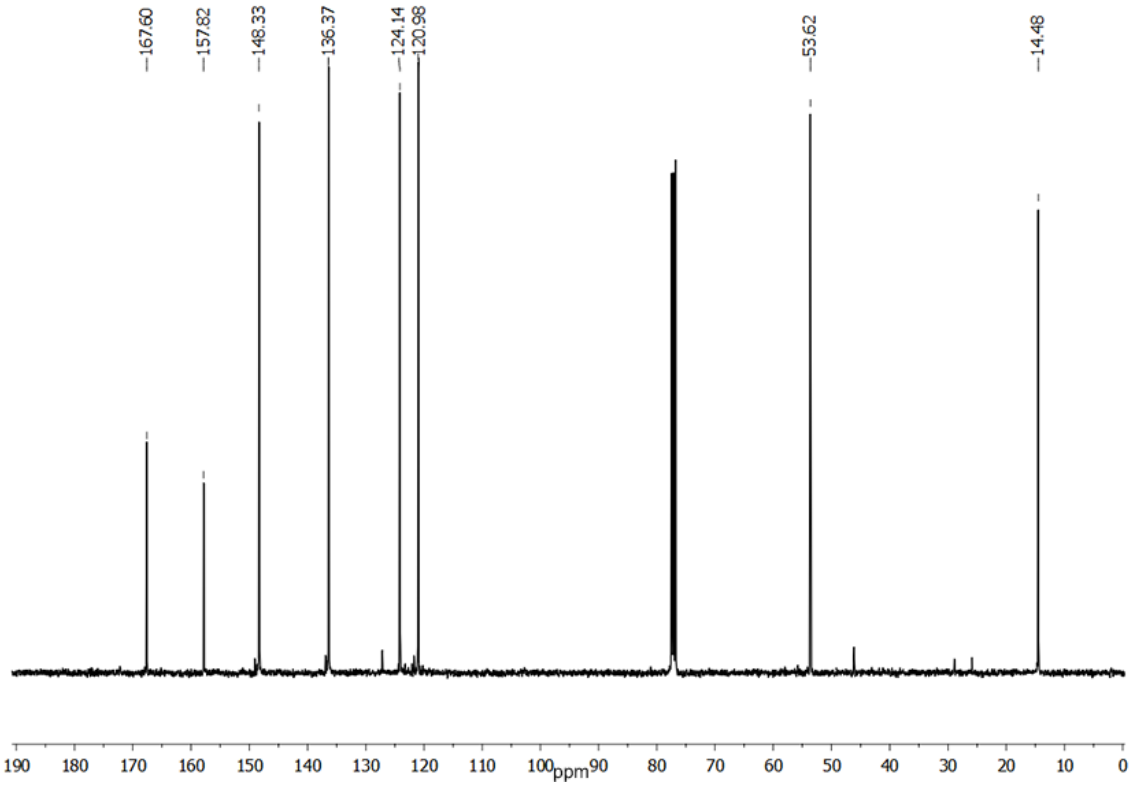

Figure S27. ^{13}C NMR in $CDCl_3$ of **L** obtained from the reaction between **L2** and $Sn[N(SiMe_3)_2]_2$

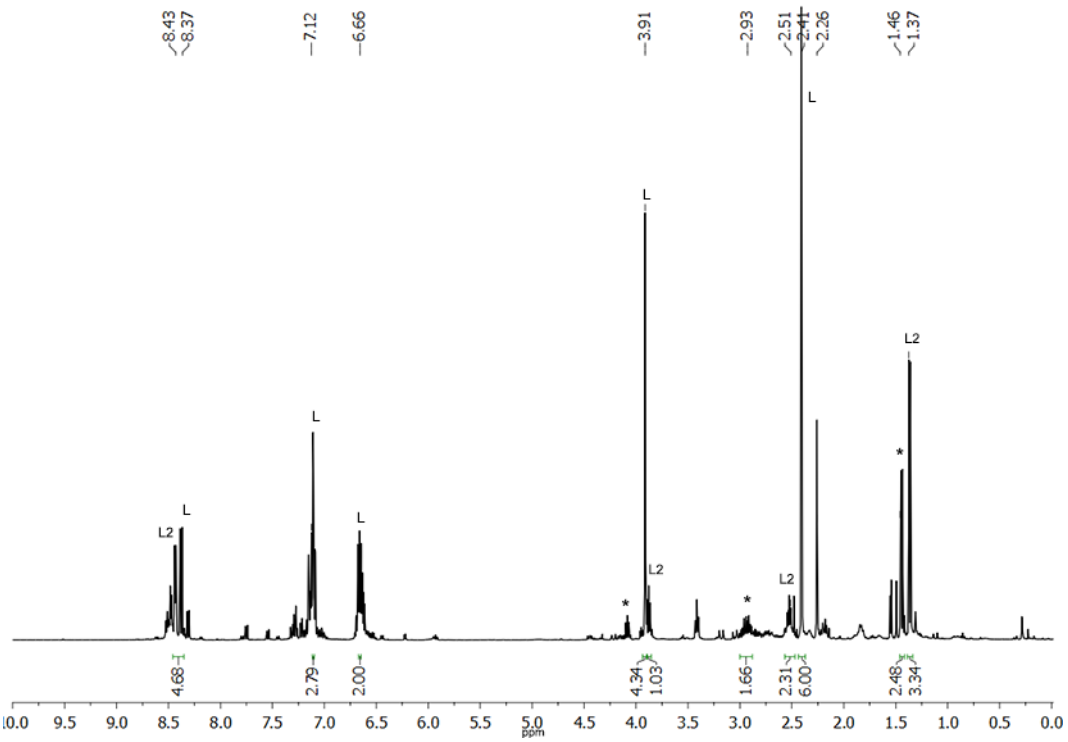

Figure S28. ^{1}H NMR in C_6D_6 of reaction mixture obtained after 4 days from the reaction between **L2** and $Sn[N(SiMe_3)_2]_2$ (* = stannylene)

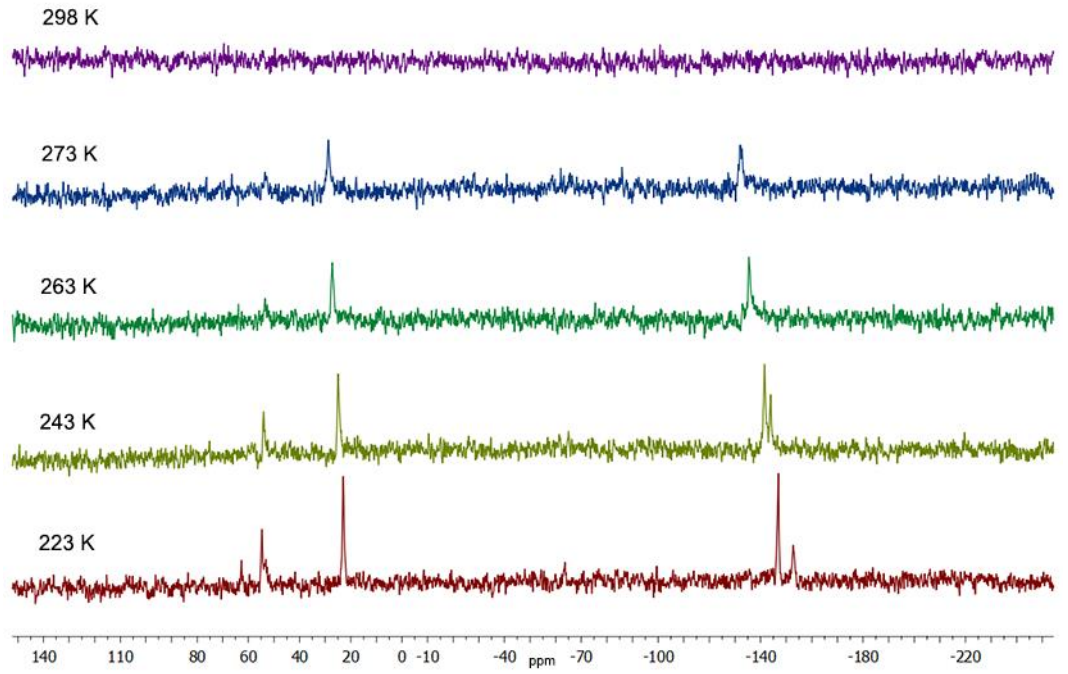

Figure S29. ^{119}Sn variable temperature NMR for the reaction between **L2** and $Sn[N(SiMe_3)_2]_2$

2. UV/Vis Spectra

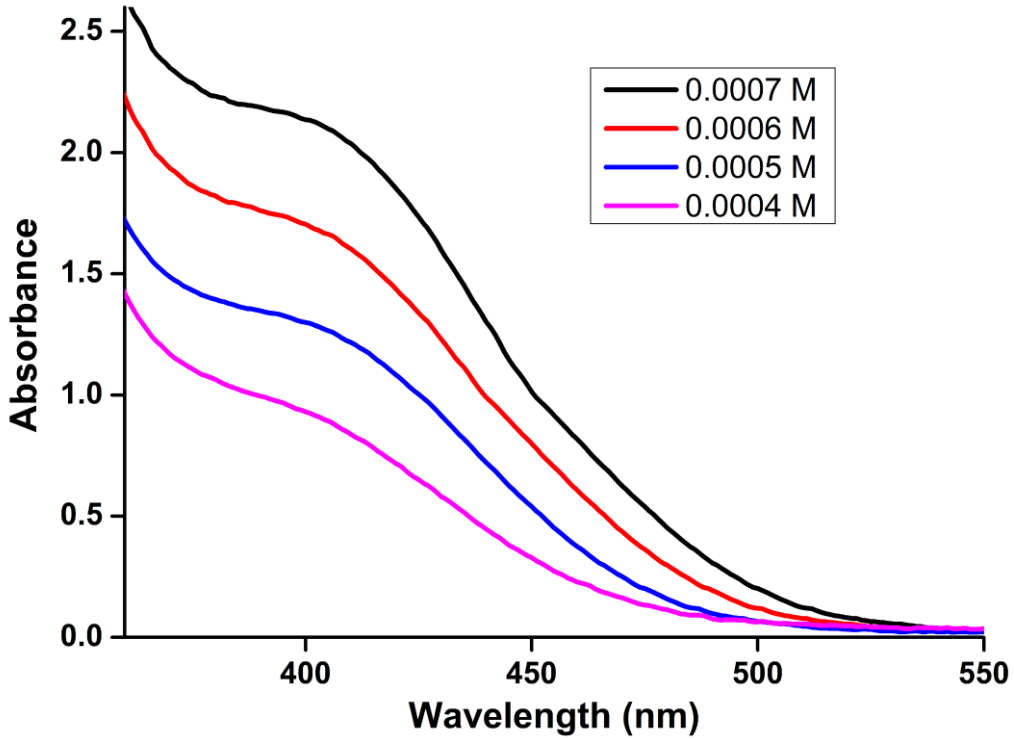

Figure S30. UV-Vis Spectra of **1** in Tetrahydrofuran

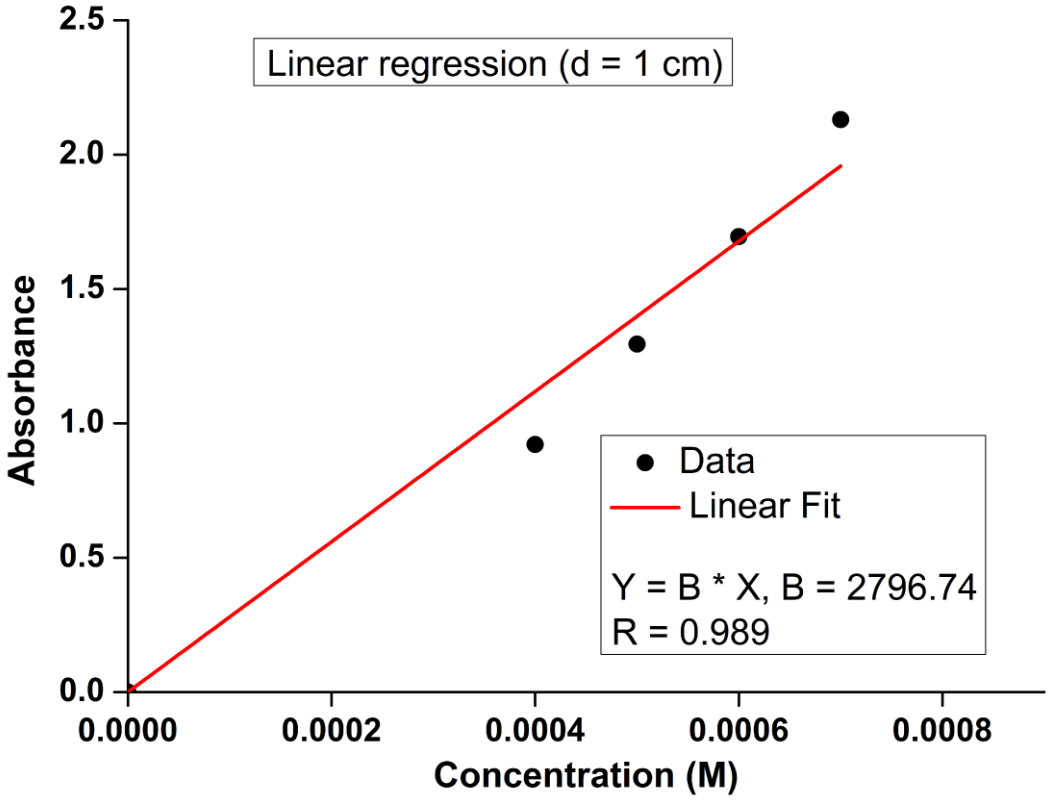

Figure S31. Linear Fit for UV-Vis data of **1**

3. DFT Calculations

DFT calculations were performed on the experimental structures **1** and **5** at the B3LYP level of theory (6-31G(d,p) basis set for C, N, H, Si, P) and LANL2DZ for Sn using *Gaussian 09* suite of programs.[S1] Compounds **1'** and **5'** were optimized at the stationary point with number of imaginary frequency NIMAG = 0. The monomer **5m** was optimized at the stationary point with number of imaginary frequency NIMAG = 0. The dissociation energy for the dimer **5'** were calculated in gas phase and in toluene, tetrahydrofuran and acetonitrile solvents using the Polarization Continumm Model (PCM).

Cartesian coordinated of the optimized structure **1'**

Sn	-1.90600400	0.23101200	-0.75255900
Sn	1.99101000	-0.14546900	-0.88792500
Si	5.01264400	0.76301600	0.67299700
Si	-4.32898600	2.29637500	-0.00429000
Si	4.54639800	-2.07585500	-0.27374700
Si	-4.62697800	-0.37134800	1.39609800
N	-1.00423800	-1.45200900	0.30885700
N	0.86050000	0.86152100	0.68072700
N	2.12390300	2.11445000	-1.29848100
N	3.93648200	-0.43121800	-0.05207700
N	-3.72580000	0.66276800	0.28744800
N	-2.68200400	-1.69863700	-1.75191900
C	0.26470700	0.13637100	1.80752000
H	-0.68451500	0.62825500	2.08318900
C	0.16959500	3.01406700	1.64715500
H	-0.26893100	2.60060600	2.54387200
H	0.13244000	4.08998100	1.55932100
C	0.76558700	2.23566100	0.69681700
C	1.88294500	4.79444000	-1.90700200
H	1.77339200	5.84821500	-2.14455000
C	-0.23135300	-3.76750800	-0.03005400
H	0.50357800	-3.76723500	0.76143400
H	-0.28779300	-4.67407400	-0.61461800
C	-1.02496700	-2.68994900	-0.30594500
C	1.24165400	4.26578100	-0.79652500
H	0.62358500	4.90031900	-0.17618100
C	2.66012400	3.96185900	-2.72064000
H	3.17631000	4.33890600	-3.59616000
C	-0.66777500	-2.04206600	2.69472100
H	-1.61060400	-1.54622200	2.95293700
H	-0.92156900	-3.07210600	2.42968600
C	-2.04035600	-2.82880700	-1.39032400
C	-0.08830100	-1.32665700	1.44766800
H	0.87039300	-1.82006400	1.19441200
C	1.20287600	0.15892000	3.03978500
H	2.14790600	-0.31424700	2.74394500
H	1.43799500	1.19898500	3.28526200
C	-4.20432200	0.00790200	3.21046200
H	-3.12393600	-0.01046600	3.38675600
H	-4.66354000	-0.72668900	3.88307000
H	-4.56380900	0.99813400	3.50731400
C	2.74061600	2.62245600	-2.38274700
H	3.30681000	1.91581700	-2.98286600
C	1.38415100	2.90254600	-0.48536100
C	-3.63441200	-1.71026400	-2.70137500
H	-4.09908900	-0.75316800	-2.92153600

C	-2.38222800	-4.04101600	-2.01554900
H	-1.89958300	-4.96144600	-1.71664700
C	3.53641200	-3.07680900	-1.53760200
H	2.50269300	-3.27444000	-1.23570400
H	4.03299300	-4.04945600	-1.65154700
H	3.50752500	-2.60871900	-2.52736700
C	0.62838100	-0.56514900	4.26278300
H	-0.27348500	-0.04323200	4.61348400
H	1.34831000	-0.53224900	5.08943500
C	0.26989100	-2.01099500	3.90618300
H	1.18968700	-2.56970000	3.68088700
H	-0.20119800	-2.51792100	4.75697000
C	-4.34710600	-2.22467900	1.12128900
H	-4.69949500	-2.54564000	0.13553800
H	-4.93192300	-2.77414900	1.86914300
H	-3.30359000	-2.52463100	1.22736600
C	-3.01419300	3.45011500	-0.74938800
H	-2.10528000	3.48874600	-0.13984000
H	-3.43870200	4.46200400	-0.78393100
H	-2.72152600	3.18267700	-1.76923100
C	-4.88684900	3.18092000	1.58234700
H	-5.71531700	2.68797900	2.09832700
H	-5.21443700	4.19893600	1.33844500
H	-4.05583800	3.26385300	2.29152400
C	4.14733500	2.24767300	1.47300800
H	3.75890800	2.96514400	0.74646900
H	4.89347700	2.77881700	2.07681900
H	3.32860400	1.96277300	2.13700400
C	6.07669300	0.04048900	2.07654500
H	5.44865800	-0.28897000	2.91183900
H	6.74605800	0.82091300	2.45866200
H	6.70113200	-0.80560100	1.77763200
C	6.32422800	-2.13193600	-0.94663800
H	6.38315600	-1.65382500	-1.93093300
H	6.63082500	-3.17753600	-1.07215500
H	7.06404900	-1.65164600	-0.30026100
C	-3.36275300	-4.05975800	-2.99648300
H	-3.63071000	-4.99669200	-3.47554400
C	-4.01073600	-2.87141500	-3.35404800
H	-4.78787200	-2.85030800	-4.10969800
C	-6.51428000	-0.17520500	1.21920700
H	-6.88484900	0.83252700	1.42728900
H	-7.00801900	-0.85358600	1.92618400
H	-6.84904600	-0.45369000	0.21377800
C	4.48055500	-3.08150000	1.33661600
H	5.10748500	-2.65794100	2.12632200
H	4.81305400	-4.11228600	1.16345200
H	3.45447800	-3.12751100	1.72038200
C	6.19068600	1.49733800	-0.62834900
H	6.82384200	0.73536700	-1.09225600
H	6.84934200	2.24926900	-0.17675200
H	5.63059300	1.99372200	-1.42969200
C	-5.77248300	2.31347400	-1.24245400
H	-5.46051700	1.88482000	-2.20282400
H	-6.10469800	3.34072900	-1.43651700
H	-6.63865800	1.74426500	-0.89355600

Time Dependent DFT Calculations of **1'**

```
 Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      2.3580 eV  525.81 nm  f=0.0030
<S**2>=0.000
     178 ->179         0.69865
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2746.92641360
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:      Singlet-A      2.7054 eV  458.28 nm  f=0.0264
<S**2>=0.000
     177 ->179         0.57394
     178 ->180         0.38002

 Excited State   3:      Singlet-A      2.7273 eV  454.60 nm  f=0.0477
<S**2>=0.000
     177 ->179        -0.38336
     178 ->180         0.56739
     178 ->182        -0.12465

 Excited State   4:      Singlet-A      2.9196 eV  424.66 nm  f=0.0189
<S**2>=0.000
     176 ->179         0.69263

 Excited State   5:      Singlet-A      2.9759 eV  416.63 nm  f=0.0049
<S**2>=0.000
     177 ->180         0.17901
     178 ->180         0.13550
     178 ->181         0.20399
     178 ->182         0.63292

 Excited State   6:      Singlet-A      3.0128 eV  411.53 nm  f=0.0040
<S**2>=0.000
     177 ->181         0.15119
     178 ->181         0.64777
     178 ->182        -0.20297

 Excited State   7:      Singlet-A      3.1234 eV  396.95 nm  f=0.0249
<S**2>=0.000
     177 ->180         0.66888
     178 ->182        -0.17884

 Excited State   8:      Singlet-A      3.2549 eV  380.92 nm  f=0.0214
<S**2>=0.000
     177 ->181         0.66563
     178 ->181        -0.15531

 Excited State   9:      Singlet-A      3.4178 eV  362.76 nm  f=0.0066
<S**2>=0.000
     176 ->180         0.62996
     177 ->182         0.28347

 Excited State  10:      Singlet-A      3.4397 eV  360.45 nm  f=0.0064
<S**2>=0.000
     176 ->180        -0.27491
     176 ->182        -0.13562
```

```
     177 ->182         0.62404

 Excited State  11:      Singlet-A      3.4535 eV  359.01 nm  f=0.0098
<S**2>=0.000
     174 ->179         0.53599
     175 ->179         0.43738
     176 ->180        -0.11394

 Excited State  12:      Singlet-A      3.4906 eV  355.19 nm  f=0.0003
<S**2>=0.000
     174 ->179        -0.44417
     175 ->179         0.54695

 Excited State  13:      Singlet-A      3.5606 eV  348.21 nm  f=0.0012
<S**2>=0.000
     176 ->181         0.69244

 Excited State  14:      Singlet-A      3.7746 eV  328.47 nm  f=0.0013
<S**2>=0.000
     175 ->180         0.67311
     178 ->183        -0.19413

 Excited State  15:      Singlet-A      3.7786 eV  328.12 nm  f=0.0024
<S**2>=0.000
     175 ->180         0.15340
     176 ->182        -0.33801
     178 ->183         0.58673

 Excited State  16:      Singlet-A      3.7974 eV  326.49 nm  f=0.0016
<S**2>=0.000
     175 ->180         0.12495
     176 ->182         0.59736
     177 ->182         0.11696
     178 ->183         0.32785

 Excited State  17:      Singlet-A      3.8753 eV  319.93 nm  f=0.0384
<S**2>=0.000
     173 ->179         0.68678

 Excited State  18:      Singlet-A      4.0377 eV  307.07 nm  f=0.0142
<S**2>=0.000
     173 ->180         0.13360
     174 ->180         0.48056
     177 ->183         0.48502

 Excited State  19:      Singlet-A      4.0454 eV  306.48 nm  f=0.0046
<S**2>=0.000
     173 ->180        -0.11864
     174 ->180        -0.46800
     177 ->183         0.50509

 Excited State  20:      Singlet-A      4.1125 eV  301.48 nm  f=0.0028
<S**2>=0.000
     174 ->181         0.44416
     175 ->181         0.51603
     175 ->182         0.17145
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370.
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Cartesian Coordinates of optimized structure 5'

Sn	-0.33149300	1.42124100	0.94841600
P	1.33389100	3.51458800	4.18394200
P	-4.38614100	-2.25113900	2.50627500
N	-0.20532700	-0.81019900	1.25889000
N	1.59335200	1.28730100	1.70170300
C	0.55457600	2.08060000	5.05986300
C	3.10709200	2.98325100	4.01516000
C	-0.84868400	2.00642500	5.03485100
H	-1.41564800	2.77695000	4.51822100
C	-1.68948300	-2.86743400	1.81461500
C	2.62548400	2.30496800	1.57423200
H	2.13529200	3.26965700	1.39779700
H	3.27106300	2.12066000	0.69593400
C	-5.84941400	-3.36519300	2.26656600
C	4.03094200	3.13479200	5.06133100
H	3.70466700	3.57327700	5.99911700
C	-2.95655900	-3.39936500	2.17985800
C	3.54701100	2.44367100	2.78322900
C	-4.34971900	-2.04549000	4.34787700
C	-0.80106900	-0.05445900	6.30043700
H	-1.32746900	-0.87950000	6.77008900
C	1.26659500	1.06370100	5.71394500
H	2.35094400	1.09566400	5.74061700
C	0.92615200	-0.99598800	2.21002900
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C	-1.48291400	-1.35022800	1.78015500
H	-2.29768200	-0.92790200	1.18138500
H	-1.63682200	-0.96579400	2.80211500
C	-3.13217600	-4.79166500	2.20944400
H	-4.10247600	-5.19717200	2.47641500
C	-0.85905500	-5.14895000	1.51672800
H	-0.03977100	-5.80990400	1.24886100
C	-0.66682100	-3.76600000	1.48688500
H	0.30419100	-3.38925300	1.19191800
C	2.08620200	-0.07043400	1.85227300
H	2.83408500	-0.13432500	2.65709600
H	2.59641900	-0.44498100	0.93904400
C	1.44797200	4.78130800	5.53749600
C	0.59347000	0.00395900	6.32703200
H	1.16187800	-0.77649400	6.82629400
C	1.82090600	6.08341700	5.15919500
H	2.04760400	6.29425000	4.11667100
C	-6.62607100	-3.88710600	3.31175200
H	-6.35147100	-3.68823900	4.34229200
C	4.88523800	2.04595300	2.66227800
H	5.21919700	1.61801100	1.71966400
C	-2.09552400	-5.66753200	1.88643000
H	-2.26025300	-6.74073500	1.91781400
C	-5.05622300	-0.95432500	4.88285700
H	-5.56753500	-0.26765000	4.21274900
C	-6.23825300	-3.63856900	0.94263800
H	-5.65884100	-3.23759900	0.11511700
C	-3.68025900	-2.90765800	5.22980700
H	-3.12294200	-3.75262600	4.83793200
C	1.13373200	4.54423700	6.88453400
H	0.83328600	3.55081000	7.20191100
C	5.36249100	2.74050700	4.91906300

H	6.05601700	2.86592700	5.74608400
C	-1.52239200	0.95272600	5.65444300
H	-2.60693100	0.90762000	5.62611800
C	5.79114000	2.18627000	3.71459900
H	6.82273400	1.86819900	3.59060200
C	1.20109400	5.57541500	7.82534100
H	0.95216700	5.37216700	8.86357400
C	-5.11174600	-0.74285900	6.26134200
H	-5.67007900	0.10100300	6.65700100
C	-4.44575400	-1.61227600	7.12890000
H	-4.48446200	-1.44791000	8.20199900
C	1.90098600	7.10940500	6.09948700
H	2.19701000	8.10701500	5.78651000
C	-3.72771100	-2.69162900	6.60927400
H	-3.20805600	-3.37216300	7.27854300
C	-7.75527600	-4.66453200	3.04033000
H	-8.34533700	-5.05859900	3.86339800
C	1.58847400	6.85838400	7.43799300
H	1.64083100	7.65873200	8.17080100
C	-8.12183100	-4.93936500	1.72297000
H	-8.99903000	-5.54524900	1.51433500
C	-7.35608700	-4.42606200	0.67294900
H	-7.63331300	-4.63137800	-0.35724700
Sn	0.33149300	-1.42124100	-0.94841600
P	-1.33389100	-3.51458800	-4.18394200
P	4.38614100	2.25113900	-2.50627500
N	0.20532700	0.81019900	-1.25889000
N	-1.59335200	-1.28730100	-1.70170300
C	-0.55457600	-2.08060000	-5.05986300
C	-3.10709200	-2.98325100	-4.01516000
C	0.84868400	-2.00642500	-5.03485100
H	1.41564800	-2.77695000	-4.51822100
C	1.68948300	2.86743400	-1.81461500
C	-2.62548400	-2.30496800	-1.57423200
H	-2.13529200	-3.26965700	-1.39779700
H	-3.27106300	-2.12066000	-0.69593400
C	5.84941400	3.36519300	-2.26656600
C	-4.03094200	-3.13479200	-5.06133100
H	-3.70466700	-3.57327700	-5.99911700
C	2.95655900	3.39936500	-2.17985800
C	-3.54701100	-2.44367100	-2.78322900
C	4.34971900	2.04549000	-4.34787700
C	0.80106900	0.05445900	-6.30043700
H	1.32746900	0.87950000	-6.77008900
C	-1.26659500	-1.06370100	-5.71394500
H	-2.35094400	-1.09566400	-5.74061700
C	-0.92615200	0.99598800	-2.21002900
H	-1.28643400	2.03209000	-2.22606300
H	-0.58329700	0.75920700	-3.22710600
C	1.48291400	1.35022800	-1.78015500
H	2.29768200	0.92790200	-1.18138500
H	1.63682200	0.96579400	-2.80211500
C	3.13217600	4.79166500	-2.20944400
H	4.10247600	5.19717200	-2.47641500
C	0.85905500	5.14895000	-1.51672800
H	0.03977100	5.80990400	-1.24886100
C	0.66682100	3.76600000	-1.48688500
H	-0.30419100	3.38925300	-1.19191800
C	-2.08620200	0.07043400	-1.85227300
H	-2.83408500	0.13432500	-2.65709600

H	-2.59641900	0.44498100	-0.93904400
C	-1.44797200	-4.78130800	-5.53749600
C	-0.59347000	-0.00395900	-6.32703200
H	-1.16187800	0.77649400	-6.82629400
C	-1.82090600	-6.08341700	-5.15919500
H	-2.04760400	-6.29425000	-4.11667100
C	6.62607100	3.88710600	-3.31175200
H	6.35147100	3.68823900	-4.34229200
C	-4.88523800	-2.04595300	-2.66227800
H	-5.21919700	-1.61801100	-1.71966400
C	2.09552400	5.66753200	-1.88643000
H	2.26025300	6.74073500	-1.91781400
C	5.05622300	0.95432500	-4.88285700
H	5.56753500	0.26765000	-4.21274900
C	6.23825300	3.63856900	-0.94263800
H	5.65884100	3.23759900	-0.11511700
C	3.68025900	2.90765800	-5.22980700
H	3.12294200	3.75262600	-4.83793200
C	-1.13373200	-4.54423700	-6.88453400
H	-0.83328600	-3.55081000	-7.20191100
C	-5.36249100	-2.74050700	-4.91906300
H	-6.05601700	-2.86592700	-5.74608400
C	1.52239200	-0.95272600	-5.65444300
H	2.60693100	-0.90762000	-5.62611800
C	-5.79114000	-2.18627000	-3.71459900
H	-6.82273400	-1.86819900	-3.59060200
C	-1.20109400	-5.57541500	-7.82534100
H	-0.95216700	-5.37216700	-8.86357400
C	5.11174600	0.74285900	-6.26134200
H	5.67007900	-0.10100300	-6.65700100
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H	4.48446200	1.44791000	-8.20199900
C	-1.90098600	-7.10940500	-6.09948700
H	-2.19701000	-8.10701500	-5.78651000
C	3.72771100	2.69162900	-6.60927400
H	3.20805600	3.37216300	-7.27854300
C	7.75527600	4.66453200	-3.04033000
H	8.34533700	5.05859900	-3.86339800
C	-1.58847400	-6.85838400	-7.43799300
H	-1.64083100	-7.65873200	-8.17080100
C	8.12183100	4.93936500	-1.72297000
H	8.99903000	5.54524900	-1.51433500
C	7.35608700	4.42606200	-0.67294900
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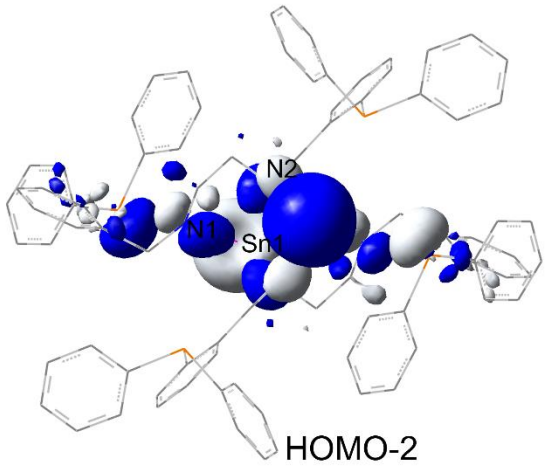
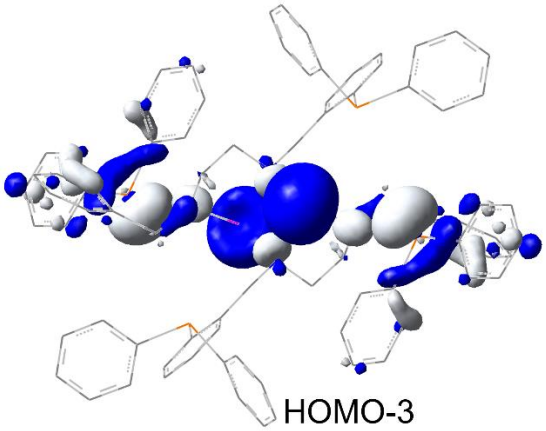
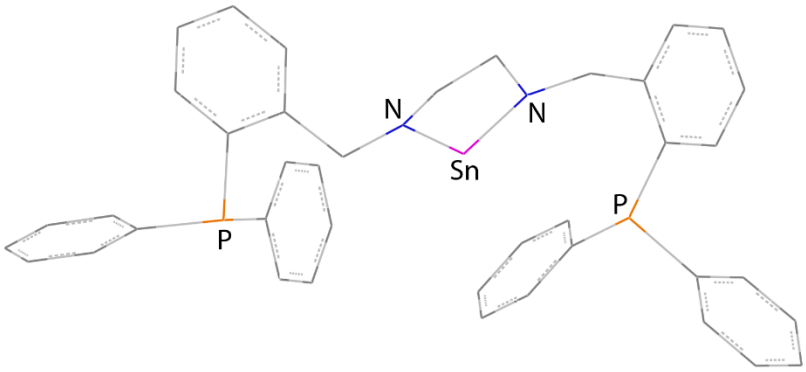
Contour Plots of 5' at 0.03 a.u.





Cartesian Coordinates of optimized structure 5m



Optimized structure 5m

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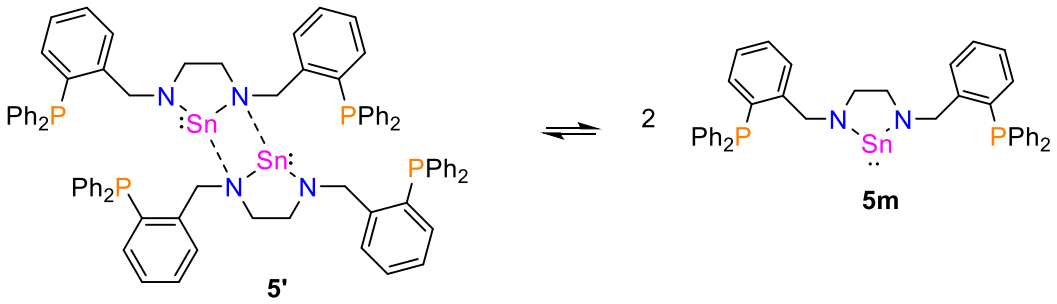
N	-0.49594800	-1.70552200	-0.31787900
N	2.07859600	-2.24696700	0.12587800
C	2.74856400	1.29862300	-0.23653800
C	4.67833600	-0.57143600	0.91267800
C	1.97097300	1.81483500	-1.28879300
H	2.23156600	1.57427700	-2.31713700
C	-3.01108200	-1.80336900	-0.13288600
C	3.43614100	-2.74021100	0.28598500
H	3.91047000	-2.76550400	-0.70275300
H	3.44074300	-3.77777900	0.66350300
C	-6.25274200	0.85922800	-0.75335600
C	5.49708100	0.12906600	1.81220700
H	5.81189800	1.13916600	1.56962900
C	-4.27208300	-1.15834600	-0.08338400
C	4.29978900	-1.90014200	1.22289500
C	-3.91218400	1.60517300	0.75341900
C	0.51367200	2.93519200	0.28346900
H	-0.35934800	3.54744600	0.48832700

C	2.38867400	1.62147800	1.08042200
H	2.97094000	1.23254400	1.90948500
C	-0.06423000	-1.55484000	1.07682400
H	-0.84219900	-1.90336900	1.77092500
H	0.11710100	-0.49069000	1.30347600
C	-1.76184200	-1.06809500	-0.63026700
H	-1.85069900	-0.95911900	-1.72084200
H	-1.77203100	-0.04063200	-0.23158600
C	-5.39147500	-1.88760900	0.34666700
H	-6.36236000	-1.40524200	0.38267800
C	-4.04183600	-3.85676500	0.67757000
H	-3.94348300	-4.89963800	0.96717500
C	-2.92036700	-3.14455800	0.25022600
H	-1.94726200	-3.62294600	0.19954200
C	1.21936000	-2.35946100	1.30487800
H	1.72916100	-1.98280500	2.20296100
H	0.97102100	-3.41937800	1.50354200
C	5.51991200	1.38075200	-1.03562400
C	1.27960100	2.43205800	1.33638900
H	1.00878900	2.66461500	2.36269300
C	6.66482500	0.87895500	-1.67880800
H	6.71320200	-0.17491000	-1.94247600
C	-7.01053400	1.33808400	0.32710500
H	-6.52433800	1.55403900	1.27321300
C	4.74169400	-2.46503000	2.42549500
H	4.45169300	-3.48650600	2.66058900
C	-5.28278700	-3.22619700	0.72737700
H	-6.16464300	-3.76718600	1.05936700
C	-3.71240700	2.98064700	0.54080900
H	-3.86986100	3.39768500	-0.45103200
C	-6.90780700	0.60042000	-1.96925800
H	-6.33259300	0.24928400	-2.82234100
C	-3.68527400	1.08680200	2.03721700
H	-3.83117500	0.02696100	2.22136600
C	5.47051300	2.75016000	-0.73252200
H	4.59289100	3.16370200	-0.24591000
C	5.92636800	-0.44973100	3.00779000
H	6.55678200	0.11639000	3.68786200
C	0.86767500	2.63004000	-1.03295900
H	0.27846800	3.01637900	-1.85992800
C	5.54519700	-1.75354800	3.31737100
H	5.87286700	-2.21769700	4.24349600
C	6.54023100	3.58980500	-1.05319600
H	6.48376800	4.64796500	-0.81213800
C	-3.31800100	3.81700700	1.58515500
H	-3.18188300	4.87999100	1.40466600
C	-3.09269100	3.28712700	2.85883900
H	-2.77815200	3.93540800	3.67194300
C	7.73748800	1.71417900	-1.98797800
H	8.61548400	1.30581100	-2.48084700
C	-3.27347100	1.92120600	3.07974900
H	-3.10000500	1.50204500	4.06722300
C	-8.38544500	1.54340000	0.19601500
H	-8.95676300	1.91691700	1.04157600
C	7.67701600	3.07485700	-1.67726200
H	8.50767900	3.72928500	-1.92604300
C	-9.02577300	1.26889800	-1.01387400
H	-10.09552000	1.42980700	-1.11392200
C	-8.28348900	0.79410900	-2.09712200
H	-8.77299000	0.58483400	-3.04424100

Dissociation Energy of the Dimer 5'



Medium	$E_{5'}$ (in Hartrees)	E_{5m} (in Hartrees)	ΔE (in Hartrees)	ΔE (in Kcal/mol)
Gas-phase	-4683.1152923	-2341.5438911	0.0275101	17.3
Toluene	-4683.1242152	-2341.5487781	0.026659	16.7
Tetrahydrofuran	-4683.1318814	-2341.5529881	0.0259052	16.3
Acetonitrile	-4683.135949	-2341.5552483	0.0254524	16.0

4. X-ray Data

Experimental Detail

Single-crystal data was collected on a Bruker SMART APEX four-circle diffractometer equipped with a CMOS photon 100 detector (Bruker Systems Inc.) and with a Cu Kα radiation (1.5418 Å). The incident X-ray beam was focused and monochromated using Microfocus (IμS). Crystals were mounted on nylon Cryo loops with Paratone-N oil. Data was collected at 100(2) K. Data was integrated using Bruker SAINT software and was corrected for absorption using SADABS. Structure was solved by Intrinsic Phasing module of the Direct methods and refined using the SHELXL-2017/1 (Sheldrick, 2017) software suite. All non-hydrogen atoms were located from iterative examination of difference F-maps following which the structure was refined using least-squares method. Hydrogen atoms were placed geometrically and placed in a riding model.

Table S1: Crystal data and structure refinement for compound **1**

	1
Empirical Formula	$C_{32}H_{58}N_6Si_4Sn_2$
Formula Weight [g mol^{-1}]	876.58
Crystal colour, shape	Orange. Plates
Crystal Size (mm)	0.09 x 0.08 x 0.07
Crystal System	Monoclinic
Space Group	P 21/n
Formula units	4
Temperature [K]	100 (2)
Unit cell dimensions [Å] and [°]	a = 11.7813(13) b = 25.808(3) c = 14.0899(15) α= 90 β= 109.687(6) γ = 90
Cell volume [Å^3]	4033.7 (8)
$\rho_{calc.}$ [g cm^{-3}]	1.443
μ (Cu K$_\alpha$)[mm $^{-1}$]	11.209
θ_{min} / θ_{max} [°]	3.425 – 66.676
Reflections measured	36575
Independent Reflections	7100 [R(int) = 0.1359]
R_1 ($I > 2\sigma(I)$)	0.0543
wR_2 (all data)	0.1567
GooF	0.982
Largest diff. peak and hole [e Å^{-3}]	1.333/ -0.957

Table S2: Crystal data and structure refinement for compound **2**

	2
Empirical Formula	$C_{74}H_{43}B_2F_{30}N_4Sn$
Formula Weight [g mol^{-1}]	1692.43
Crystal colour, shape	Colourless, Plate
Crystal Size (mm)	0.09 x 0.08 x 0.06
Crystal System	Monoclinic
Space Group	P 21/n
Formula units	4
Temperature [K]	100 (2)
Unit cell dimensions [Å] and [°]	a = 10.2239(8) b = 15.6566(12) c = 41.352(3) α= 90 β= 95.994(4) γ = 90
Cell volume [Å^3]	6583.1 (9)
$\rho_{calc.}$ [g cm^{-3}]	1.708
μ (Cu K$_\alpha$)[mm $^{-1}$]	4.311
θ_{min} / θ_{max} [°]	3.020 – 66.889
Reflections measured	84616
Independent Reflections	11636 [R(int) = 0.1495]
R_1 ($I > 2\sigma(I)$)	0.0392
wR_2 (all data)	0.0946
GooF	1.018
Largest diff. peak and hole [e Å^{-3}]	0.620/ -0.581

Table S3: Crystal data and structure refinement for compound **3**

	3
Empirical Formula	$C_{22}H_{23}F_6N_4O_6S_2Sn$
Formula Weight [g mol^{-1}]	736.25
Crystal colour, shape	Colourless, Blocks
Crystal Size (mm)	0.03x 0.03 x 0.02
Crystal System	Triclinic
Space Group	P -1
Formula units	2
Temperature [K]	100 (2)
Unit cell dimensions [Å] and [°]	a = 8.182(15) b = 11.154(14) c = 16.25(2) α= 72.46(13) β= 79.32(13) γ = 73.70(12)
Cell volume [Å^3]	1349 (4)
$\rho_{calc.}$ [g cm^{-3}]	1.812
μ (Cu K$_\alpha$)[mm $^{-1}$]	9.789
θ_{min} / θ_{max} [°]	2.869 – 66.826
Reflections measured	12140
Independent Reflections	4728 [R(int) = 0.1028]
R_1 ($I > 2\sigma(I)$)	0.0613
wR_2 (all data)	0.1534
GooF	0.995
Largest diff. peak and hole [e Å^{-3}]	1.321 / -0.846

Table S4: Crystal data and structure refinement for compound **4**

	4
Empirical Formula	$C_{24}H_{31}F_3N_4O_3SSiSn$
Formula Weight [g mol^{-1}]	659.37
Crystal colour, shape	Plates, Pale Yellow
Crystal Size (mm)	0.05 x 0.02 x 0.01
Crystal System	Monoclinic
Space Group	P 21/c
Formula units	4
Temperature [K]	100 (2)
Unit cell dimensions [Å] and [°]	a = 16.533(4) b = 10.968(4) c = 17.061(7) α = 90 β = 117.43(3) γ = 90
Cell volume [Å^3]	2746.1(17)
$\rho_{calc.}$ [g cm^{-3}]	1.595
μ (Cu K$_\alpha$)[mm^{-1}]	9.004
θ_{min} / θ_{max} [°]	3.011 – 66.956
Reflections measured	28820
Independent Reflections	4857 [R (int) = 0.1443]
R_1 ($I > 2\sigma(I)$)	0.0571
wR_2 (all data)	0.1125
GooF	1.045
Largest diff. peak and hole [e Å^{-3}]	0.717 /-0.866

Table S5: Crystal data and structure refinement for compound **5**

	5
Empirical Formula	$C_{80}H_{72}N_4P_4Sn_2$
Formula Weight [g mol^{-1}]	1450.67
Crystal colour, shape	Colourless. Block
Crystal Size (mm)	0.05 x 0.04 x 0.03
Crystal System	Triclinic
Space Group	P -1
Formula units	1
Temperature [K]	100 (2)
Unit cell dimensions [Å] and [°]	a = 10.4508(7) b = 11.1315(7) c = 15.4211(10) α = 81.375 (4) β = 75.530 (4) γ = 81.525 (4)
Cell volume [Å^3]	1706.1 (2)
$\rho_{calc.}$ [g cm^{-3}]	1.412
μ (Cu K$_\alpha$)[mm^{-1}]	7.072
θ_{min} / θ_{max} [°]	2.980 – 67.134
Reflections measured	19241
Independent Reflections	6039 [R (int) = 0.0780]
R_1 ($I > 2\sigma(I)$)	0.0439
wR_2 (all data)	0.0985
GooF	1.045
Largest diff. peak and hole [e Å^{-3}]	1.941 /-0.648

X-Ray Structure

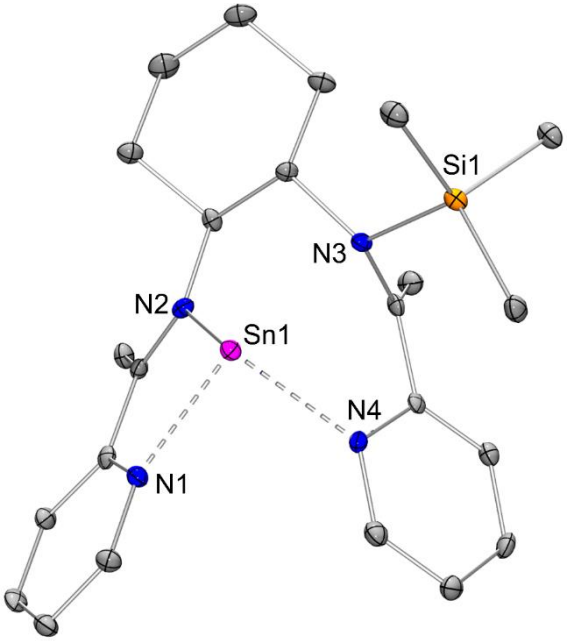


Figure S32. Molecular structure of **4** in the solid state (thermal ellipsoids at 30%, H atoms and triflate counter anions are omitted for clarity). Selected bond lengths [Å]**:** Sn1-N1 2.323(5), Sn1-N2 2.095(6), Sn1-N4 2.323(5), Si1-N3 1.791(6).

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[S1] Gaussian 09, Revision **E.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.