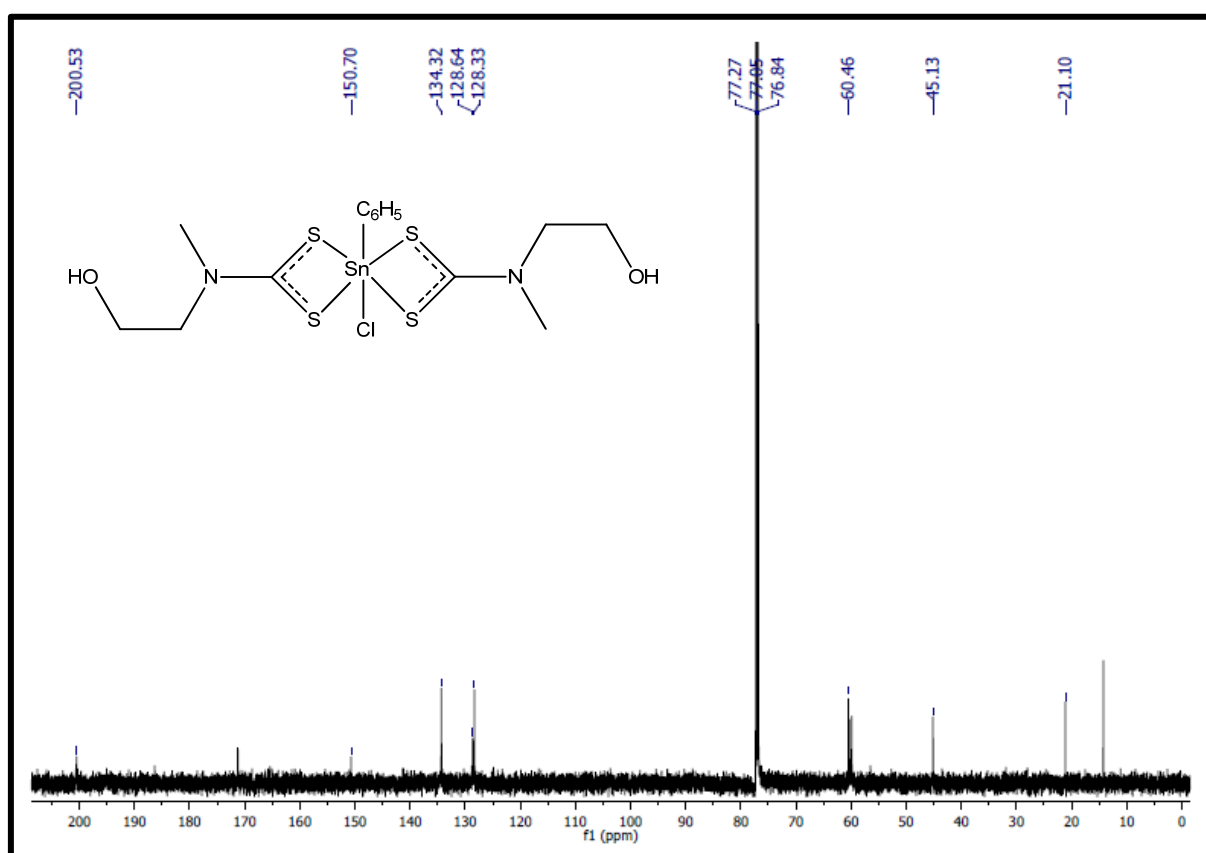
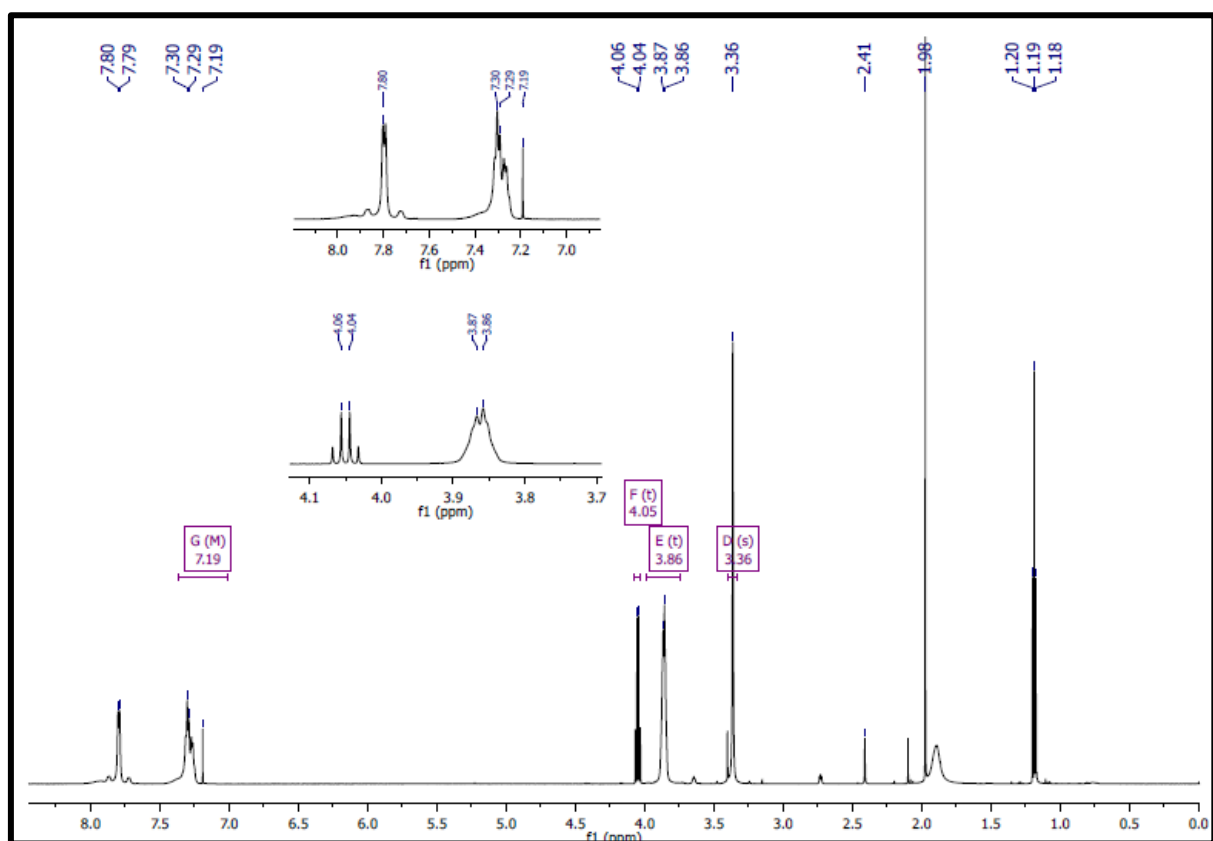


(a)



(b)

Figure S1. ¹H and ¹³C spectra of (a) [(C₆H₅)₂Sn(L)₂] and (b) [(C₆H₅)(Cl)Sn(L)₂]

Table S1. Gaussian input file for conformer A of [(C₆H₅)₂Sn(L)₂]

```
%mem=10GB
%CPU=0-23
%chk=Sncomplx_ph_cis.chk
# opt freq genecp m06

Sncomplx_ph_cis

0 1
Sn      0.03602369  0.23682095 -0.19792621
S      -1.32976711 -0.29117480  1.86099494
S      -2.86002604  0.36528424 -0.62733089
S       2.67062277  0.54379565 -1.54091413
S       2.03095240 -0.18694520  1.29502620
C      -2.84624659 -0.04211809  1.01364285
N      -3.96377195 -0.19478392  1.73580510
C      -3.91448186 -0.47248789  3.16408186
H      -2.99767444 -0.04096803  3.57051031
H      -4.76117810  0.00550277  3.65403128
C      -3.93711956 -1.95890527  3.43640383
H      -3.14290744 -2.45092986  2.85479924
H      -4.89767358 -2.36601851  3.09893800
O      -3.74356678 -2.12004747  4.81799216
H      -3.95055388 -3.02217688  5.06233305
C      -5.28091654 -0.01711719  1.14542309
H      -5.45871101 -0.74989411  0.35660063
H      -6.03038016 -0.14560544  1.92254137
H      -5.38924760  0.97901051  0.71357574
C       3.18801093  0.12659156  0.00799738
N       4.49130652  0.01805816  0.30633139
C       4.98199761 -0.38510785  1.61531213
H       5.92129148  0.14407102  1.80332274
H       4.27751354 -0.07792846  2.38718545
C       5.20513975 -1.88437654  1.69300255
H       4.24811381 -2.39449898  1.56444395
H       5.85597212 -2.20714365  0.86824973
O       5.71048473 -2.26606038  2.94439343
H       6.61013061 -1.94487824  3.02787156
C       5.48401983  0.20478813 -0.73892074
H       6.47417846  0.07621316 -0.30663798
H       5.34436408 -0.51727531 -1.54509616
H       5.40239731  1.20227560 -1.17227069
C      -0.10323978 -1.48871374 -1.42053492
C      -0.17652414 -1.38909859 -2.80425394
C      -0.14820146 -2.74156421 -0.82671957
C      -0.29524982 -2.52596060 -3.58344983
H      -0.13471790 -0.41715966 -3.28722649
C      -0.26099496 -3.88222849 -1.60753504
H      -0.09552164 -2.83827706  0.25301062
C      -0.33631425 -3.77504870 -2.98445828
H      -0.35259392 -2.43838022 -4.66113320
H      -0.29011927 -4.85674484 -1.13618317
H      -0.42554933 -4.66528704 -3.59398339
C      -0.03281228  2.34079236 -0.44074079
C      -0.52918907  2.91803930 -1.60251940
C       0.45533436  3.15798458  0.56873156
```

C	-0.53180839	4.29324388	-1.75591152
H	-0.92800564	2.29597427	-2.39800060
C	0.44179995	4.53638504	0.42049570
H	0.85129612	2.72374149	1.48131844
C	-0.04804670	5.10403828	-0.74208937
H	-0.91752477	4.73387592	-2.66661108
H	0.81709838	5.16724289	1.21658917
H	-0.05546997	6.18025067	-0.85901215

C H N O S 0

cc-pVTZ

Sn 0

LANL2DZ

Sn 0

LANL2DZ

Gaussian input file for conformer B of [(C₆H₅)₂Sn(L)₂]

%mem=10GB

%CPU=0-23

%chk=Sncomplx_ph_new.chk

opt freq genecp m06

Sncomplx_ph_cis

0 1

Sn	0.00350940	-0.00534824	-0.22932078
S	1.78299587	-1.83929104	-0.16929713
S	2.30109057	1.11251539	-0.25298463
S	-1.78346176	1.82635658	-0.26885192
S	-2.29344910	-1.12618958	-0.17351114
C	2.88654872	-0.51305742	-0.20618026
N	4.19424558	-0.76013419	-0.19280287
C	5.18522462	0.30746628	-0.16617447
H	6.07363902	-0.03030463	-0.70209169
H	4.79763601	1.18093013	-0.68914564
C	5.55522233	0.67438128	1.25342093
H	5.87131238	-0.23004197	1.79412639
H	4.66857754	1.07076058	1.76328129
O	6.58878254	1.61762560	1.16369577
H	6.74270994	2.00311513	2.02662455
C	4.68578499	-2.12654798	-0.09378012
H	4.34030318	-2.72050074	-0.94097219
H	5.77241556	-2.10655649	-0.09032731
H	4.33369350	-2.60200264	0.82318596
C	-2.88209677	0.49691491	-0.22671151
N	-4.19174613	0.74084686	-0.23103898
C	-5.18069557	-0.32622800	-0.14636589
H	-6.05432797	-0.02292019	-0.72991948
H	-4.78204010	-1.23204083	-0.60182491
C	-5.57755159	-0.60454154	1.29281343
H	-4.70056439	-0.94788641	1.84568634

H	-5.91725973	0.32391666	1.77265026
O	-6.53819187	-1.62116090	1.36703576
H	-7.37694056	-1.28630754	1.04485693
C	-4.68569322	2.10932357	-0.20779873
H	-5.77246821	2.08899026	-0.22189612
H	-4.35017553	2.63084980	0.69023024
H	-4.32695322	2.66140051	-1.07746302
C	0.00780523	0.06482999	1.93953987
C	0.12626757	1.28934326	2.59757129
C	-0.10796998	-1.11418602	2.67579085
C	0.12962354	1.33466955	3.99154260
H	0.21829896	2.21860195	2.01683874
C	-0.10562104	-1.06892170	4.07019234
H	-0.20152443	-2.07936223	2.15732054
C	0.01328600	0.15521462	4.72813489
H	0.22362415	2.29974512	4.51028100
H	-0.19733353	-1.99864539	4.65043100
H	0.01589750	0.19120717	5.82722272
C	-0.00459955	-0.06776420	-2.39840780
C	0.16565503	1.10750815	-3.13067804
C	-0.17990371	-1.28280879	-3.06058846
C	0.15991813	1.06774839	-4.52481146
H	0.30306885	2.06537649	-2.60832999
C	-0.18468144	-1.32289462	-4.45514222
H	-0.31392653	-2.20922785	-2.48360090
C	-0.01494766	-0.14787632	-5.18730302
H	0.29348113	1.99415993	-5.10206278
H	-0.32251099	-2.28110778	-4.97697053
H	-0.01937679	-0.17898660	-6.28653406

C H N O S 0

cc-pVTZ

Sn 0

LANL2DZ

Sn 0

LANL2DZ

Gaussian input file for conformer A of [(C6H5)(Cl)Sn(L)2]

%mem=10GB

%CPU=0-23

%chk=Sncomplx_Clph_cis.chk

opt freq genecp m06

Sncomplx_Clph_cis

0 1

Sn	-0.00531159	-0.18538193	-0.00061126
S	-1.82576199	-0.23254840	1.85094375
S	-2.35236716	-0.23600488	-1.11102484
S	1.82392790	-0.24916921	-1.84927723
S	2.34044025	-0.25602360	1.11425515

C	-2.92423916	-0.21807786	0.51979785
N	-4.23498356	-0.20839437	0.77100216
C	-4.76782031	-0.08556753	2.12079579
H	-4.05835477	0.48427488	2.72329335
H	-5.70341914	0.47128272	2.09726627
C	-4.99062895	-1.44318515	2.74803334
H	-4.06062042	-2.02830579	2.69385092
H	-5.75386312	-1.98152124	2.17319043
O	-5.38402756	-1.21083699	4.07475229
H	-5.69970285	-2.02908675	4.45894457
C	-5.19675700	-0.21278099	-0.32052262
H	-5.09821809	-1.11977306	-0.91860657
H	-6.19871376	-0.16748308	0.09870670
H	-5.04469737	0.64468438	-0.97803882
C	2.91634552	-0.23426672	-0.51408736
N	4.22925271	-0.22101644	-0.76093639
C	5.22248094	-0.25693920	0.30407369
H	6.08955154	0.32357853	-0.02406236
H	4.82279357	0.22566944	1.19490940
C	5.63680346	-1.68014568	0.63267148
H	4.76983094	-2.22706400	1.00884509
H	5.96947259	-2.19246424	-0.28094796
O	6.61225769	-1.70746562	1.63883384
H	7.43967458	-1.37972927	1.28197519
C	4.72334827	-0.28255284	-2.12743819
H	5.81045007	-0.28532822	-2.10554837
H	4.37418696	-1.18638250	-2.62941317
H	4.37890880	0.57832100	-2.70215712
Cl	-0.01462071	-2.59730485	-0.00597580
C	0.00727251	1.97664287	-0.00466490
C	-0.19911511	2.68072334	-1.18173122
C	0.21998890	2.68199725	1.17051307
C	-0.19320447	4.06659242	-1.18686196
H	-0.36886104	2.15226499	-2.11530767
C	0.22681394	4.06790566	1.17179447
H	0.38416143	2.15457398	2.10565892
C	0.02002569	4.76122048	-0.00847959
H	-0.35624991	4.60411013	-2.11283117
H	0.39399601	4.60641917	2.09644617
H	0.02464514	5.84391937	-0.00990617

C H N O Cl S O

cc-pVTZ

Sn 0

LANL2DZ

Sn 0

LANL2DZ

Gaussian input file for conformer B of [(C₆H₅)(Cl)Sn(L)₂]

%mem=10GB

%CPU=0-23
%chk=Sncomplx_Cl.chk
opt freq genecp m06

Sncomplx_Cl

0 1

Sn	-1.31715670	1.37373368	-0.54579608
S	-1.32111749	1.37375680	-2.95599589
S	-3.72715217	1.37373368	-0.54112295
S	-1.11821625	1.38524547	1.82718094
S	1.09121442	1.37589272	-0.51920488
C	-3.19640868	1.31288680	-2.41806065
N	-4.17172175	1.29887522	-3.51781884
C	-5.08899245	2.43851560	-3.37382483
H	-5.68114595	2.31052432	-2.49185405
H	-4.52373986	3.34365693	-3.29566667
C	-6.01122503	2.51390910	-4.60484184
H	-6.59666164	1.62044394	-4.66716342
H	-5.41773365	2.61387598	-5.48953083
O	-6.87834824	3.64438700	-4.48229768
H	-7.51581946	3.63858658	-5.20006979
C	-4.93793093	0.04500858	-3.47729800
H	-5.61277239	0.06606826	-2.64721035
H	-5.49305181	-0.06326934	-4.38560230
H	-4.26568522	-0.78045126	-3.36958659
C	0.79591324	1.49867199	1.46243553
N	1.95206931	1.57322994	2.36722516
C	2.06044555	0.32014115	3.12809510
H	2.90588085	0.37184460	3.78190387
H	1.17132948	0.17545855	3.70553735
C	2.23685019	-0.85879756	2.15311566
H	1.28839802	-1.32240444	1.97873922
H	2.63378007	-0.49924079	1.22679736
O	3.13773567	-1.81446833	2.71879998
H	4.01972622	-1.43772627	2.76072963
C	1.77458985	2.69753552	3.29746061
H	2.62966840	2.77004225	3.93658771
H	1.66605718	3.60590498	2.74249613
H	0.89885826	2.53503105	3.89040790
Cl	-1.39518704	3.76242511	-0.55862245
Cl	-1.39205614	-1.01509197	-0.54723678

C H N O Cl 0

cc-pVTZ

Sn 0

LANL2DZ

Sn 0

LANL2DZ