Supplementary Information

Synthesis and structure of stannane-based molecular bevel gears having substituents on a tin linker

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(Total 30 pages including this cover page)

1. Copies of NMR and HRMS Spectra for New Compounds

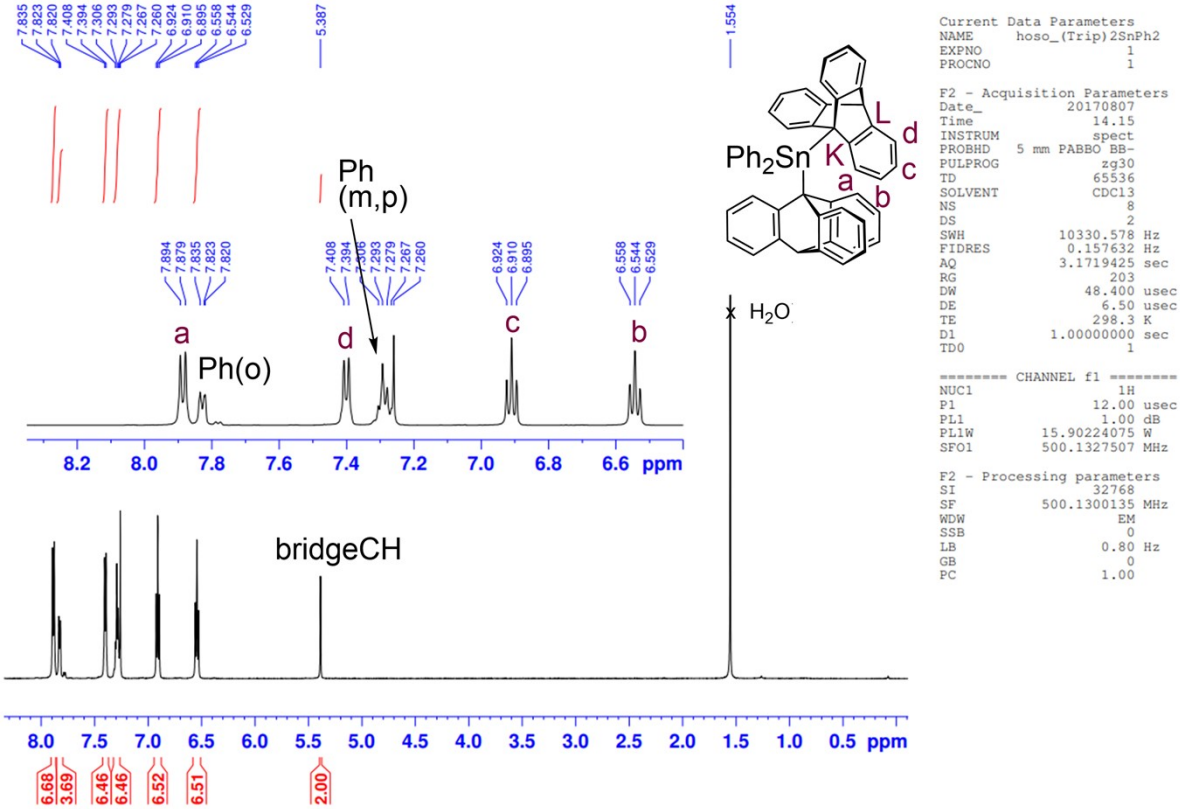
2. Appended Data of X-ray Crystallography

3. Appended Data of VT-NMR Study

4. Appended Data of DFT Calculations

1. **Copies of NMR and HRMS Spectra for New Compounds**

1. **Spectra of SnPh2**

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PROCNO                   1

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TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH             10330.578 Hz
FIDRES              0.157632 Hz
AQ                3.1719425 sec
RG                    203
DW                 48.400 usec
DE                  6.50 usec
TE                 298.3 K
D1              1.00000000 sec
TD0                     1

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PL1                 1.00 dB
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SFO1         500.1327507 MHz

F2 - Processing parameters
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WDW                    EM
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PC                 1.00
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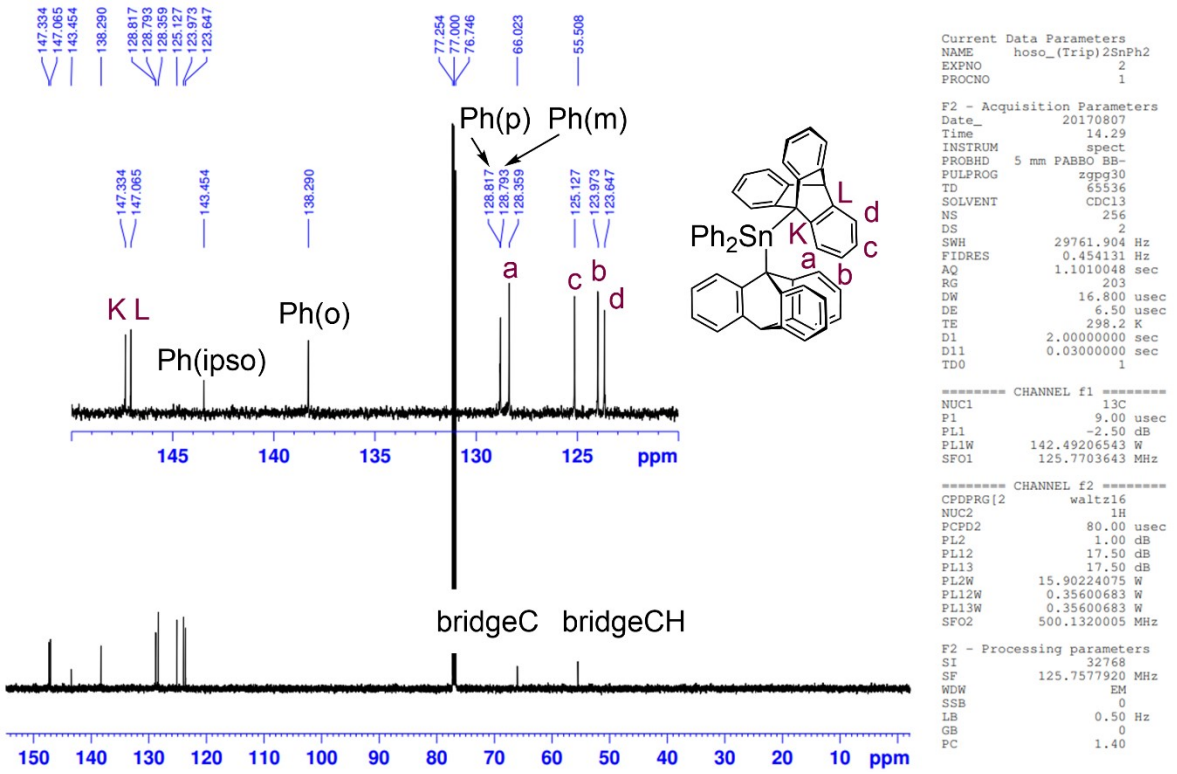
Fig. S1. ^{1}H NMR spectrum of **SnPh2** in $CDCl_3$.

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PROCNO                   1

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SOLVENT             CDCl3
NS                    256
DS                      2
SWH             29761.904 Hz
FIDRES              0.454131 Hz
AQ                1.1010048 sec
RG                    203
DW                 16.800 usec
DE                  6.50 usec
TE                 298.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.00 usec
PL1                -2.50 dB
PL1W         142.49206543 W
SFO1          125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 1.00 dB
PL12               17.50 dB
PL13               17.50 dB
PL2W         15.90224075 W
PL12W         0.35600683 W
PL13W         0.35600683 W
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                  32768
SF            125.7577920 MHz
WDW                    EM
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LB                 0.50 Hz
GB                      0
PC                 1.40
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Fig. S2. ^{13}C NMR spectrum of **SnPh2** in $CDCl_3$.

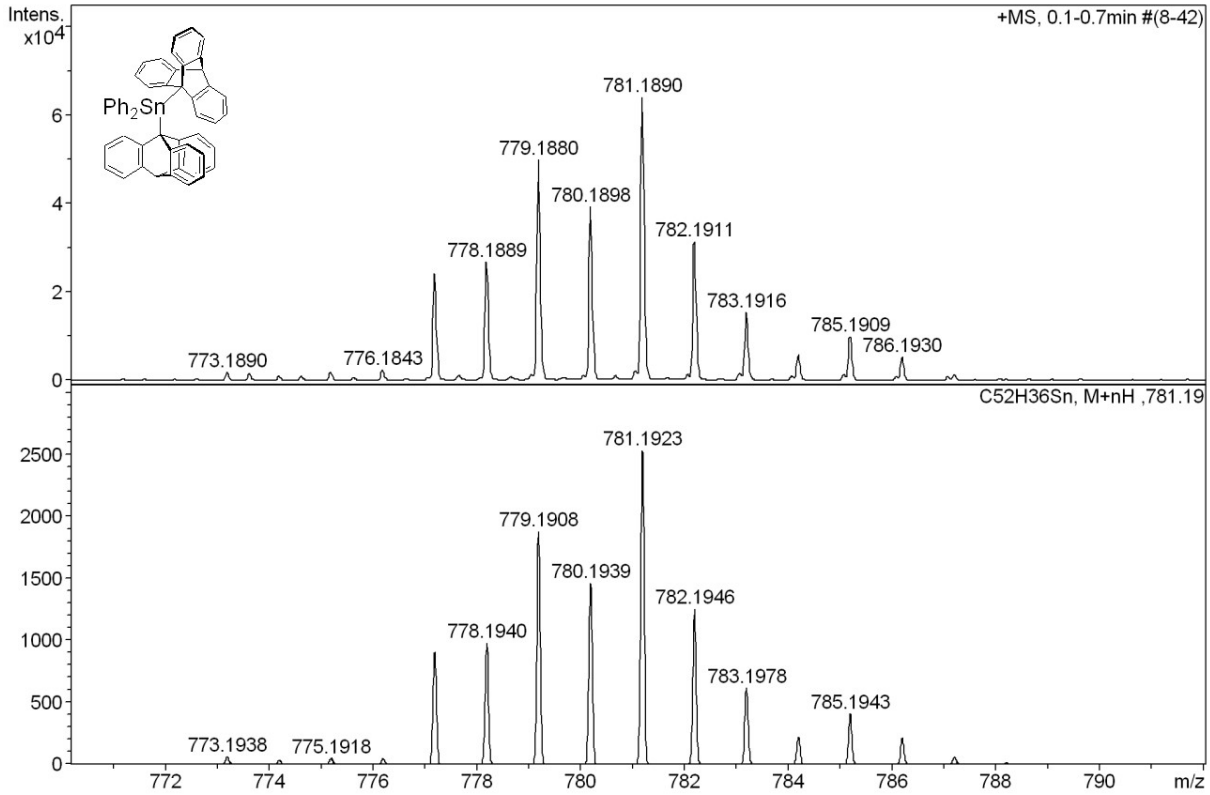
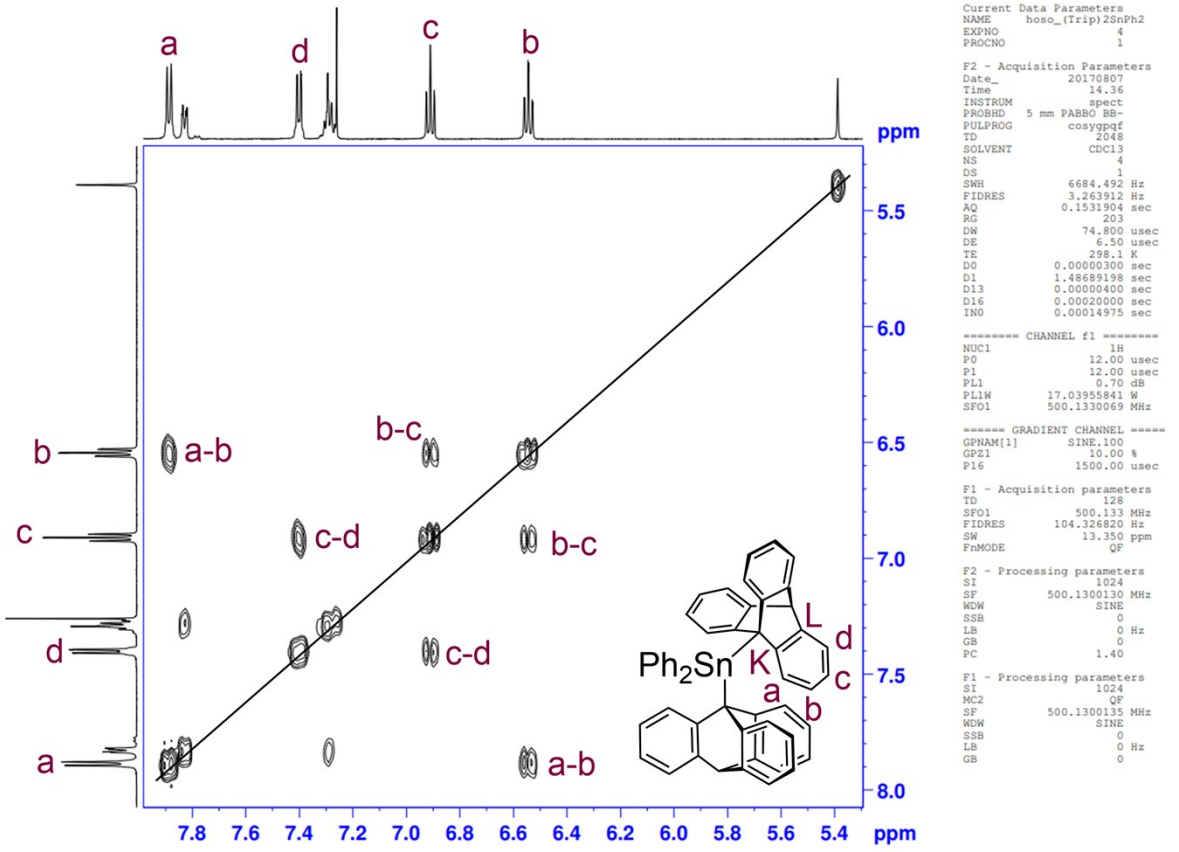


Fig. S3. HRMS spectrum of **SnPh2** (ESI, positive). Top: obsd. Bottom: sim.

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EXPNO                     4
PROCNO                    1

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Time                  14.36
INSTRUM                spect
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PULPROG           cosygpqf
TD                    2048
SOLVENT              CDCl3
NS                        4
DS                        1
SWH                6684.492 Hz
FIDRES             3.263912 Hz
AQ                 0.1531904 sec
RG                      203
DW                   74.800 usec
DE                    6.50 usec
TE                   298.1 K
D0                0.00000300 sec
D1                1.48689198 sec
D13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00014975 sec

======== CHANNEL f1 ========
NUC1                      1H
P0                    12.00 usec
P1                    12.00 usec
PL1                    0.70 dB
PL1W          17.03955841 W
SFO1          500.1330069 MHz

====== GRADIENT CHANNEL =====
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GPZ1                 10.00 %
P16                1500.00 usec

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TD                      128
SFO1              500.133 MHz
FIDRES          104.326820 Hz
SW                 13.350 ppm
FnMODE                   QF

F2 - Processing parameters
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SF            500.1300130 MHz
WDW                     SINE
SSB                        0
LB                         0 Hz
GB                         0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                      QF
SF            500.1300135 MHz
WDW                     SINE
SSB                        0
LB                         0 Hz
GB                         0
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Fig. S4. ^{1}H-^{1}H COSY NMR spectrum of **SnPh2** in $CDCl_3$.

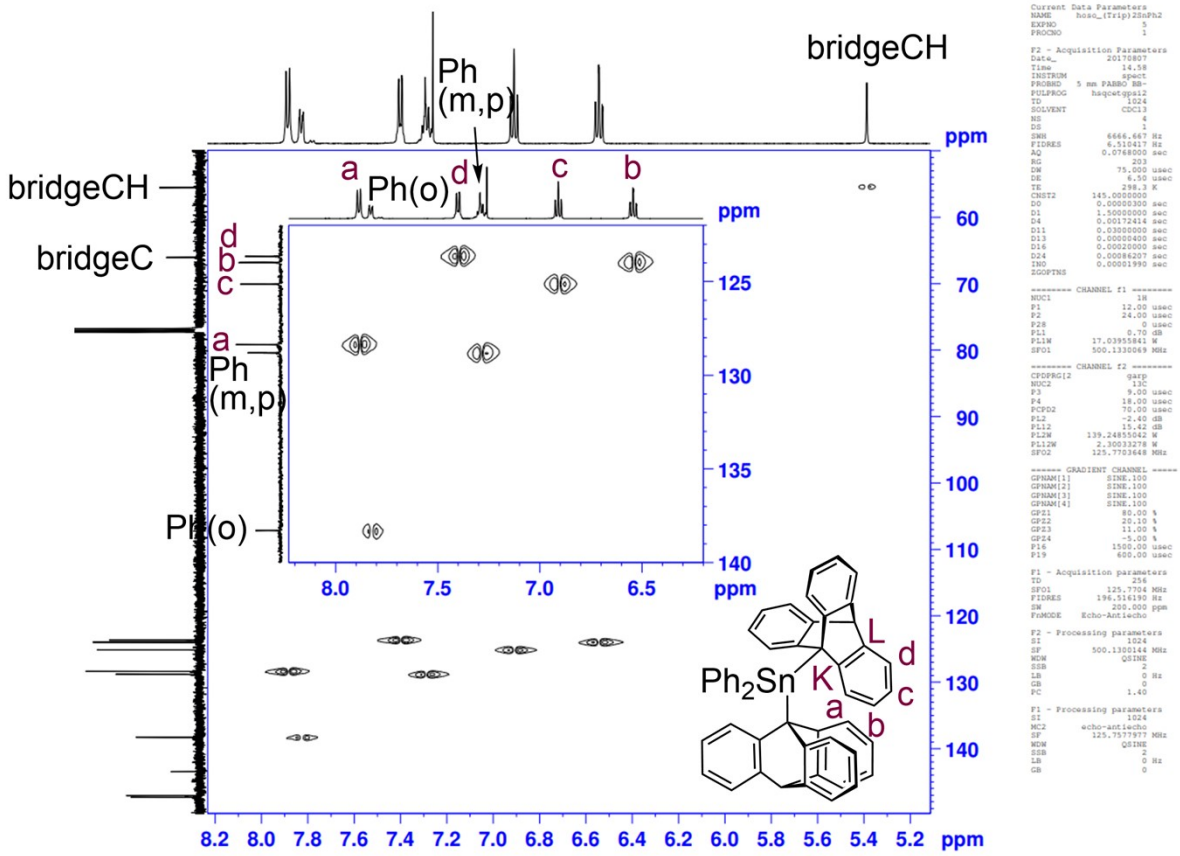


Fig. S5. ^{1}H-^{13}C HSQC NMR spectrum of **SnPh2** in $CDCl_3$.

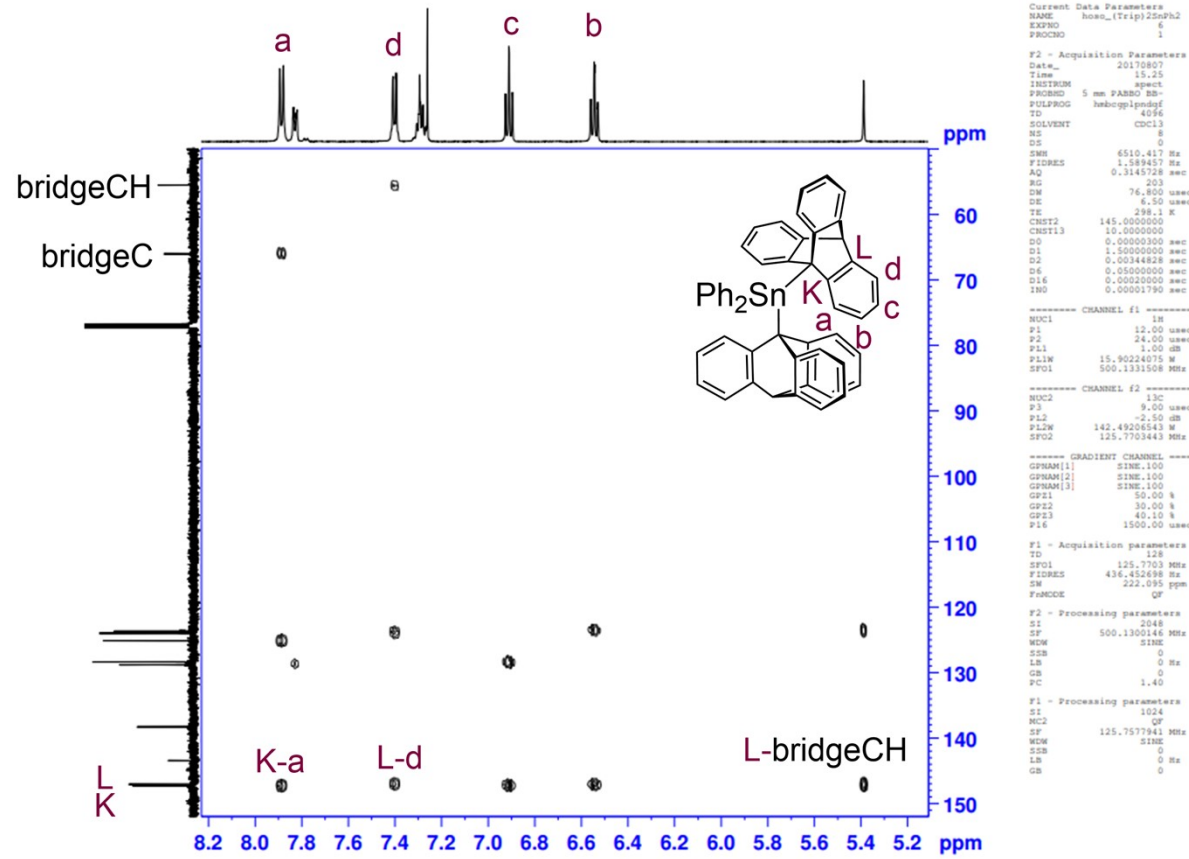
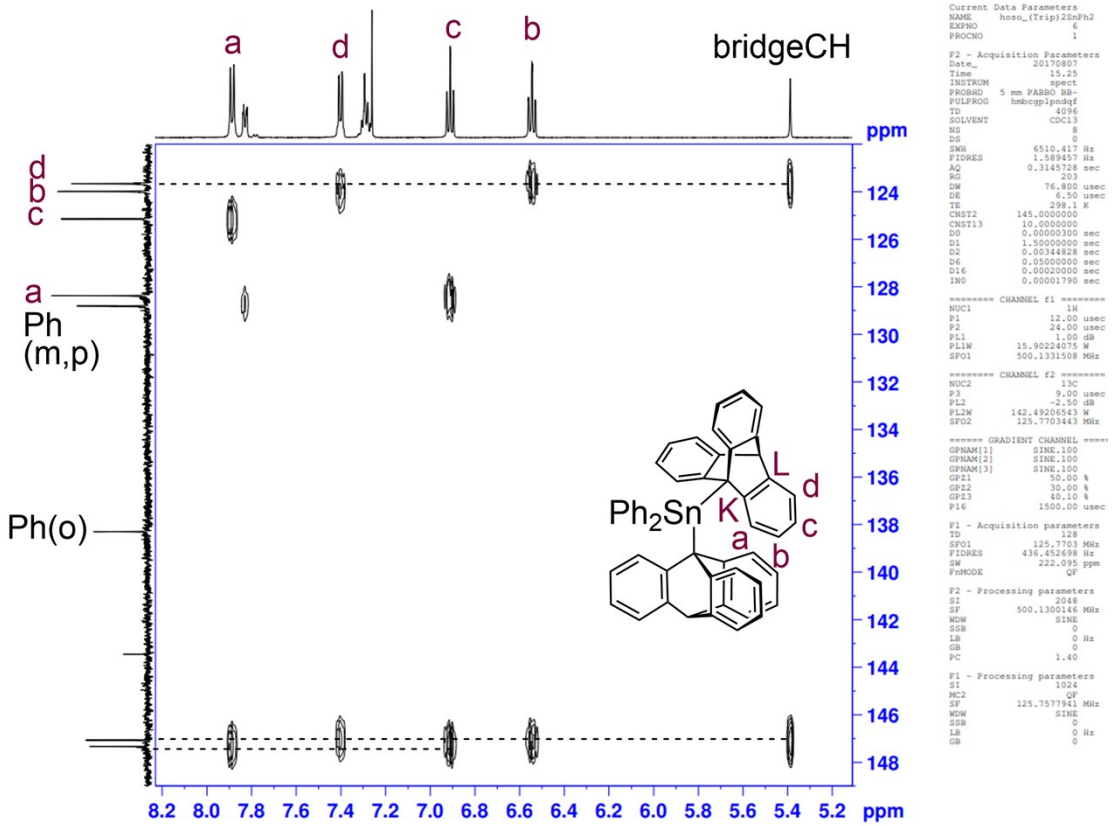


Fig. S6. ^{1}H-^{13}C HMBC NMR spectrum (the whole region) of **SnPh2** in $CDCl_3$.



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PROCNO 1

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INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgplpndqf
TD 4096
SOLVENT CDCl3
NS 8
DS 0
SWH 6510.417 Hz
FIDRES 1.589457 Hz
AQ 0.3145728 sec
RG 203
DW 76.800 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00344828 sec
D6 0.05000000 sec
D16 0.00020000 sec
IN0 0.00001790 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
P2 24.00 usec
PL1 1.00 dB
PL1W 15.90224075 W
SFO1 500.1331508 MHz

======== CHANNEL f2 ========
NUC2 13C
P3 9.00 usec
PL2 -2.50 dB
PL2W 142.49206543 W
SFO2 125.7703443 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPNAM[3] SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1500.00 usec

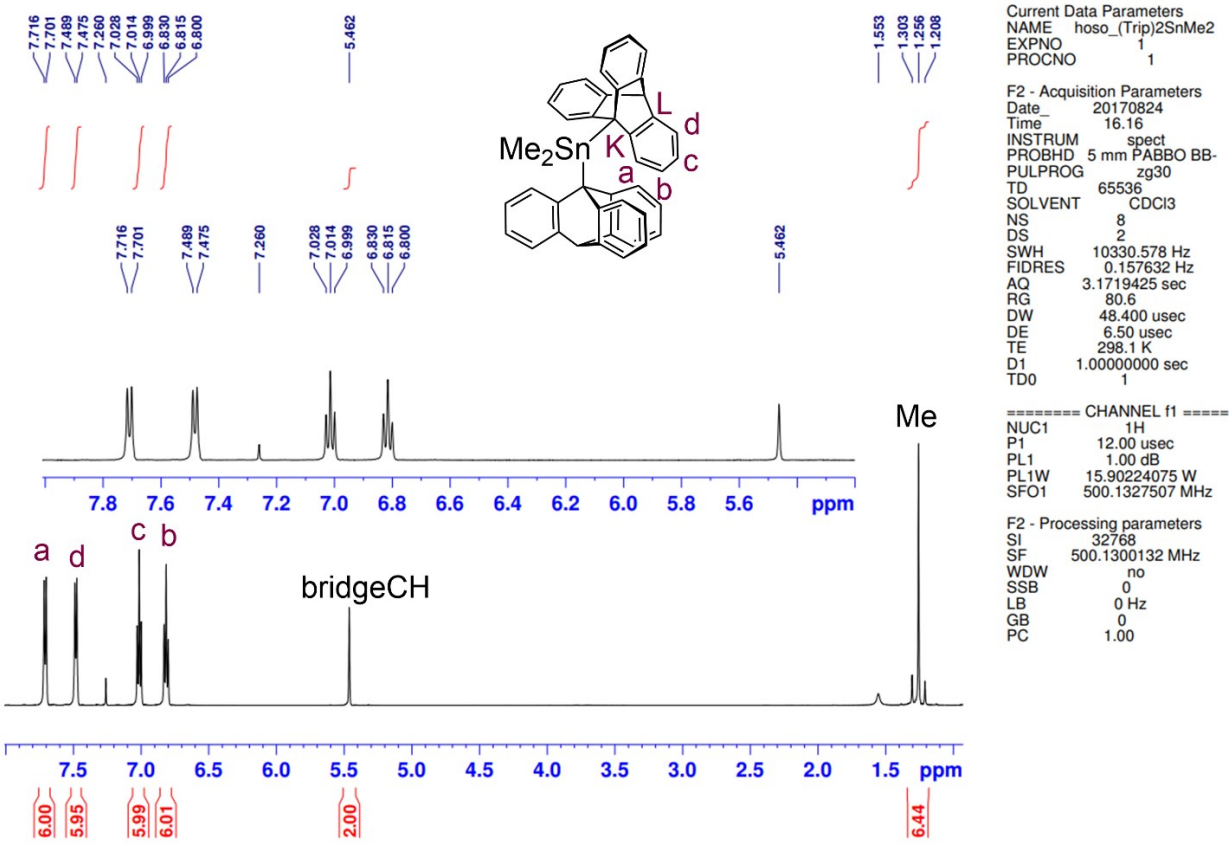
F1 - Acquisition parameters
TD 128
SFO1 125.7703 MHz
FIDRES 436.452698 Hz
SW 222.095 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 500.1300146 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 125.7577941 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Fig. S7. ^{1}H-^{13}C HMBC NMR spectrum (the aromatic region) of **SnPh2** in $CDCl_3$.

b. Spectra of SnMe2



Current Data Parameters
NAME hoso_(Trip)2SnMe2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170824
Time 16.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 80.6
DW 48.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 1.00 dB
PL1W 15.90224075 W
SFO1 500.1327507 MHz

F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Fig. S8. ^{1}H NMR spectrum of **SnMe2** in $CDCl_3$.

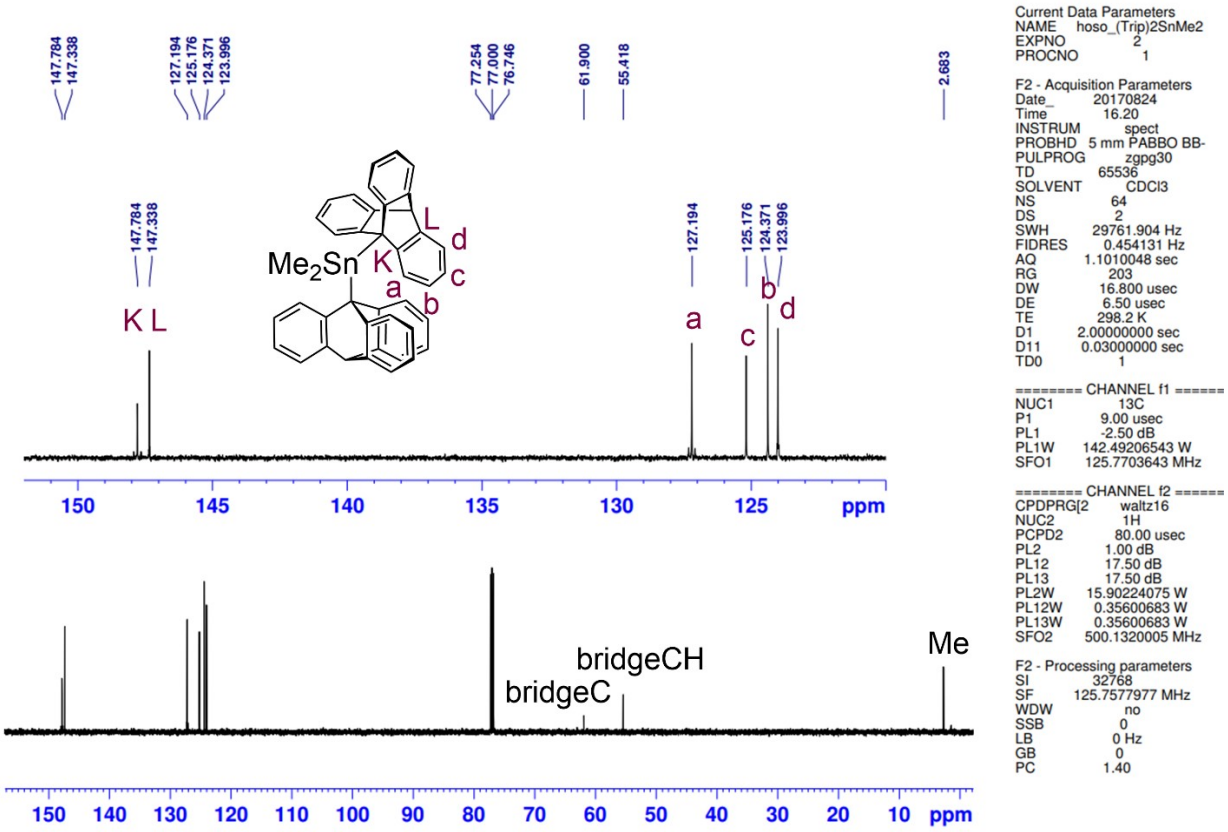


Fig. S9. ^{13}C NMR spectrum of **SnMe2** in $CDCl_3$.

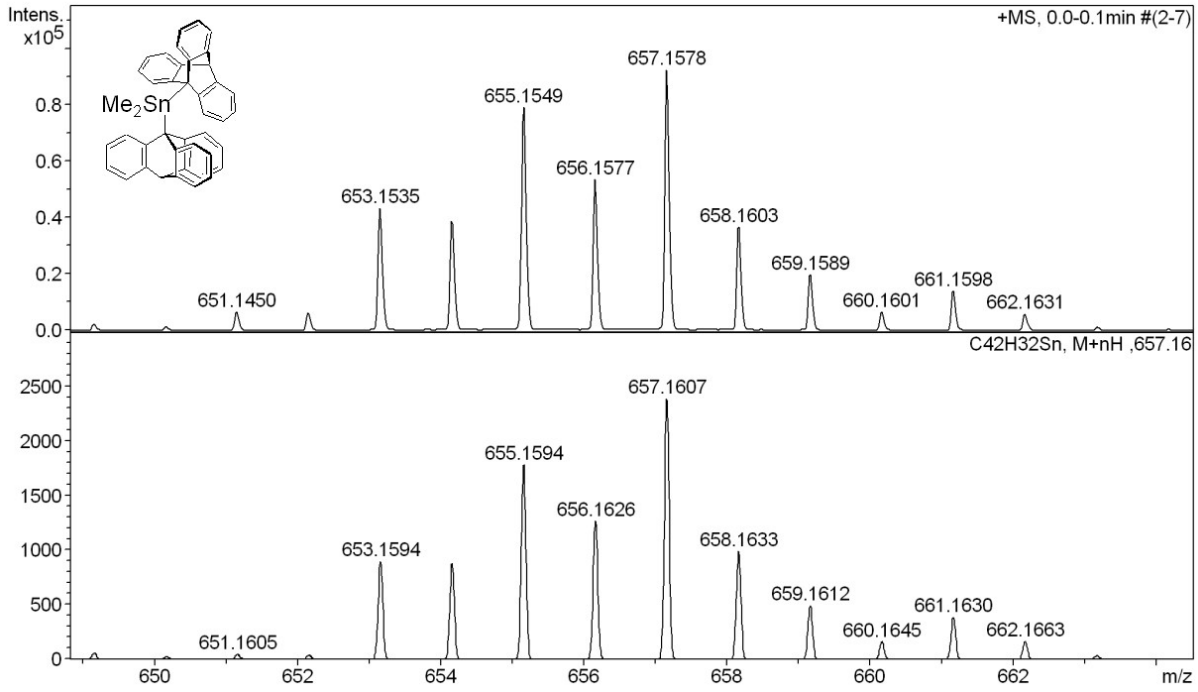


Fig. S10. HRMS spectrum of **SnMe2** (ESI, positive). Top: obsd. Bottom: sim.

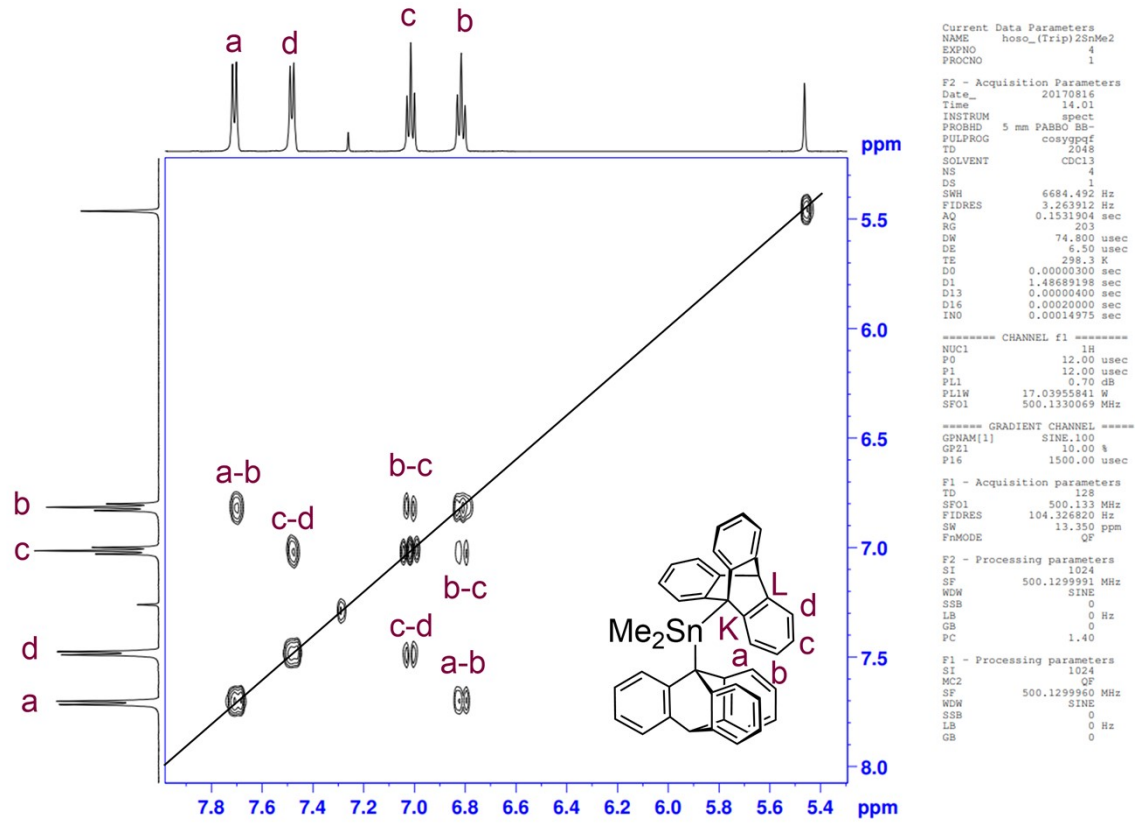


Fig. S11. ^{1}H-^{1}H COSY NMR spectrum of **SnMe2** in $CDCl_3$.

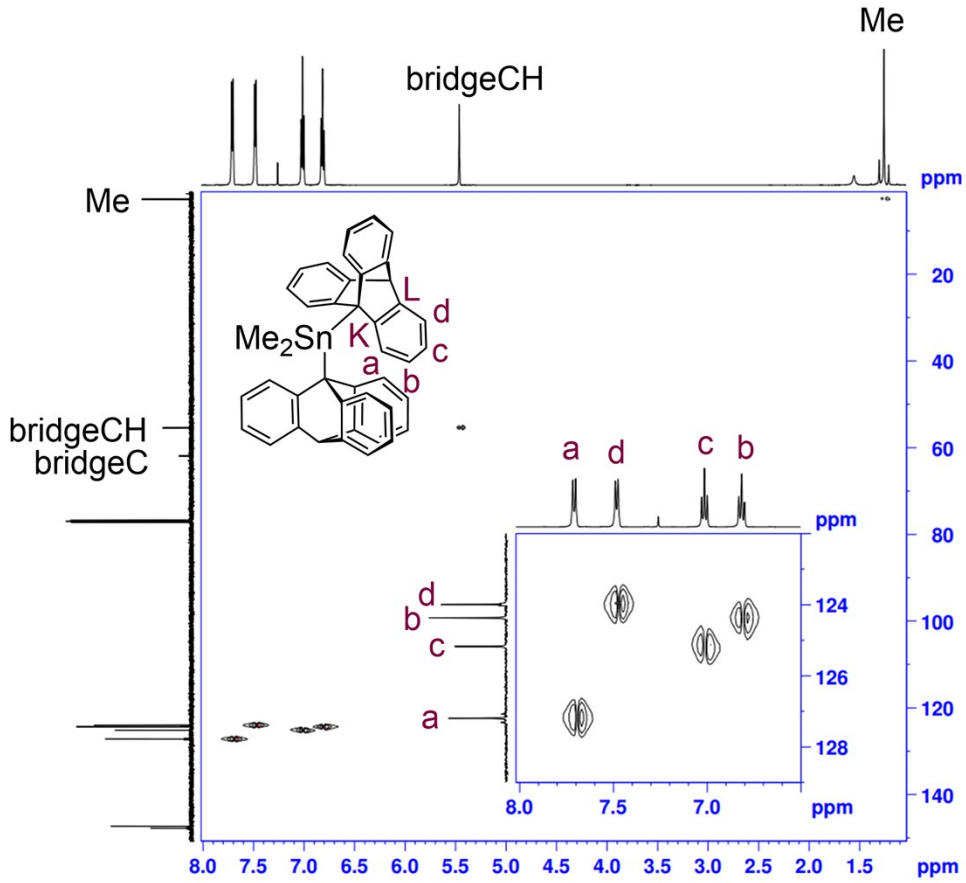


Fig. S12. ^{1}H-^{13}C HSQC NMR spectrum of **SnMe2** in $CDCl_3$.

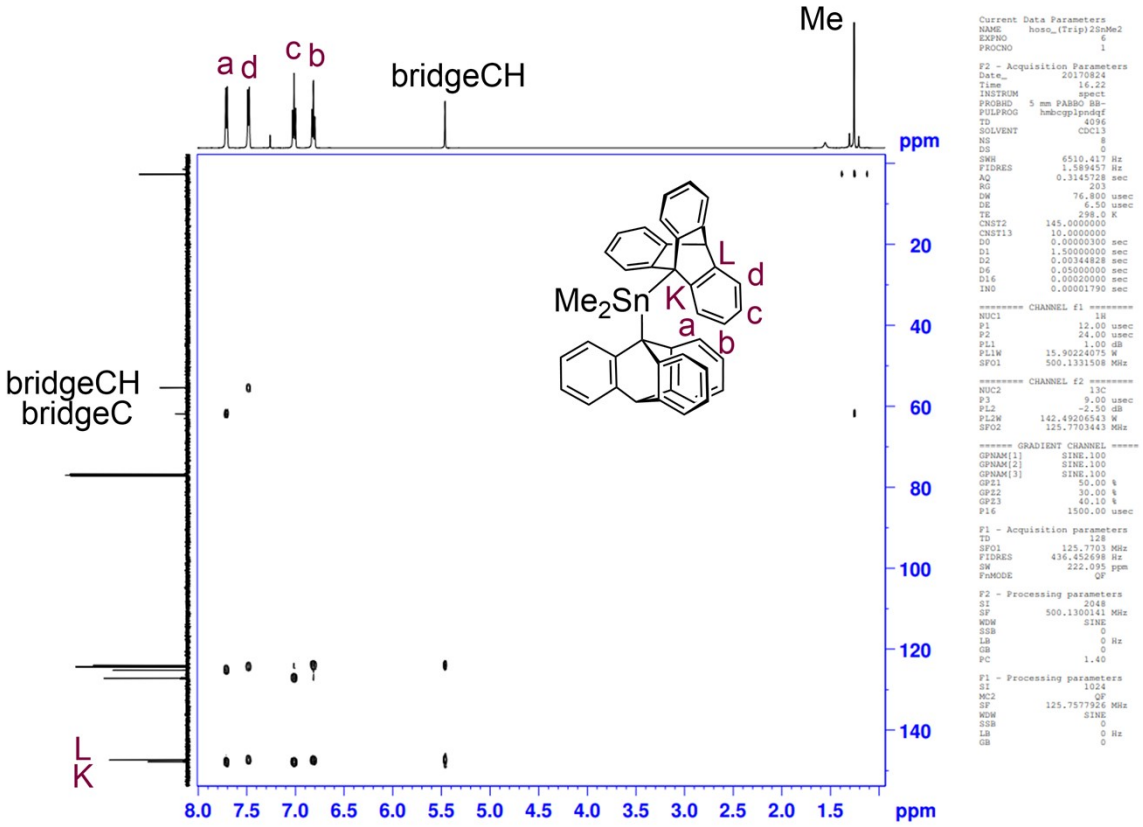


Fig. S13. ^{1}H-^{13}C HMBC NMR spectrum (the whole region) of **SnMe2** in $CDCl_3$.

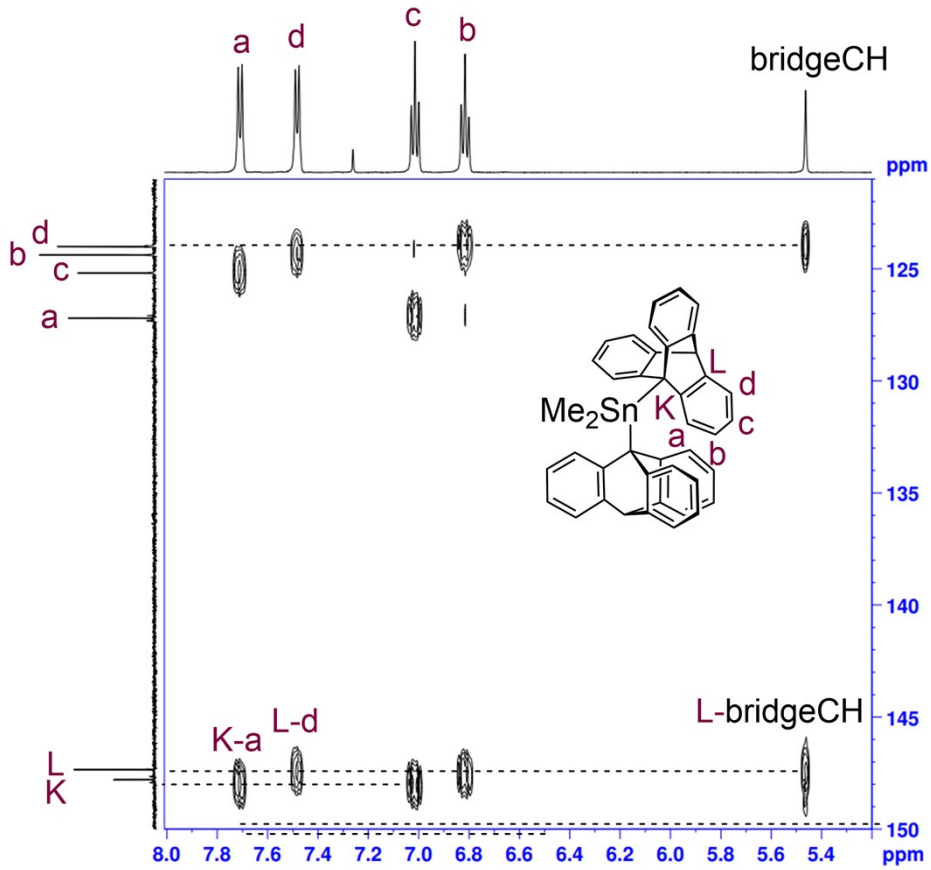
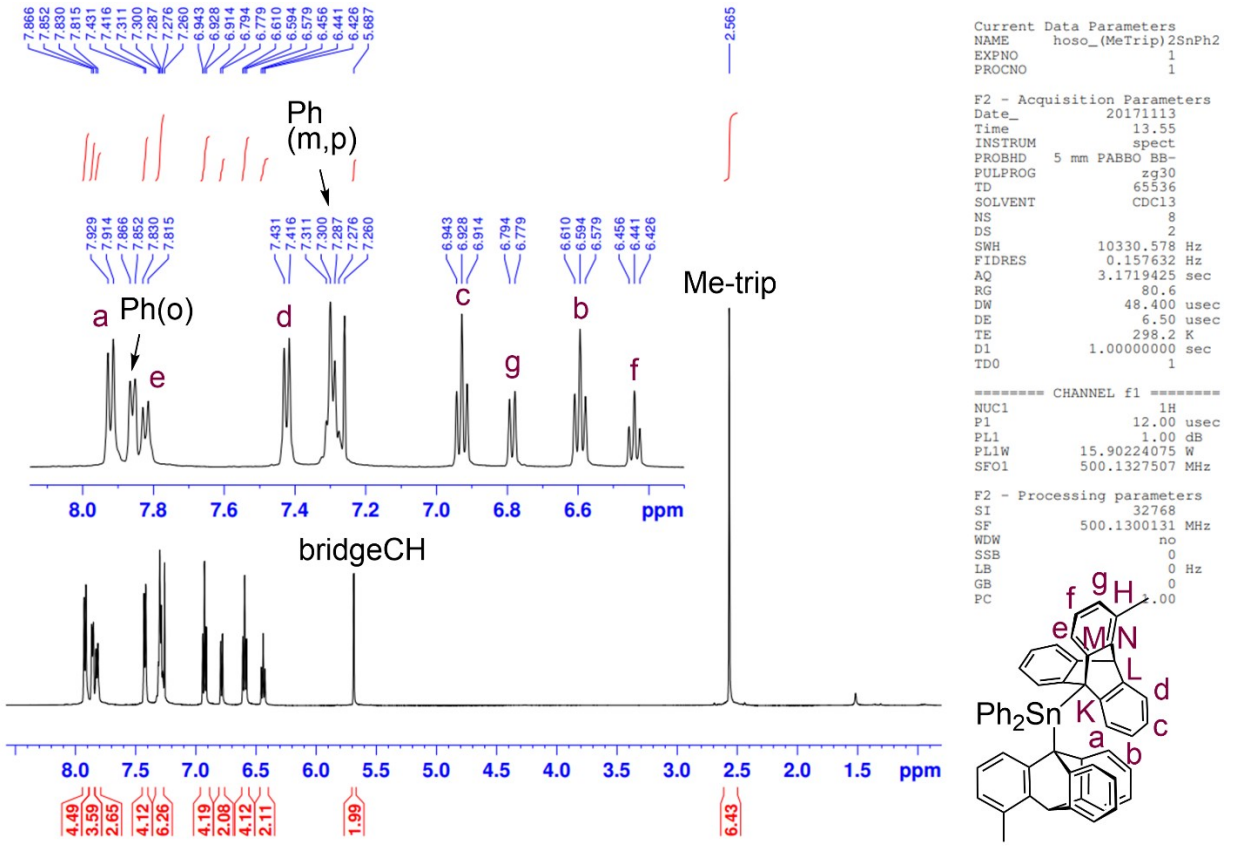


Fig. S14. ^{1}H-^{13}C HMBC NMR spectrum (the aromatic region) of **SnMe2** in $CDCl_3$.

c. Spectra of SnPh2me

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EXPNO                      1
PROCNO                     1

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PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719425 sec
RG                  80.6
DW                48.400 usec
DE                 6.50 usec
TE                298.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                12.00 usec
PL1                1.00 dB
PL1W        15.90224075 W
SFO1        500.1327507 MHz

F2 - Processing parameters
SI                 32768
SF          500.1300131 MHz
WDW                   no
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
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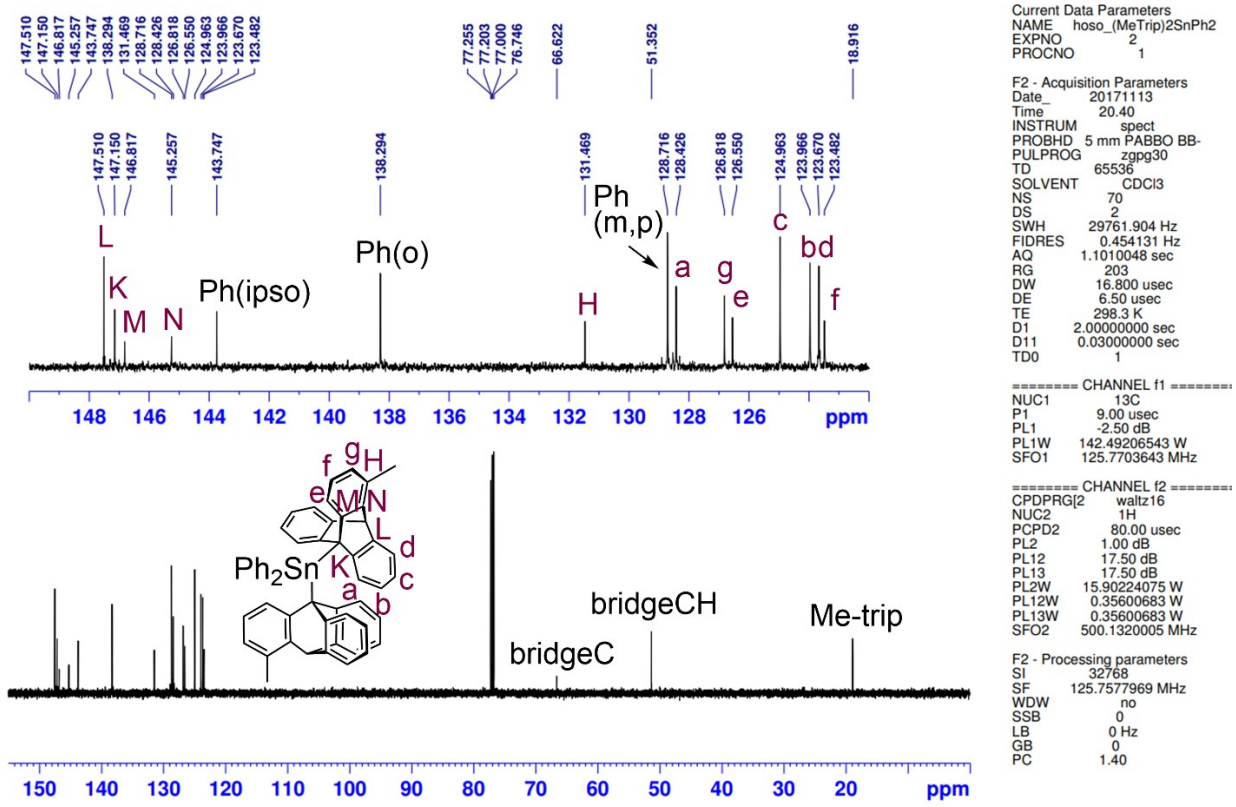
Fig. S15. ^{1}H NMR spectrum of **SnPh2me** in $CDCl_3$.

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Current Data Parameters
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EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
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Time                20.40
INSTRUM             spect
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PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    70
DS                     2
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                   203
DW                16.800 usec
DE                 6.50 usec
TE                298.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.00 usec
PL1                -2.50 dB
PL1W       142.49206543 W
SFO1       125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2            80.00 usec
PL2                1.00 dB
PL12              17.50 dB
PL13              17.50 dB
PL2W       15.90224075 W
PL12W       0.35600683 W
PL13W       0.35600683 W
SFO2       500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577969 MHz
WDW                   no
SSB                    0
LB                  0 Hz
GB                     0
PC                  1.40
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Fig. S16. ^{13}C NMR spectrum of **SnPh2me** in $CDCl_3$.

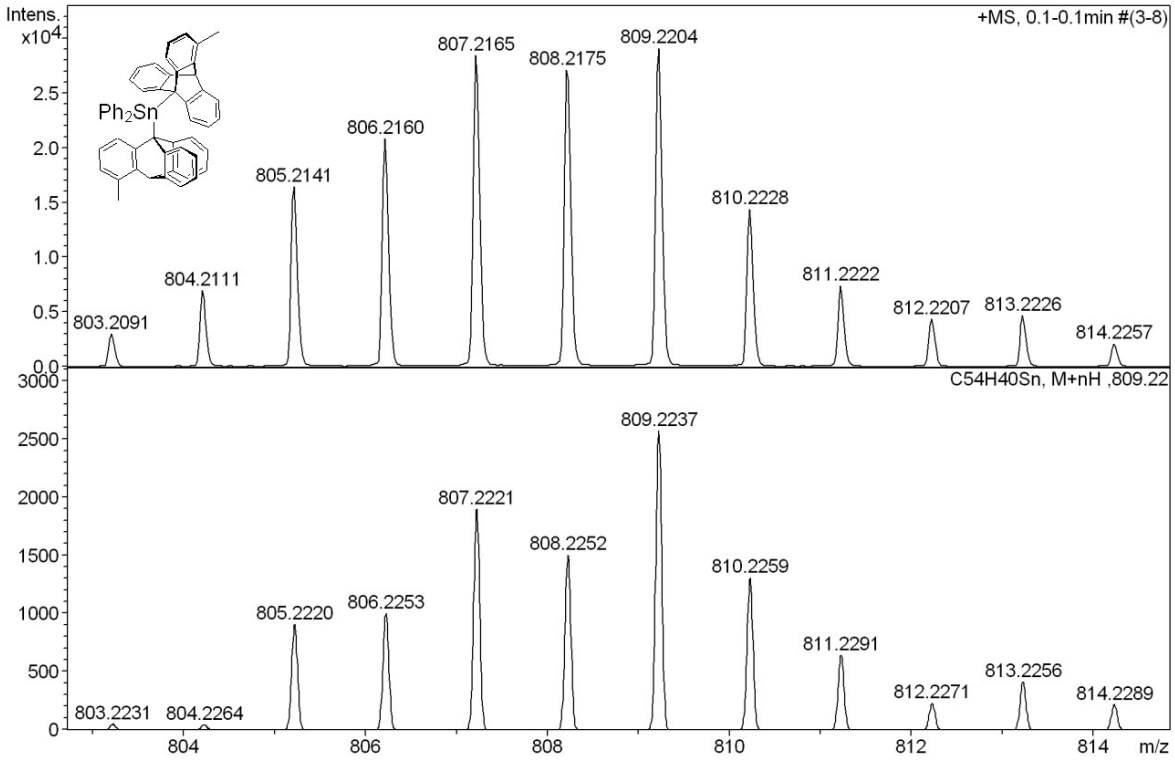

Fig. S17. HRMS spectrum of **SnPh2me** (ESI, positive). Top: obsd. Bottom: sim.

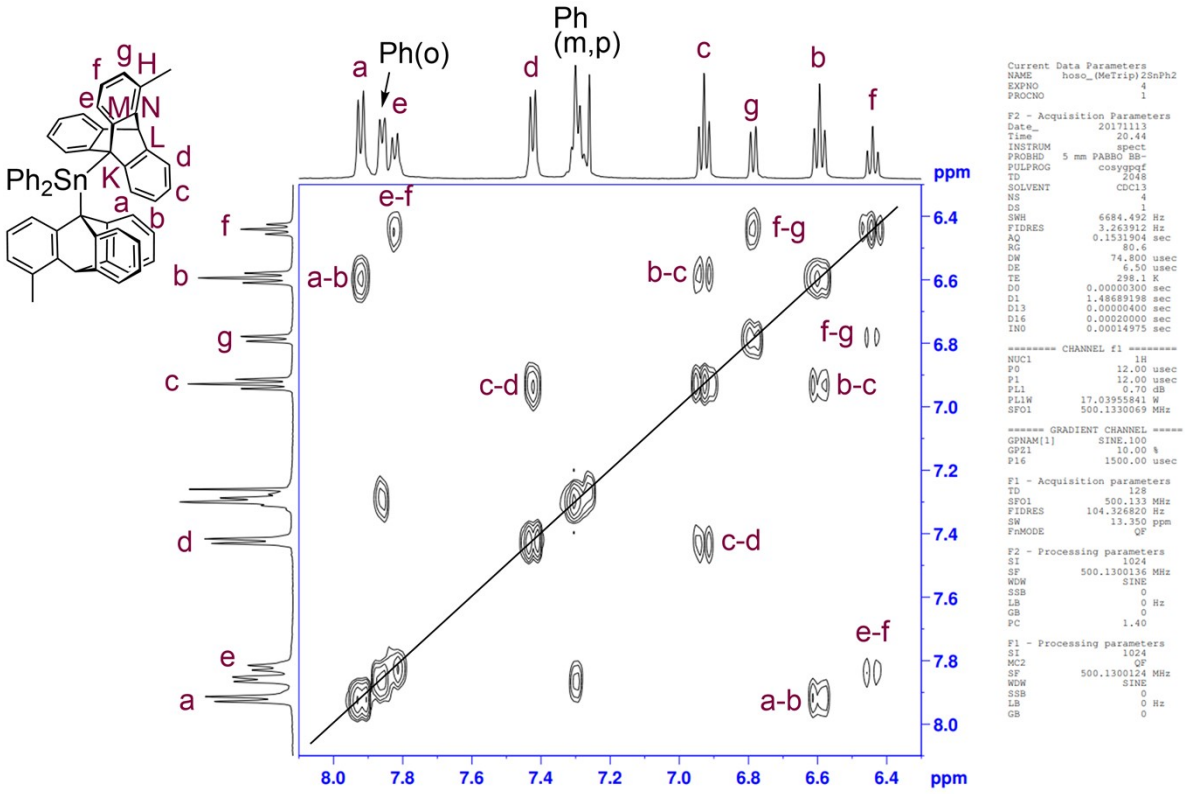

Fig. S18. ^{1}H-^{1}H COSY NMR spectrum of **SnPh2me** in $CDCl_3$.

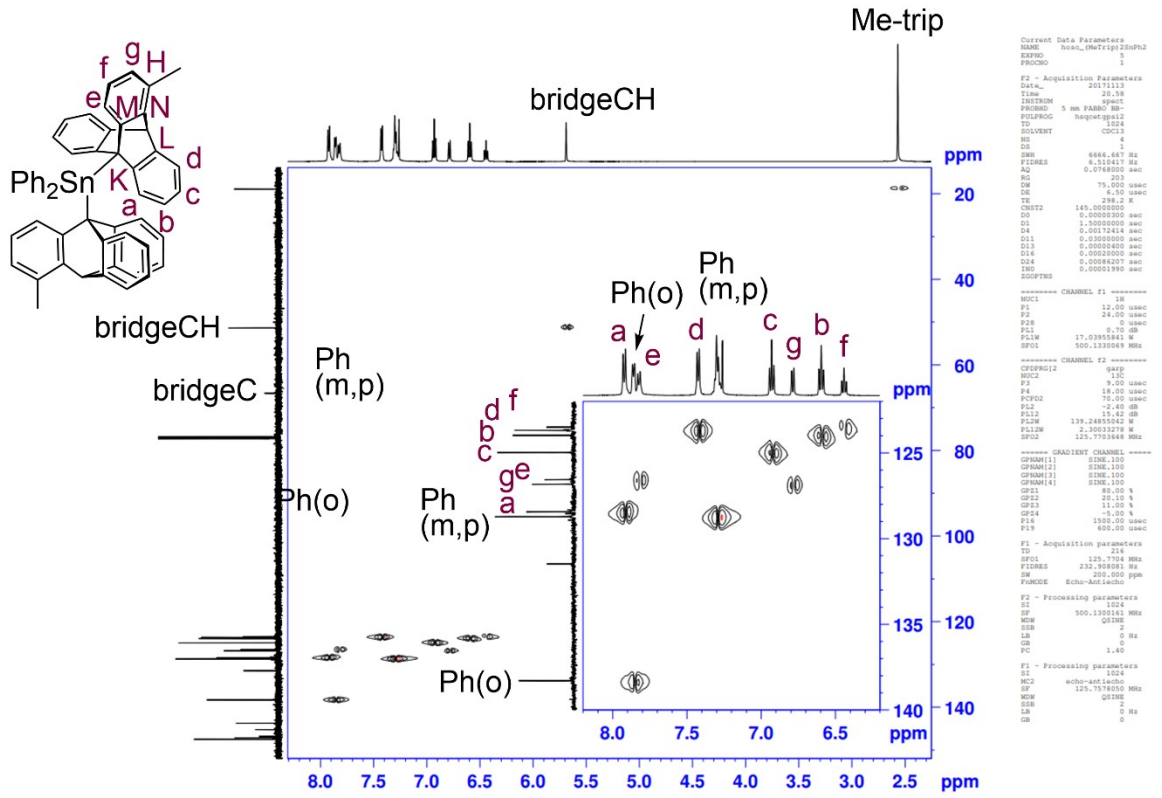

Fig. S19. ^{1}H-^{13}C HSQC NMR spectrum of **SnPh2me** in $CDCl_3$.

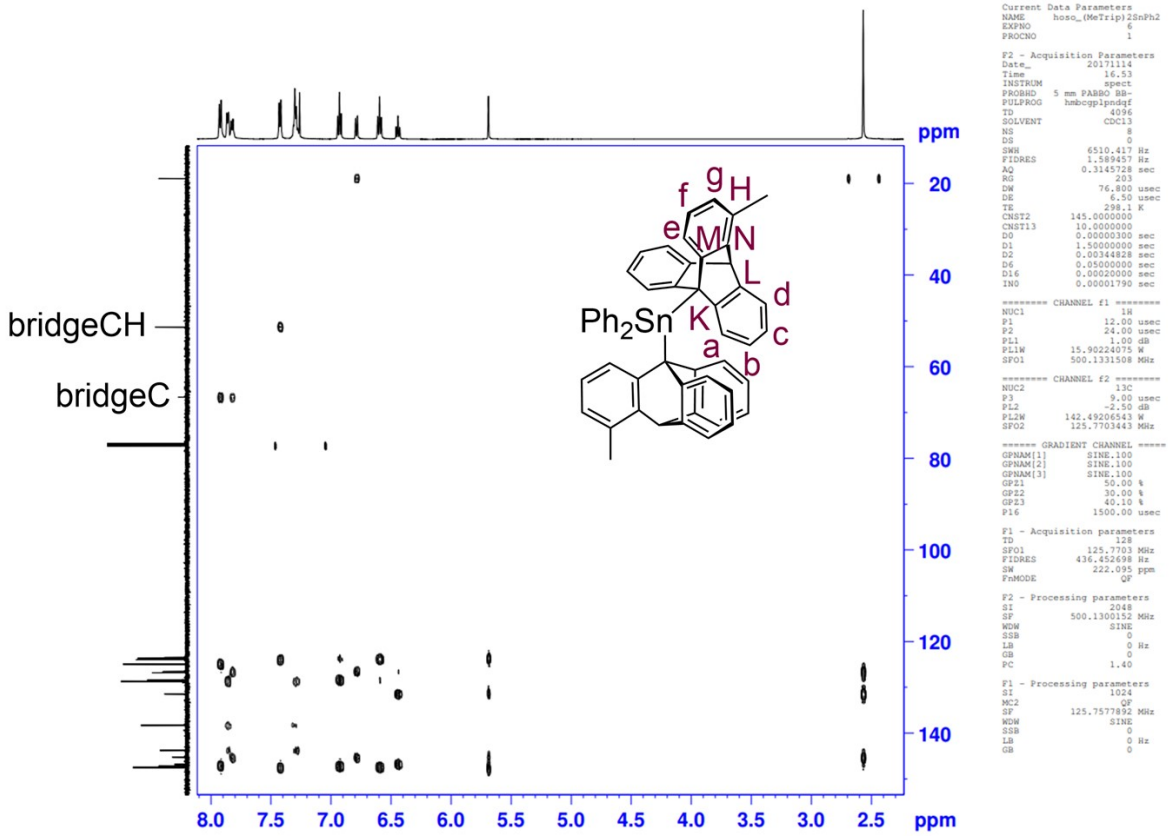

Fig. S20. ^{1}H-^{13}C HMBC NMR spectrum (the whole region) of **SnPh2me** in $CDCl_3$.

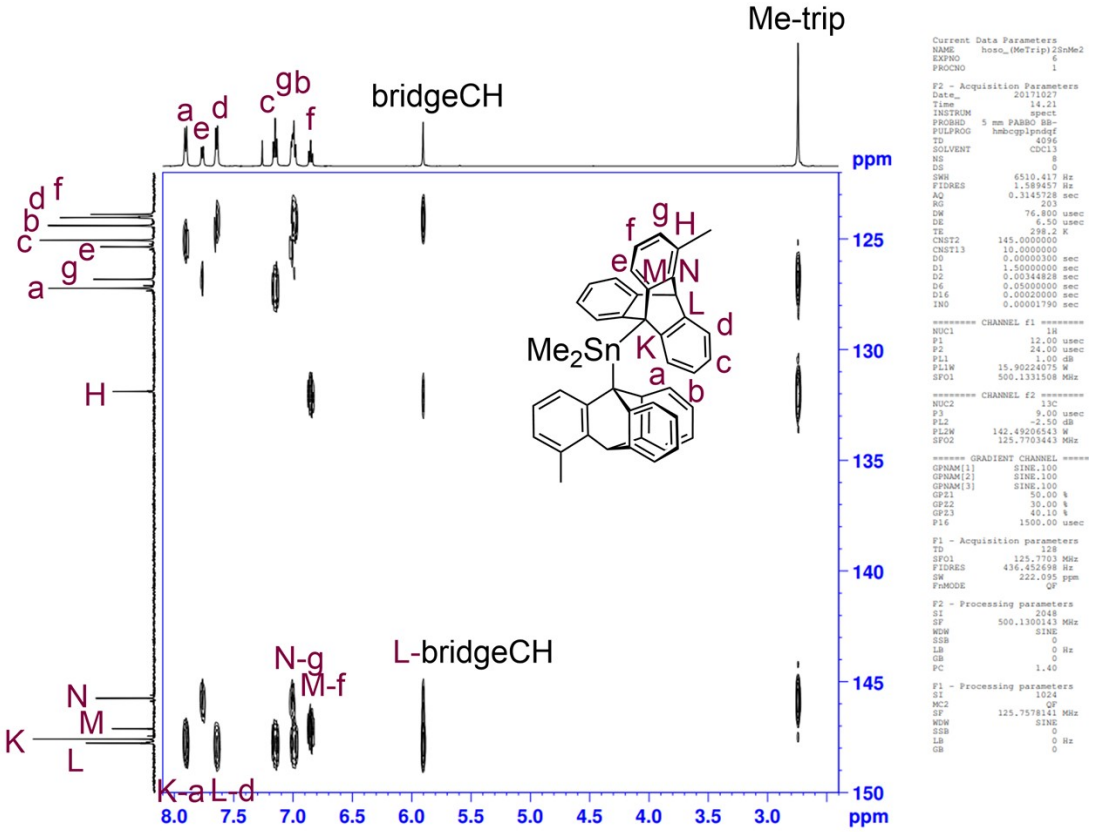

Fig. S21. ^{1}H-^{13}C HMBC NMR spectrum (the aromatic region) of **SnPh2me** in $CDCl_3$.

d. Spectra of SnMe2me

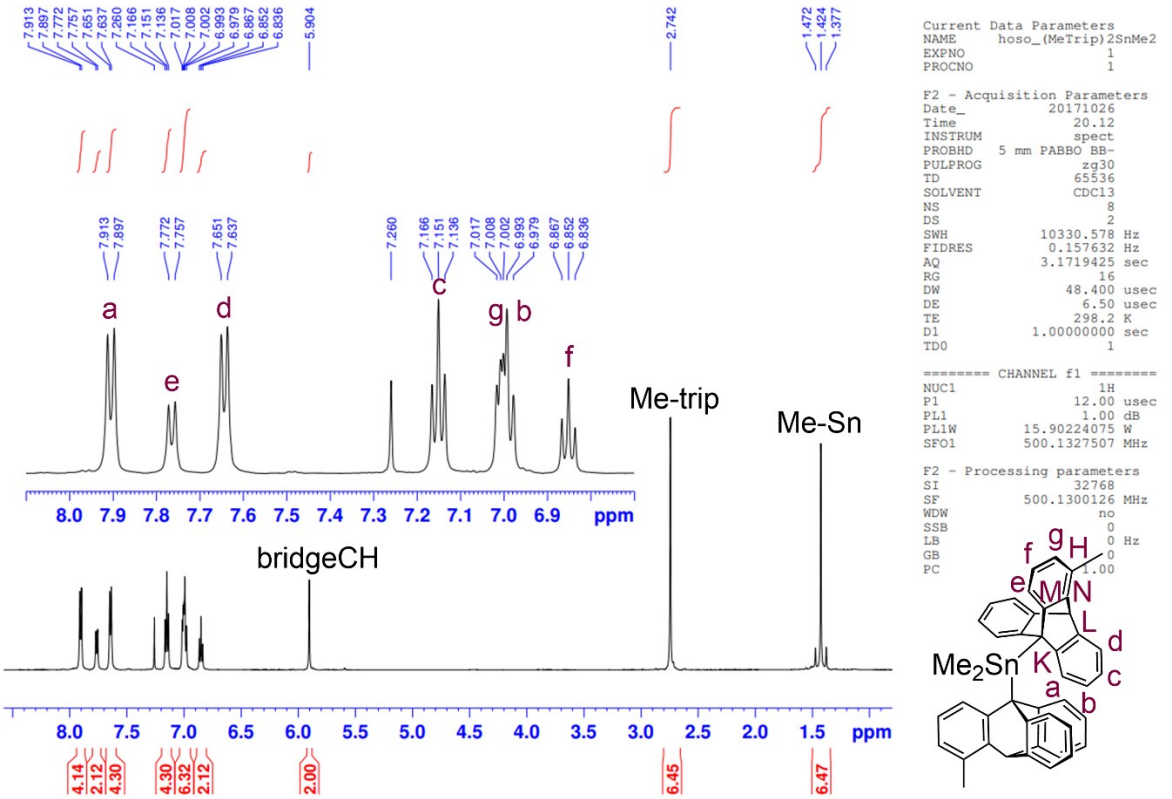

Fig. S22. ^{1}H NMR spectrum of **SnMe2me** in $CDCl_3$.

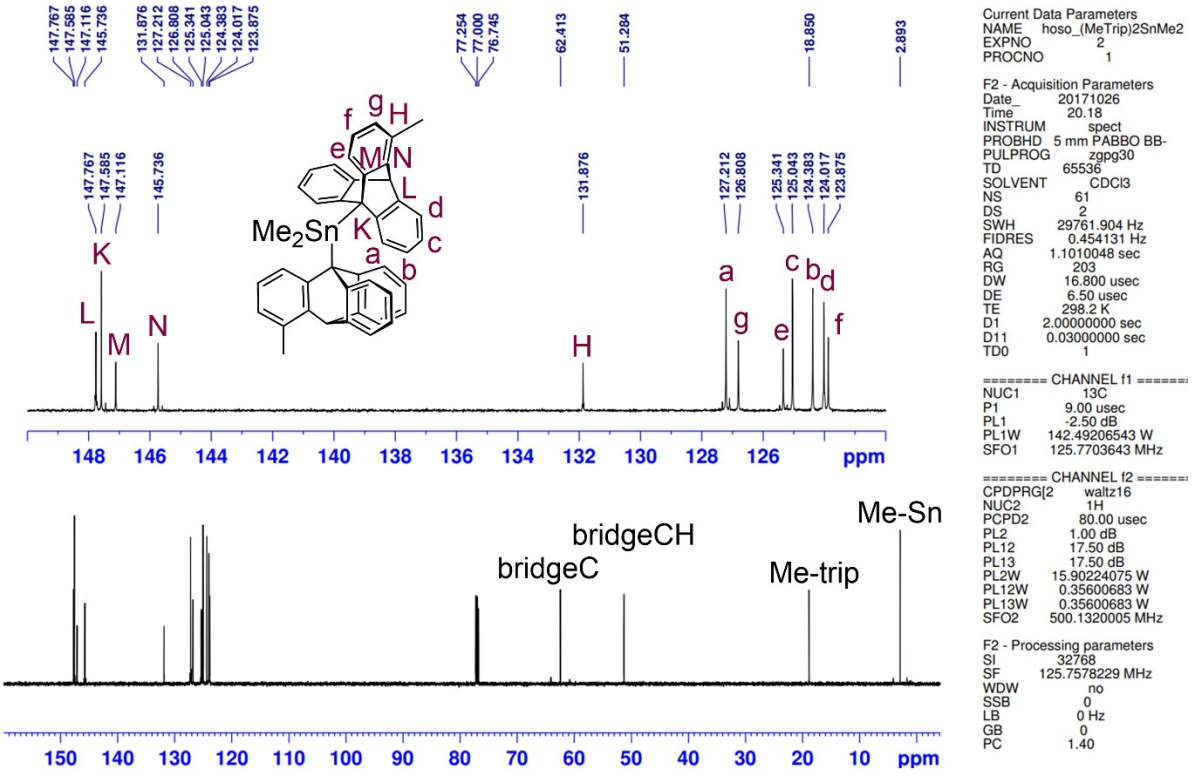

Fig. S23. ^{13}C NMR spectrum of **SnMe2me** in $CDCl_3$.

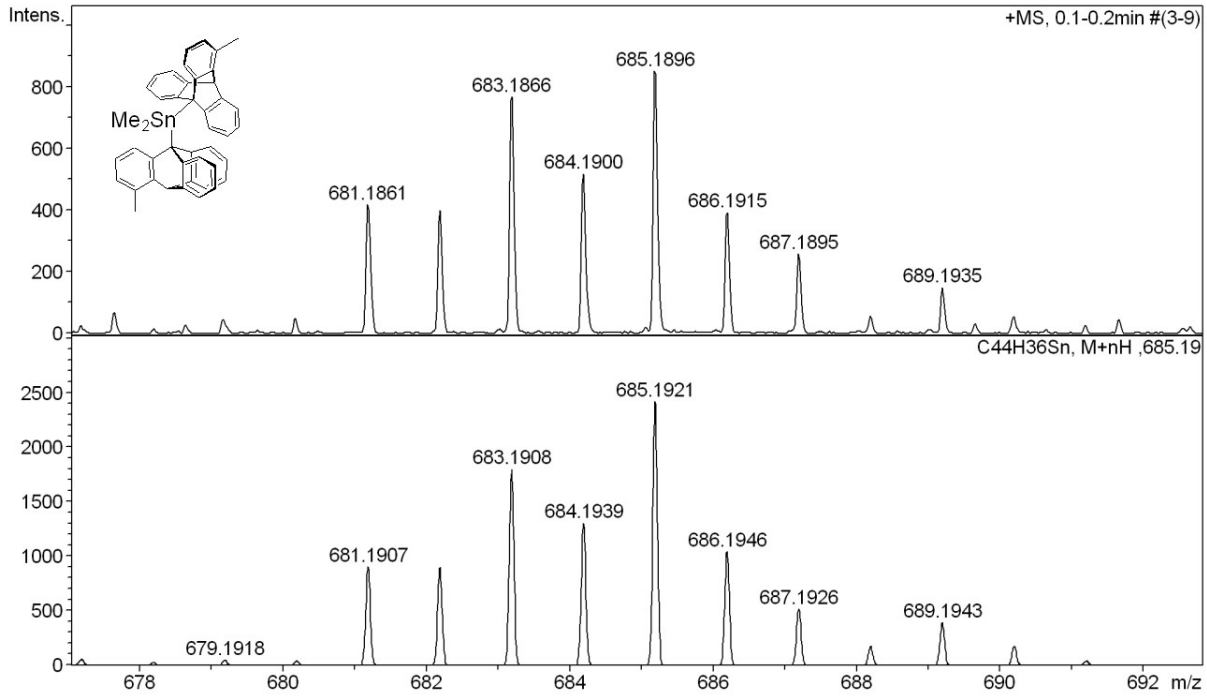

Fig. S24. HRMS spectrum of **SnMe2me** (ESI, positive). Top: obsd. Bottom: sim.

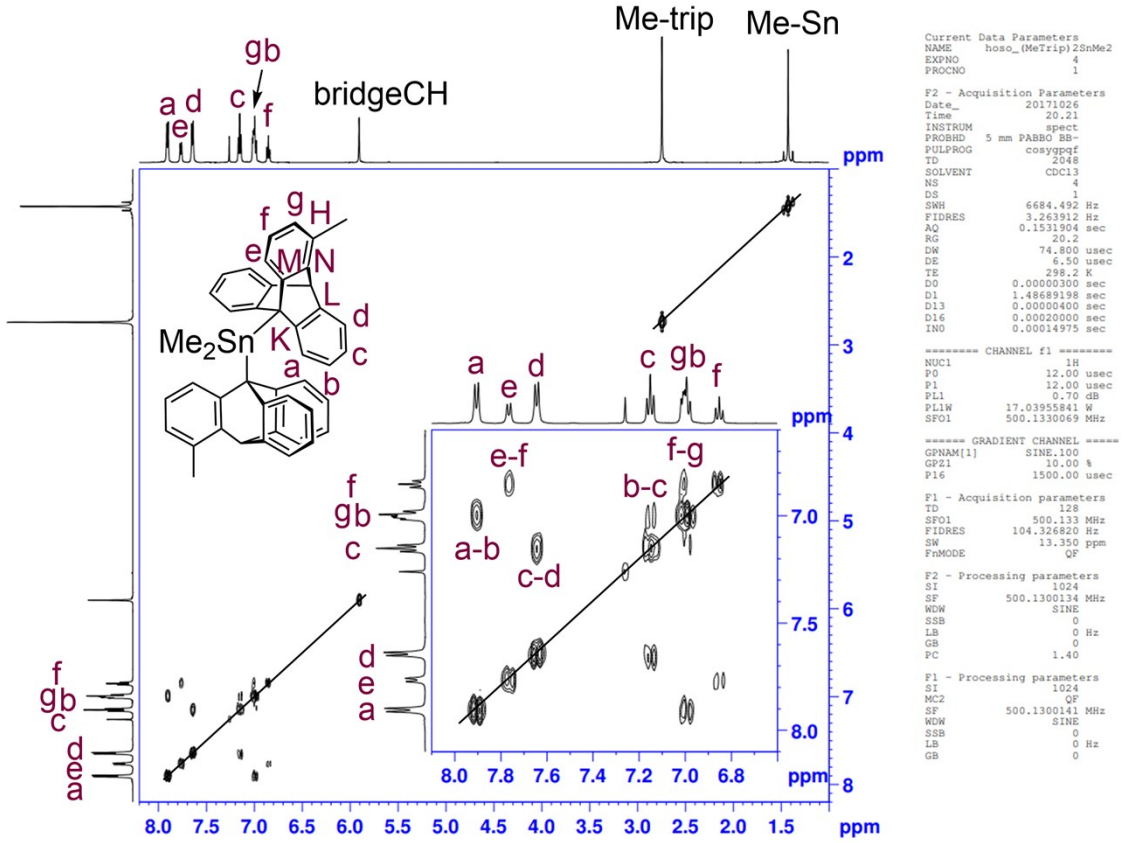

Fig. S25. ^{1}H-^{1}H COSY NMR spectrum of **SnMe2me** in $CDCl_3$.

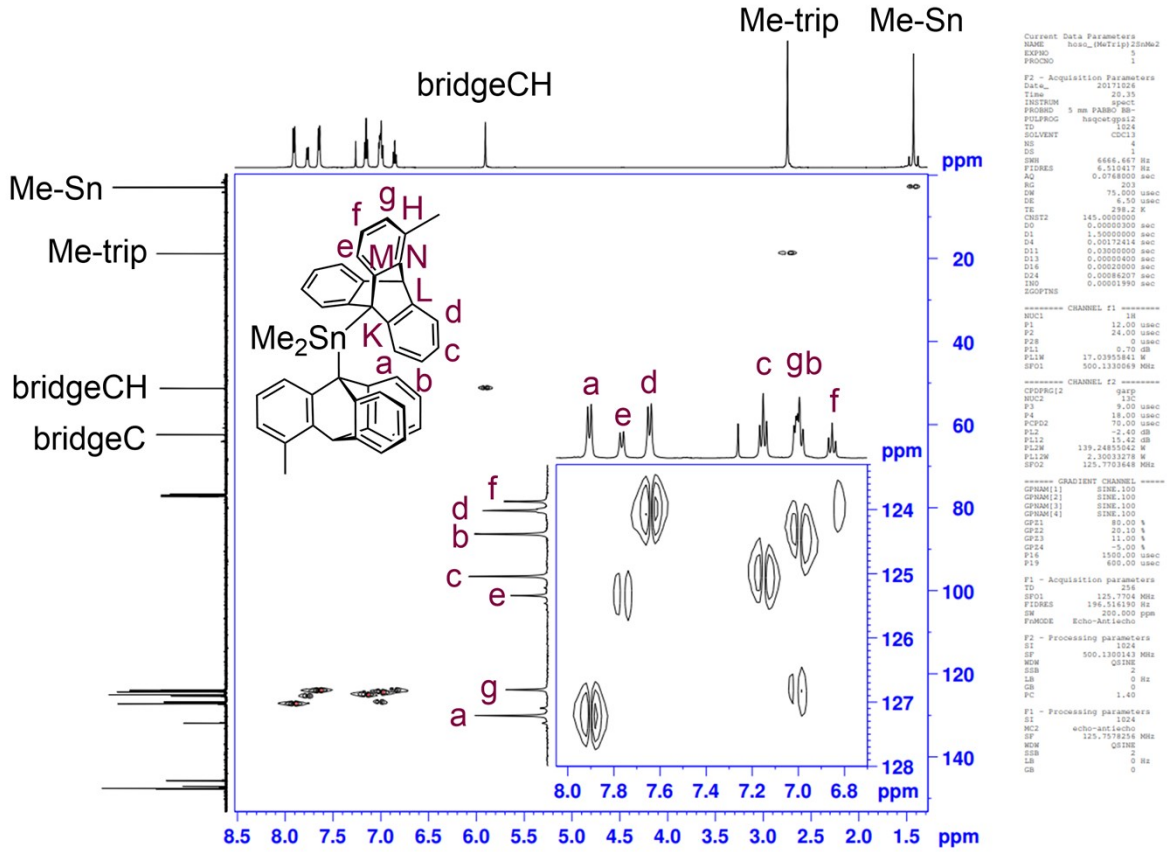

Fig. S26. ^{1}H-^{13}C HSQC NMR spectrum of **SnMe2me** in $CDCl_3$.

Fig. S27. ^{1}H-^{13}C HMBC NMR spectrum (the whole region) of **SnMe2me** in $CDCl_3$.

Fig. S28. ^{1}H-^{13}C HMBC NMR spectrum (the aromatic region) of **SnMe2me** in $CDCl_3$.

2. Appended Data of X-ray Crystallography

2-1. Crystal Data

Table S1. Crystal Data

Compound		**SnPh2**	**SnMe2** (with 4MeOH)
CCDC #		2259574	2259575
Empirical formula		C52 H36 Sn	C46 H48 O4 Sn
Temperature		200(2) K	100(2) K
Crystal shape & Color		Prism, colorless	Prism, colorless
Crystal size		0.330 x 0.280 x 0.260 mm^3	0.400 x 0.300 x 0.200 mm^3
Formula weight / g mol^{-1}		779.50	783.53
Crystal system		Orthorhombic	Monoclinic
Space group		*Fdd*2	*C*2/*c*
Z		16	4
Calculated density		1.410 Mg/m^3	1.385 Mg/m^3
Cell parameter	*a*	18.4107(4) Å	24.8807(14) Å
	b	30.9552(6) Å	11.0845(6) Å
	c	25.7752(5) Å	16.1241(9) Å
	α	90°	90°
	β	90°	122.3220(10)°
	γ	90°	90°
	V	14689.5(5) $Å^3$	3757.9(4) $Å^3$
F(000)		6368	1624
Absorption coefficient		0.733 mm^{-1}	5.746 mm^{-1}
***θ* range for collection**		2.397 to 32.560° (MoKα)	4.205 to 71.273° (CuKα)
Index ranges		-27<=h<=24, -46<=k<=46, -38<=l<=37	-30<=h<=30, -13<=k<=13, -19<=l<=19
Reflections collected		48405	17172
Independent reflections		12621 [R(int) = 0.0281]	3541 [R(int) = 0.0256]
Completeness		99.7 %	98.6 %
Goodness-of-fit on F^2		1.040	1.136
Final R indices [I>2sigma(I)]		R1 = 0.0210, wR2 = 0.0492	R1 = 0.0258, wR2 = 0.0691
R indices (all data)		R1 = 0.0233, wR2 = 0.0501	R1 = 0.0259, wR2 = 0.0692

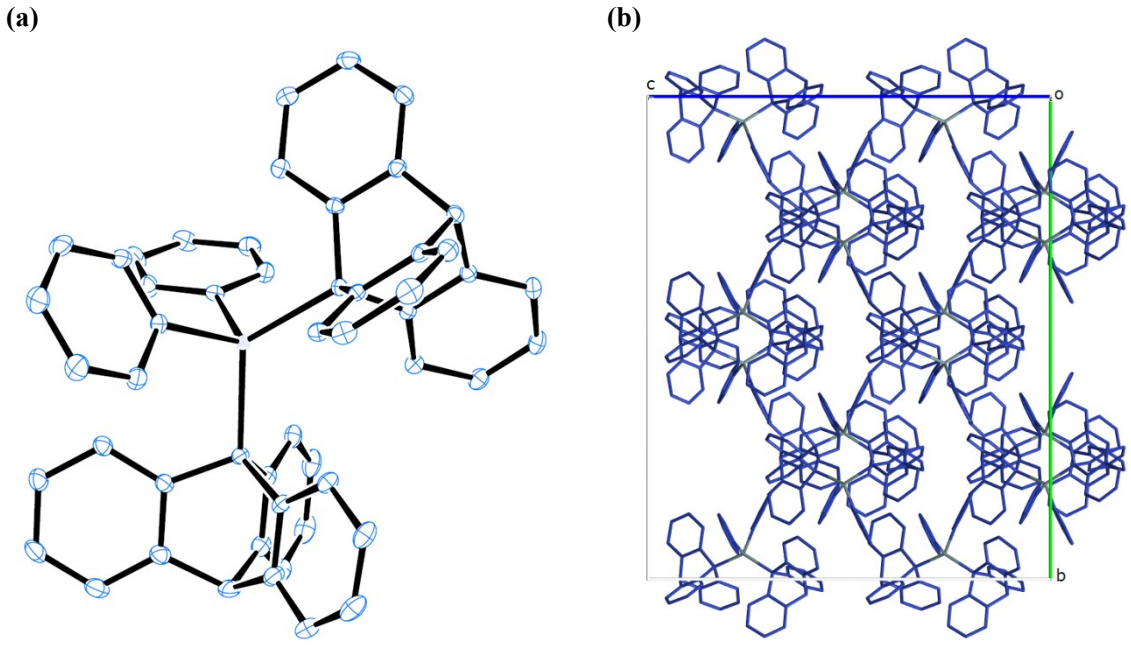

Fig. S29. (a) An ORTEP drawing (50% thermal ellipsoids) of molecular structure and (b) crystal packing of **SnPh2** determined by X-ray crystallography.

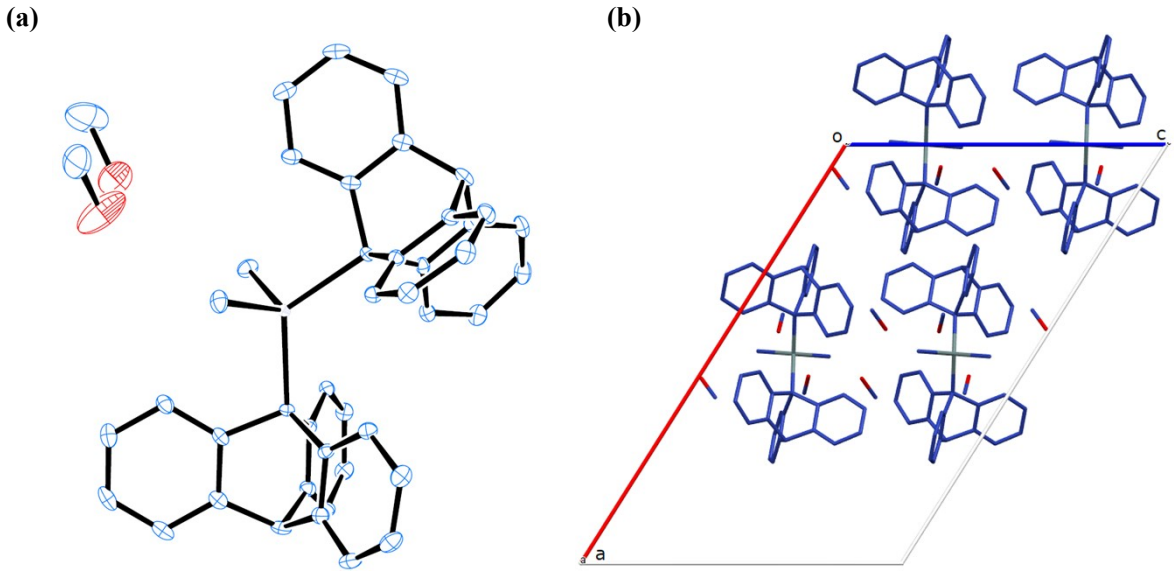

Fig. S30. (a) An ORTEP drawing (50% thermal ellipsoids) of molecular structure and (b) crystal packing of **SnMe2** determined by X-ray crystallography.

3. Appended Data of VT-NMR Study

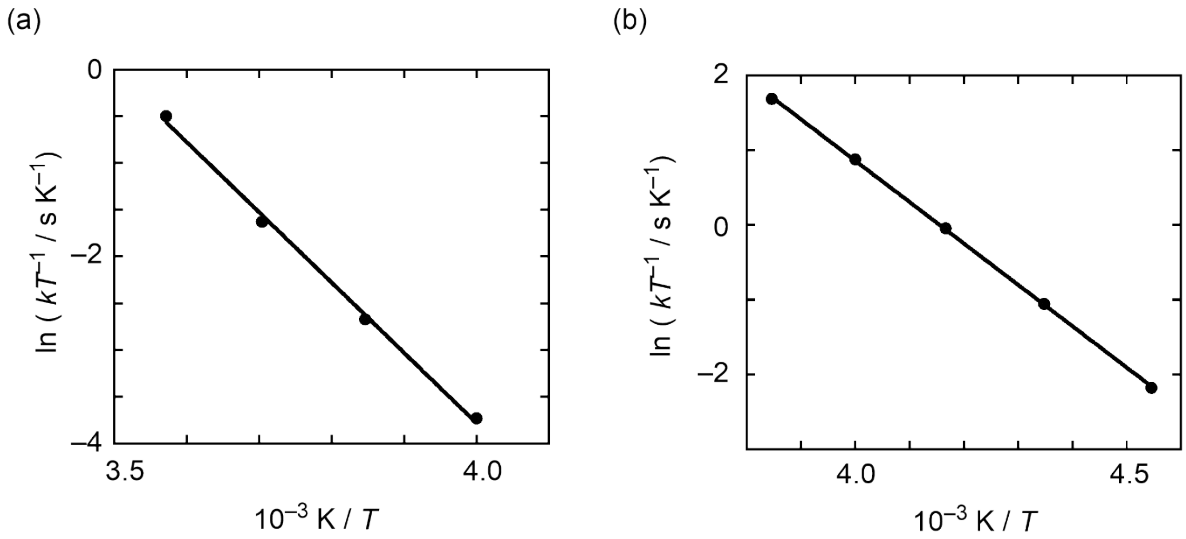

Fig. S31. Eyring plot of gear slippage (k_{ex} values taken from Fig. 5): (a) **SnPh2me** and (b) **SnMe2me**.

4. Appended Data of DFT Calculations

Table S2. Optimized Structural Coordinate and its Total Energy of **SnPh2** (Ground State) at B3LYP-D3/B1(Sn:LanL2DZ, C,H:6-31G(d)) level **HF=-2006.6423324, NImg=0**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	0.000000	-0.000000	0.723330
2	6	0	0.607862	1.627833	1.981488
3	6	0	-0.607862	-1.627833	1.981488
4	6	0	-1.860003	0.652124	-0.365346
5	6	0	1.860003	-0.652124	-0.365346
6	6	0	-2.130587	-0.218824	-1.614285
7	6	0	2.130587	0.218824	-1.614285
8	6	0	-3.140909	0.545473	0.518855
9	6	0	3.140909	-0.545473	0.518855
10	6	0	-1.947221	2.121458	-0.875486
11	6	0	1.947221	-2.121458	-0.875486
12	6	0	-3.336241	0.070701	-2.279142
13	6	0	3.336241	-0.070701	-2.279142
14	6	0	-4.330326	0.820931	-0.187772
15	6	0	4.330326	-0.820931	-0.187772
16	6	0	-3.138552	2.390273	-1.583380
17	6	0	3.138552	-2.390273	-1.583380
18	6	0	-4.102403	1.210685	-1.640316
19	6	0	4.102403	-1.210685	-1.640316
20	1	0	-5.031142	1.449432	-2.165437
21	1	0	5.031142	-1.449432	-2.165437
22	6	0	-1.304786	-1.205978	-2.141642
23	6	0	1.304786	1.205978	-2.141642
24	6	0	-3.230749	0.303673	1.887954
25	6	0	3.230749	-0.303673	1.887954
26	6	0	-1.042634	3.162468	-0.680026
27	6	0	1.042634	-3.162468	-0.680026
28	6	0	-3.720951	-0.630850	-3.414785
29	6	0	3.720951	0.630850	-3.414785
30	6	0	-5.568672	0.796200	0.440472
31	6	0	5.568672	-0.796200	0.440472
32	6	0	-3.390394	3.645939	-2.119450
33	6	0	3.390394	-3.645939	-2.119450
34	6	0	-1.684099	-1.922331	-3.283568
35	6	0	1.684099	1.922331	-3.283568
36	6	0	-4.476686	0.281884	2.528571
37	6	0	4.476686	-0.281884	2.528571
38	6	0	-1.293343	4.431697	-1.220109
39	6	0	1.293343	-4.431697	-1.220109
40	6	0	-2.892349	-1.642104	-3.917239
41	6	0	2.892349	1.642104	-3.917239
42	6	0	-5.645715	0.514589	1.809390
43	6	0	5.645715	-0.514589	1.809390
44	6	0	-2.456015	4.674631	-1.946137
45	6	0	2.456015	-4.674631	-1.946137
46	1	0	-0.345157	-1.427786	-1.698004
47	1	0	0.345157	1.427786	-1.698004
48	1	0	-2.346949	0.107045	2.478917
49	1	0	2.346949	-0.107045	2.478917
50	1	0	-0.140937	3.013778	-0.101854
51	1	0	0.140937	-3.013778	-0.101854
52	1	0	-4.658662	-0.388281	-3.909340
53	1	0	4.658662	0.388281	-3.909340
54	1	0	-6.468659	1.010625	-0.131141
55	1	0	6.468659	-1.010625	-0.131141
56	1	0	-4.315589	3.826521	-2.661773
57	1	0	4.315589	-3.826521	-2.661773
58	1	0	-1.021592	-2.692808	-3.667825
59	1	0	1.021592	2.692808	-3.667825
60	1	0	-4.521059	0.078823	3.595052
61	1	0	4.521059	-0.078823	3.595052
62	1	0	-0.570858	5.227379	-1.059918
63	1	0	0.570858	-5.227379	-1.059918
64	1	0	-3.188207	-2.196232	-4.803953
65	1	0	3.188207	2.196232	-4.803953
66	1	0	-6.611070	0.493425	2.307845
67	1	0	6.611070	-0.493425	2.307845

68	1	0	-2.646980	5.659175	-2.364521
69	1	0	2.646980	-5.659175	-2.364521
70	6	0	-0.000000	1.852462	3.226394
71	6	0	1.637156	2.500822	1.581591
72	6	0	1.411540	3.778240	3.623212
73	6	0	0.397182	2.916906	4.042190
74	6	0	2.032998	3.567297	2.389302
75	1	0	-0.788397	1.193433	3.582118
76	1	0	2.148708	2.343259	0.634049
77	1	0	1.719830	4.607110	4.255196
78	1	0	-0.087690	3.071831	5.002905
79	1	0	2.830901	4.228114	2.060008
80	6	0	0.000000	-1.852462	3.226394
81	6	0	-1.637156	-2.500822	1.581591
82	6	0	-1.411540	-3.778240	3.623212
83	6	0	-0.397182	-2.916906	4.042190
84	6	0	-2.032998	-3.567297	2.389302
85	1	0	0.788397	-1.193433	3.582118
86	1	0	-2.148708	-2.343259	0.634049
87	1	0	-1.719830	-4.607110	4.255196
88	1	0	0.087690	-3.071831	5.002905
89	1	0	-2.830901	-4.228114	2.060008

Table S3. Optimized Structural Coordinate and its Total Energy of **SnPh2** (Ground State) at ωB97XD/B1(Sn;LanL2DZ, C,H;6-31G(d)) level **HF=-2005.9287733, NImg=0**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	0.000000	-0.000000	0.721153
2	6	0	0.601833	1.630695	1.976923
3	6	0	-0.601833	-1.630695	1.976923
4	6	0	-1.849717	0.642783	-0.364992
5	6	0	1.849717	-0.642783	-0.364992
6	6	0	-2.114492	-0.224236	-1.610921
7	6	0	2.114492	0.224236	-1.610921
8	6	0	-3.125672	0.529948	0.513757
9	6	0	3.125672	-0.529948	0.513757
10	6	0	-1.941552	2.106273	-0.870237
11	6	0	1.941552	-2.106273	-0.870237
12	6	0	-3.315180	0.060413	-2.274885
13	6	0	3.315180	-0.060413	-2.274885
14	6	0	-4.311390	0.799975	-0.189845
15	6	0	4.311390	-0.799975	-0.189845
16	6	0	-3.127903	2.372140	-1.575983
17	6	0	3.127903	-2.372140	-1.575983
18	6	0	-4.084668	1.193012	-1.636948
19	6	0	4.084668	-1.193012	-1.636948
20	1	0	-5.013518	1.429405	-2.162428
21	1	0	5.013518	-1.429405	-2.162428
22	6	0	-1.285759	-1.204570	-2.135234
23	6	0	1.285759	1.204570	-2.135234
24	6	0	-3.213297	0.286579	1.878289
25	6	0	3.213297	-0.286579	1.878289
26	6	0	-1.041856	3.144797	-0.670994
27	6	0	1.041856	-3.144797	-0.670994
28	6	0	-3.694132	-0.639343	-3.408543
29	6	0	3.694132	0.639343	-3.408543
30	6	0	-5.546450	0.767048	0.435482
31	6	0	5.546450	-0.767048	0.435482
32	6	0	-3.381779	3.624792	-2.107786
33	6	0	3.381779	-3.624792	-2.107786
34	6	0	-1.658554	-1.919335	-3.274898
35	6	0	1.658554	1.919335	-3.274898
36	6	0	-4.455397	0.255465	2.516394
37	6	0	4.455397	-0.255465	2.516394
38	6	0	-1.293830	4.410878	-1.206180
39	6	0	1.293830	-4.410878	-1.206180
40	6	0	-2.862910	-1.643844	-3.908477
41	6	0	2.862910	1.643844	-3.908477
42	6	0	-5.621798	0.481749	1.799380
43	6	0	5.621798	-0.481749	1.799380
44	6	0	-2.452608	4.651827	-1.930862
45	6	0	2.452608	-4.651827	-1.930862

46	1	0	-0.324794	-1.424555	-1.690320
47	1	0	0.324794	1.424555	-1.690320
48	1	0	-2.328794	0.095933	2.471506
49	1	0	2.328794	-0.095933	2.471506
50	1	0	-0.139724	2.996177	-0.091664
51	1	0	0.139724	-2.996177	-0.091664
52	1	0	-4.631142	-0.401072	-3.905446
53	1	0	4.631142	0.401072	-3.905446
54	1	0	-6.447632	0.977955	-0.134633
55	1	0	6.447632	-0.977955	-0.134633
56	1	0	-4.305867	3.805637	-2.650941
57	1	0	4.305867	-3.805637	-2.650941
58	1	0	-0.992094	-2.685575	-3.659036
59	1	0	0.992094	2.685575	-3.659036
60	1	0	-4.499207	0.050210	3.581703
61	1	0	4.499207	-0.050210	3.581703
62	1	0	-0.574468	5.207706	-1.042759
63	1	0	0.574468	-5.207706	-1.042759
64	1	0	-3.154209	-2.197820	-4.795886
65	1	0	3.154209	2.197820	-4.795886
66	1	0	-6.586363	0.453379	2.297399
67	1	0	6.586363	-0.453379	2.297399
68	1	0	-2.645079	5.636541	-2.346210
69	1	0	2.645079	-5.636541	-2.346210
70	6	0	-0.000000	1.850423	3.219872
71	6	0	1.622924	2.504245	1.573872
72	6	0	1.401773	3.774937	3.611186
73	6	0	0.395231	2.912876	4.032625
74	6	0	2.017538	3.567945	2.378215
75	1	0	-0.783911	1.187299	3.578385
76	1	0	2.130632	2.349860	0.623181
77	1	0	1.709553	4.603877	4.242072
78	1	0	-0.086115	3.065473	4.994514
79	1	0	2.811248	4.231182	2.046461
80	6	0	0.000000	-1.850423	3.219872
81	6	0	-1.622924	-2.504245	1.573872
82	6	0	-1.401773	-3.774937	3.611186
83	6	0	-0.395231	-2.912876	4.032625
84	6	0	-2.017538	-3.567945	2.378215
85	1	0	0.783911	-1.187299	3.578385
86	1	0	-2.130632	-2.349860	0.623181
87	1	0	-1.709553	-4.603877	4.242072
88	1	0	0.086115	-3.065473	4.994514
89	1	0	-2.811248	-4.231182	2.046461

Table S4. Optimized Structural Coordinate and its Total Energy of **SnPh2** (Transition State) at B3LYP-D3/B1(Sn:LanL2DZ, C,H:6-31G(d)) level **HF=-2006.6180576, NImg=1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	0.612895	0.025172	0.000000
2	6	0	-0.345073	-2.069232	0.000000
3	6	0	0.840191	-3.100444	0.000000
4	6	0	0.426934	-4.446174	0.000000
5	6	0	-1.075790	-4.615952	0.000000
6	1	0	-1.386685	-5.664084	0.000000
7	6	0	-1.236001	-2.481273	1.201286
8	6	0	-1.590081	-3.846955	1.207879
9	6	0	-1.236001	-2.481273	-1.201286
10	6	0	-1.590081	-3.846955	-1.207879
11	6	0	-0.298649	2.120894	-0.000000
12	6	0	0.701926	3.321627	-0.000000
13	6	0	0.045444	4.574862	-0.000000
14	6	0	-1.482994	4.486825	-0.000000
15	1	0	-1.958743	5.471174	-0.000000
16	6	0	-1.154651	2.427271	-1.260528
17	6	0	-1.830887	3.661560	-1.220149
18	6	0	-1.154651	2.427271	1.260528
19	6	0	-1.830887	3.661560	1.220149
20	6	0	2.214552	-2.845747	0.000000
21	6	0	3.141165	-3.893841	0.000000
22	6	0	1.340894	-5.494353	0.000000
23	6	0	2.710756	-5.218605	0.000000

24	1	0	2.601793	-1.834715	0.000000
25	1	0	4.202256	-3.661460	0.000000
26	1	0	0.982012	-6.520821	0.000000
27	1	0	3.431977	-6.031320	0.000000
28	6	0	2.094269	3.304351	-0.000000
29	6	0	2.825856	4.501729	-0.000000
30	6	0	0.766337	5.760747	-0.000000
31	6	0	2.167354	5.727166	-0.000000
32	1	0	2.638137	2.365470	-0.000000
33	1	0	3.911555	4.461900	-0.000000
34	1	0	0.239504	6.712068	-0.000000
35	1	0	2.733529	6.654433	-0.000000
36	6	0	-1.777269	-1.656379	2.177974
37	6	0	-2.595676	-2.180798	3.186604
38	6	0	-2.395358	-4.377069	2.207318
39	6	0	-2.891730	-3.540955	3.215465
40	1	0	-1.596575	-0.594126	2.152463
41	1	0	-3.002441	-1.512870	3.941170
42	1	0	-2.652035	-5.433758	2.190729
43	1	0	-3.523157	-3.949951	3.999560
44	6	0	-1.777269	-1.656379	-2.177974
45	6	0	-2.595676	-2.180798	-3.186604
46	6	0	-2.395358	-4.377069	-2.207318
47	6	0	-2.891730	-3.540955	-3.215465
48	1	0	-1.596575	-0.594126	-2.152463
49	1	0	-3.002441	-1.512870	-3.941170
50	1	0	-2.652035	-5.433758	-2.190729
51	1	0	-3.523157	-3.949951	-3.999560
52	6	0	-1.194151	1.708356	-2.453172
53	6	0	-1.993077	2.132507	-3.522939
54	6	0	-2.629460	4.091637	-2.272865
55	6	0	-2.734676	3.307136	-3.426726
56	1	0	-0.562821	0.843634	-2.594921
57	1	0	-2.012857	1.543061	-4.435603
58	1	0	-3.144069	5.047252	-2.204768
59	1	0	-3.357931	3.634545	-4.254365
60	6	0	-1.194151	1.708356	2.453172
61	6	0	-1.993077	2.132507	3.522939
62	6	0	-2.629460	4.091637	2.272865
63	6	0	-2.734676	3.307136	3.426726
64	1	0	-0.562821	0.843634	2.594921
65	1	0	-2.012857	1.543061	4.435603
66	1	0	-3.144069	5.047252	2.204768
67	1	0	-3.357931	3.634545	4.254365
68	6	0	1.661864	-0.036414	-1.913040
69	6	0	2.214129	1.111582	-2.512421
70	6	0	1.658755	-1.215932	-2.683042
71	6	0	2.777760	-0.111427	-4.524668
72	6	0	2.771921	1.075737	-3.792491
73	6	0	2.208960	-1.255825	-3.966502
74	1	0	2.190940	2.067484	-2.006379
75	1	0	1.216474	-2.126396	-2.301109
76	1	0	3.207118	-0.140591	-5.522944
77	1	0	3.190722	1.984205	-4.218481
78	1	0	2.184854	-2.186227	-4.528319
79	6	0	1.661864	-0.036414	1.913040
80	6	0	2.214129	1.111582	2.512421
81	6	0	1.658755	-1.215932	2.683042
82	6	0	2.777760	-0.111427	4.524668
83	6	0	2.771921	1.075737	3.792491
84	6	0	2.208960	-1.255825	3.966502
85	1	0	2.190940	2.067484	2.006379
86	1	0	1.216474	-2.126396	2.301109
87	1	0	3.207118	-0.140591	5.522944
88	1	0	3.190722	1.984205	4.218481
89	1	0	2.184854	-2.186227	4.528319

Table S5. Optimized Structural Coordinate and its Total Energy of **SnPh2** (Transition State) at ωB97XD/B1(Sn;LanL2DZ, C,H;6-31G(d)) level **HF=-2005.9027778, NImg=1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	0.595793	0.021362	-0.000000

2	6	0	-0.341420	-2.063079	0.000000
3	6	0	0.847913	-3.080315	0.000000
4	6	0	0.448991	-4.424165	0.000000
5	6	0	-1.047663	-4.607164	0.000000
6	1	0	-1.349339	-5.657727	0.000000
7	6	0	-1.225654	-2.481263	1.195768
8	6	0	-1.566693	-3.844150	1.204057
9	6	0	-1.225654	-2.481263	-1.195768
10	6	0	-1.566693	-3.844150	-1.204057
11	6	0	-0.302758	2.105480	-0.000000
12	6	0	0.716912	3.281112	-0.000000
13	6	0	0.090384	4.542834	-0.000000
14	6	0	-1.434351	4.486809	-0.000000
15	1	0	-1.889975	5.480359	-0.000000
16	6	0	-1.150588	2.427152	-1.255509
17	6	0	-1.798556	3.670275	-1.215801
18	6	0	-1.150588	2.427152	1.255509
19	6	0	-1.798556	3.670275	1.215801
20	6	0	2.216219	-2.814151	0.000000
21	6	0	3.148894	-3.850511	0.000000
22	6	0	1.368912	-5.462023	0.000000
23	6	0	2.731740	-5.175171	0.000000
24	1	0	2.600250	-1.800936	-0.000000
25	1	0	4.207115	-3.608852	-0.000000
26	1	0	1.019828	-6.491346	0.000000
27	1	0	3.459993	-5.980578	0.000000
28	6	0	2.104301	3.230408	-0.000000
29	6	0	2.859952	4.407307	-0.000000
30	6	0	0.835044	5.709158	-0.000000
31	6	0	2.230595	5.643327	-0.000000
32	1	0	2.628361	2.278789	-0.000000
33	1	0	3.943792	4.343838	-0.000000
34	1	0	0.331246	6.672325	-0.000000
35	1	0	2.817601	6.556705	-0.000000
36	6	0	-1.775681	-1.659780	2.163909
37	6	0	-2.587978	-2.186643	3.170137
38	6	0	-2.366319	-4.377610	2.200582
39	6	0	-2.869409	-3.545357	3.202781
40	1	0	-1.607637	-0.594919	2.131475
41	1	0	-3.003933	-1.520970	3.920604
42	1	0	-2.614867	-5.435780	2.187244
43	1	0	-3.498141	-3.957162	3.986539
44	6	0	-1.775681	-1.659780	-2.163909
45	6	0	-2.587978	-2.186643	-3.170137
46	6	0	-2.366319	-4.377610	-2.200582
47	6	0	-2.869409	-3.545357	-3.202781
48	1	0	-1.607637	-0.594919	-2.131475
49	1	0	-3.003933	-1.520970	-3.920604
50	1	0	-2.614867	-5.435780	-2.187244
51	1	0	-3.498141	-3.957162	-3.986539
52	6	0	-1.207542	1.709420	-2.443094
53	6	0	-1.998520	2.146400	-3.507808
54	6	0	-2.589209	4.114095	-2.263299
55	6	0	-2.714141	3.331879	-3.411491
56	1	0	-0.591367	0.833661	-2.588688
57	1	0	-2.031435	1.557348	-4.419534
58	1	0	-3.084251	5.079487	-2.196051
59	1	0	-3.332409	3.670042	-4.237558
60	6	0	-1.207542	1.709420	2.443094
61	6	0	-1.998520	2.146400	3.507808
62	6	0	-2.589209	4.114095	2.263299
63	6	0	-2.714141	3.331879	3.411491
64	1	0	-0.591367	0.833661	2.588688
65	1	0	-2.031435	1.557348	4.419534
66	1	0	-3.084251	5.079487	2.196051
67	1	0	-3.332409	3.670042	4.237558
68	6	0	1.632150	-0.032938	-1.919877
69	6	0	2.131696	1.123224	-2.538822
70	6	0	1.659060	-1.216593	-2.673799
71	6	0	2.709711	-0.099540	-4.537869
72	6	0	2.670970	1.092283	-3.822226
73	6	0	2.190996	-1.252960	-3.960663
74	1	0	2.077644	2.084767	-2.044498
75	1	0	1.254220	-2.138261	-2.275285
76	1	0	3.125749	-0.125510	-5.541051

77	1	0	3.049147	2.009620	-4.264633
78	1	0	2.191267	-2.189589	-4.510818
79	6	0	1.632150	-0.032938	1.919877
80	6	0	2.131696	1.123224	2.538822
81	6	0	1.659060	-1.216593	2.673799
82	6	0	2.709711	-0.099540	4.537869
83	6	0	2.670970	1.092283	3.822226
84	6	0	2.190996	-1.252960	3.960663
85	1	0	2.077644	2.084767	2.044498
86	1	0	1.254220	-2.138261	2.275285
87	1	0	3.125749	-0.125510	5.541051
88	1	0	3.049147	2.009620	4.264633
89	1	0	2.191267	-2.189589	4.510818

Table S6. Optimized Structural Coordinate and its Total Energy of **SnMe2** (Ground State) at B3LYP-D3/B1(Sn:LanL2DZ, C,H:6-31G(d)) level **HF=-1623.1661381, NImg=0**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	-0.000000	0.000000	1.312261
2	6	0	0.831659	1.502528	2.618211
3	6	0	-0.831659	-1.502528	2.618211
4	6	0	-1.574889	1.131697	0.197814
5	6	0	1.574889	-1.131697	0.197814
6	6	0	-2.094936	0.450815	-1.089433
7	6	0	2.094936	-0.450815	-1.089433
8	6	0	-2.824317	1.361761	1.096979
9	6	0	2.824317	-1.361761	1.096979
10	6	0	-1.209443	2.574679	-0.260478
11	6	0	1.209443	-2.574679	-0.260478
12	6	0	-3.164495	1.125067	-1.708262
13	6	0	3.164495	-1.125067	-1.708262
14	6	0	-3.882147	2.020938	0.438893
15	6	0	3.882147	-2.020938	0.438893
16	6	0	-2.277322	3.236610	-0.904253
17	6	0	2.277322	-3.236610	-0.904253
18	6	0	-3.553546	2.406414	-0.993205
19	6	0	3.553546	-2.406414	-0.993205
20	1	0	-4.369866	2.940049	-1.487364
21	1	0	4.369866	-2.940049	-1.487364
22	6	0	-1.588535	-0.692292	-1.699126
23	6	0	1.588535	0.692292	-1.699126
24	6	0	-2.976878	1.057054	2.448447
25	6	0	2.976878	-1.057054	2.448447
26	6	0	-0.000000	3.252458	-0.115482
27	6	0	-0.000000	-3.252458	-0.115482
28	6	0	-3.741571	0.643951	-2.876558
29	6	0	3.741571	-0.643951	-2.876558
30	6	0	-5.070481	2.317480	1.093424
31	6	0	5.070481	-2.317480	1.093424
32	6	0	-2.135580	4.529243	-1.390621
33	6	0	2.135580	-4.529243	-1.390621
34	6	0	-2.164587	-1.185908	-2.876618
35	6	0	2.164587	1.185908	-2.876618
36	6	0	-4.172041	1.357534	3.116575
37	6	0	4.172041	-1.357534	3.116575
38	6	0	0.147866	4.557066	-0.607674
39	6	0	-0.147866	-4.557066	-0.607674
40	6	0	-3.244018	-0.527556	-3.461100
41	6	0	3.244018	0.527556	-3.461100
42	6	0	-5.222217	1.974554	2.442118
43	6	0	5.222217	-1.974554	2.442118
44	6	0	-0.913069	5.196390	-1.243008
45	6	0	0.913069	-5.196390	-1.243008
46	1	0	-0.728644	-1.205505	-1.293573
47	1	0	0.728644	1.205505	-1.293573
48	1	0	-2.176969	0.593380	3.011714
49	1	0	2.176969	-0.593380	3.011714
50	1	0	0.849319	2.781342	0.364386
51	1	0	-0.849319	-2.781342	0.364386
52	1	0	-4.568102	1.182163	-3.334793
53	1	0	4.568102	-1.182163	-3.334793
54	1	0	-5.870395	2.824768	0.559140

55	1	0	5.870395	-2.824768	0.559140
56	1	0	-2.973550	5.016620	-1.883502
57	1	0	2.973550	-5.016620	-1.883502
58	1	0	-1.754505	-2.083934	-3.330217
59	1	0	1.754505	2.083934	-3.330217
60	1	0	-4.271364	1.105890	4.168997
61	1	0	4.271364	-1.105890	4.168997
62	1	0	1.100843	5.065257	-0.488645
63	1	0	-1.100843	-5.065257	-0.488645
64	1	0	-3.690725	-0.910661	-4.374659
65	1	0	3.690725	0.910661	-4.374659
66	1	0	-6.149048	2.203012	2.961227
67	1	0	6.149048	-2.203012	2.961227
68	1	0	-0.795932	6.207598	-1.623051
69	1	0	0.795932	-6.207598	-1.623051
70	1	0	0.179165	2.380424	2.618756
71	1	0	0.883191	1.114309	3.641302
72	1	0	1.837911	1.814875	2.323890
73	1	0	-0.179165	-2.380424	2.618756
74	1	0	-0.883191	-1.114309	3.641302
75	1	0	-1.837911	-1.814875	2.323890

Table S7. Optimized Structural Coordinate and its Total Energy of **SnMe2** (Ground State) at ωB97XD/B1(Sn;LanL2DZ, C,H;6-31G(d)) level **HF=-1622.5970242, NImg=0**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	-0.000000	0.000000	1.304588
2	6	0	0.828805	1.501942	2.608699
3	6	0	-0.828805	-1.501942	2.608699
4	6	0	-1.568285	1.122963	0.195531
5	6	0	1.568285	-1.122963	0.195531
6	6	0	-2.086713	0.440860	-1.084014
7	6	0	2.086713	-0.440860	-1.084014
8	6	0	-2.811082	1.353087	1.092372
9	6	0	2.811082	-1.353087	1.092372
10	6	0	-1.205360	2.559151	-0.262141
11	6	0	1.205360	-2.559151	-0.262141
12	6	0	-3.152262	1.109496	-1.702870
13	6	0	3.152262	-1.109496	-1.702870
14	6	0	-3.866031	2.007805	0.436879
15	6	0	3.866031	-2.007805	0.436879
16	6	0	-2.268034	3.216912	-0.906180
17	6	0	2.268034	-3.216912	-0.906180
18	6	0	-3.540495	2.388878	-0.992873
19	6	0	3.540495	-2.388878	-0.992873
20	1	0	-4.357243	2.921194	-1.487222
21	1	0	4.357243	-2.921194	-1.487222
22	6	0	-1.580293	-0.700934	-1.685968
23	6	0	1.580293	0.700934	-1.685968
24	6	0	-2.958691	1.053126	2.441066
25	6	0	2.958691	-1.053126	2.441066
26	6	0	-0.000000	3.234350	-0.113504
27	6	0	0.000000	-3.234350	-0.113504
28	6	0	-3.727269	0.624583	-2.865858
29	6	0	3.727269	-0.624583	-2.865858
30	6	0	-5.049547	2.305455	1.090903
31	6	0	5.049547	-2.305455	1.090903
32	6	0	-2.125789	4.504965	-1.393150
33	6	0	2.125789	-4.504965	-1.393150
34	6	0	-2.153647	-1.199007	-2.857551
35	6	0	2.153647	1.199007	-2.857551
36	6	0	-4.148770	1.354434	3.108810
37	6	0	4.148770	-1.354434	3.108810
38	6	0	0.148918	4.533947	-0.605883
39	6	0	-0.148918	-4.533947	-0.605883
40	6	0	-3.230018	-0.545759	-3.443003
41	6	0	3.230018	0.545759	-3.443003
42	6	0	-5.197269	1.967163	2.436893
43	6	0	5.197269	-1.967163	2.436893
44	6	0	-0.906959	5.169645	-1.243950
45	6	0	0.906959	-5.169645	-1.243950
46	1	0	-0.719901	-1.214107	-1.277986

47	1	0	0.719901	1.214107	-1.277986
48	1	0	-2.157747	0.590640	3.005478
49	1	0	2.157747	-0.590640	3.005478
50	1	0	0.847625	2.764694	0.372785
51	1	0	-0.847625	-2.764694	0.372785
52	1	0	-4.553795	1.158958	-3.327438
53	1	0	4.553795	-1.158958	-3.327438
54	1	0	-5.851089	2.810956	0.558372
55	1	0	5.851089	-2.810956	0.558372
56	1	0	-2.961474	4.992750	-1.888419
57	1	0	2.961474	-4.992750	-1.888419
58	1	0	-1.742759	-2.097877	-3.307077
59	1	0	1.742759	2.097877	-3.307077
60	1	0	-4.245854	1.106731	4.161605
61	1	0	4.245854	-1.106731	4.161605
62	1	0	1.100441	5.042723	-0.484505
63	1	0	-1.100441	-5.042723	-0.484505
64	1	0	-3.675629	-0.932975	-4.354492
65	1	0	3.675629	0.932975	-4.354492
66	1	0	-6.121995	2.196979	2.957595
67	1	0	6.121995	-2.196979	2.957595
68	1	0	-0.788378	6.179459	-1.625175
69	1	0	0.788378	-6.179459	-1.625175
70	1	0	0.173460	2.378039	2.611845
71	1	0	0.882528	1.114725	3.631794
72	1	0	1.833718	1.817350	2.312900
73	1	0	-0.173460	-2.378039	2.611845
74	1	0	-0.882528	-1.114725	3.631794
75	1	0	-1.833718	-1.817350	2.312900

Table S8. Optimized Structural Coordinate and its Total Energy of **SnMe2** (Transition State) at B3LYP-D3/B1(Sn:LanL2DZ, C,H:6-31G(d)) level **HF=-1623.1484911, NImg=1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	-0.907491	0.011149	-0.000000
2	6	0	-0.046364	-2.099884	0.000000
3	6	0	-1.289023	-3.056507	0.000000
4	6	0	-0.952695	-4.425295	0.000000
5	6	0	0.539050	-4.680775	0.000000
6	1	0	0.789521	-5.744982	0.000000
7	6	0	0.808142	-2.561536	-1.206166
8	6	0	1.092398	-3.943477	-1.210135
9	6	0	0.808142	-2.561536	1.206166
10	6	0	1.092398	-3.943477	1.210135
11	6	0	-0.045830	2.095755	-0.000000
12	6	0	-1.183057	3.165969	-0.000000
13	6	0	-0.685581	4.489044	-0.000000
14	6	0	0.842716	4.582345	-0.000000
15	1	0	1.200417	5.615441	-0.000000
16	6	0	0.773235	2.490995	1.251528
17	6	0	1.288924	3.801034	1.219815
18	6	0	0.773235	2.490995	-1.251528
19	6	0	1.288924	3.801034	-1.219815
20	6	0	-2.645503	-2.727235	0.000000
21	6	0	-3.630085	-3.723960	0.000000
22	6	0	-1.922262	-5.420318	0.000000
23	6	0	-3.275730	-5.069714	0.000000
24	1	0	-2.978786	-1.699548	-0.000000
25	1	0	-4.677219	-3.433739	-0.000000
26	1	0	-1.621063	-6.465224	0.000000
27	1	0	-4.040852	-5.841176	0.000000
28	6	0	-2.561151	2.968180	-0.000000
29	6	0	-3.433015	4.067176	-0.000000
30	6	0	-1.546949	5.576797	-0.000000
31	6	0	-2.932468	5.365774	-0.000000
32	1	0	-2.983247	1.969476	-0.000000
33	1	0	-4.506073	3.895868	-0.000000
34	1	0	-1.143887	6.586884	-0.000000
35	1	0	-3.610893	6.214511	-0.000000
36	6	0	1.374326	-1.770897	-2.197289
37	6	0	2.152819	-2.341132	-3.213703
38	6	0	1.859224	-4.518249	-2.214643

39	6	0	2.383388	-3.713810	-3.234730
40	1	0	1.253680	-0.699332	-2.170458
41	1	0	2.582271	-1.700464	-3.979285
42	1	0	2.062509	-5.586443	-2.195530
43	1	0	2.984453	-4.158139	-4.023380
44	6	0	1.374326	-1.770897	2.197289
45	6	0	2.152819	-2.341132	3.213703
46	6	0	1.859224	-4.518249	2.214643
47	6	0	2.383388	-3.713810	3.234730
48	1	0	1.253680	-0.699332	2.170458
49	1	0	2.582271	-1.700464	3.979285
50	1	0	2.062509	-5.586443	2.195530
51	1	0	2.984453	-4.158139	4.023380
52	6	0	0.930392	1.758565	2.424369
53	6	0	1.678813	2.264545	3.495113
54	6	0	2.036952	4.312877	2.272836
55	6	0	2.254354	3.530097	3.412785
56	1	0	0.435478	0.805115	2.543945
57	1	0	1.795966	1.665773	4.394292
58	1	0	2.428080	5.326008	2.216054
59	1	0	2.839488	3.922499	4.239913
60	6	0	0.930392	1.758565	-2.424369
61	6	0	1.678813	2.264545	-3.495113
62	6	0	2.036952	4.312877	-2.272836
63	6	0	2.254354	3.530097	-3.412785
64	1	0	0.435478	0.805115	-2.543945
65	1	0	1.795966	1.665773	-4.394292
66	1	0	2.428080	5.326008	-2.216054
67	1	0	2.839488	3.922499	-4.239913
68	6	0	-2.085870	0.044771	1.806154
69	6	0	-2.085870	0.044771	-1.806154
70	1	0	-1.950030	0.997685	2.324726
71	1	0	-3.152940	-0.074614	1.591346
72	1	0	-1.784384	-0.770321	2.471520
73	1	0	-1.950030	0.997685	-2.324726
74	1	0	-1.784384	-0.770321	-2.471520
75	1	0	-3.152940	-0.074614	-1.591346

Table S9. Optimized Structural Coordinate and its Total Energy of **SnMe2** (Transition State) at ωB97XD/B1(Sn;LanL2DZ, C,H;6-31G(d)) level **HF=-1622.577781, NImg=1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	0.920581	0.010136	-0.000000
2	6	0	0.052750	2.075993	-0.000000
3	6	0	1.170013	3.156824	-0.000000
4	6	0	0.654991	4.467768	-0.000000
5	6	0	-0.870930	4.539056	-0.000000
6	1	0	-1.243171	5.566751	-0.000000
7	6	0	-0.763387	2.459735	-1.250104
8	6	0	-1.302414	3.754013	-1.217113
9	6	0	-0.763387	2.459735	1.250104
10	6	0	-1.302414	3.754013	1.217113
11	6	0	0.050805	-2.080179	0.000000
12	6	0	1.284125	-3.038353	-0.000000
13	6	0	0.945015	-4.400518	0.000000
14	6	0	-0.542913	-4.649595	0.000000
15	1	0	-0.797932	-5.712462	0.000000
16	6	0	-0.805129	-2.535473	1.199581
17	6	0	-1.092298	-3.911015	1.206093
18	6	0	-0.805129	-2.535473	-1.199581
19	6	0	-1.092298	-3.911015	-1.206093
20	6	0	2.546033	2.977037	-0.000000
21	6	0	3.399803	4.084961	-0.000000
22	6	0	1.498413	5.564094	-0.000000
23	6	0	2.882677	5.372139	-0.000000
24	1	0	2.983715	1.984086	-0.000000
25	1	0	4.474484	3.929324	-0.000000
26	1	0	1.083194	6.568697	-0.000000
27	1	0	3.549122	6.229363	-0.000000
28	6	0	2.637858	-2.714778	-0.000000
29	6	0	3.615833	-3.711744	-0.000000
30	6	0	1.907518	-5.396811	-0.000000

31	6	0	3.258014	-5.052085	-0.000000
32	1	0	2.977567	-1.688515	-0.000000
33	1	0	4.663294	-3.425534	-0.000000
34	1	0	1.603333	-6.440340	0.000000
35	1	0	4.020179	-5.825419	-0.000000
36	6	0	-0.885922	1.735910	-2.427744
37	6	0	-1.634713	2.229420	-3.498327
38	6	0	-2.051310	4.254177	-2.269847
39	6	0	-2.241929	3.475024	-3.411816
40	1	0	-0.359132	0.799604	-2.554743
41	1	0	-1.725374	1.636937	-4.403895
42	1	0	-2.463453	5.258376	-2.212769
43	1	0	-2.828647	3.858236	-4.241134
44	6	0	-0.885922	1.735910	2.427744
45	6	0	-1.634713	2.229420	3.498327
46	6	0	-2.051310	4.254177	2.269847
47	6	0	-2.241929	3.475024	3.411816
48	1	0	-0.359132	0.799604	2.554743
49	1	0	-1.725374	1.636937	4.403895
50	1	0	-2.463453	5.258376	2.212769
51	1	0	-2.828647	3.858236	4.241134
52	6	0	-1.377834	-1.739380	2.176117
53	6	0	-2.160591	-2.301247	3.188001
54	6	0	-1.863321	-4.478163	2.206077
55	6	0	-2.389705	-3.669604	3.216163
56	1	0	-1.261361	-0.666989	2.139300
57	1	0	-2.597368	-1.656180	3.944687
58	1	0	-2.070416	-5.545192	2.191588
59	1	0	-2.995827	-4.108361	4.003054
60	6	0	-1.377834	-1.739380	-2.176117
61	6	0	-2.160591	-2.301247	-3.188001
62	6	0	-1.863321	-4.478163	-2.206077
63	6	0	-2.389705	-3.669604	-3.216163
64	1	0	-1.261361	-0.666989	-2.139300
65	1	0	-2.597368	-1.656180	-3.944687
66	1	0	-2.070416	-5.545192	-2.191588
67	1	0	-2.995827	-4.108361	-4.003054
68	6	0	2.103800	0.038063	1.800243
69	6	0	2.103800	0.038063	-1.800243
70	1	0	1.800158	-0.775612	2.466826
71	1	0	3.168975	-0.089015	1.581149
72	1	0	1.979514	0.991624	2.321260
73	1	0	1.800158	-0.775612	-2.466826
74	1	0	1.979514	0.991624	-2.321260
75	1	0	3.168975	-0.089015	-1.581149

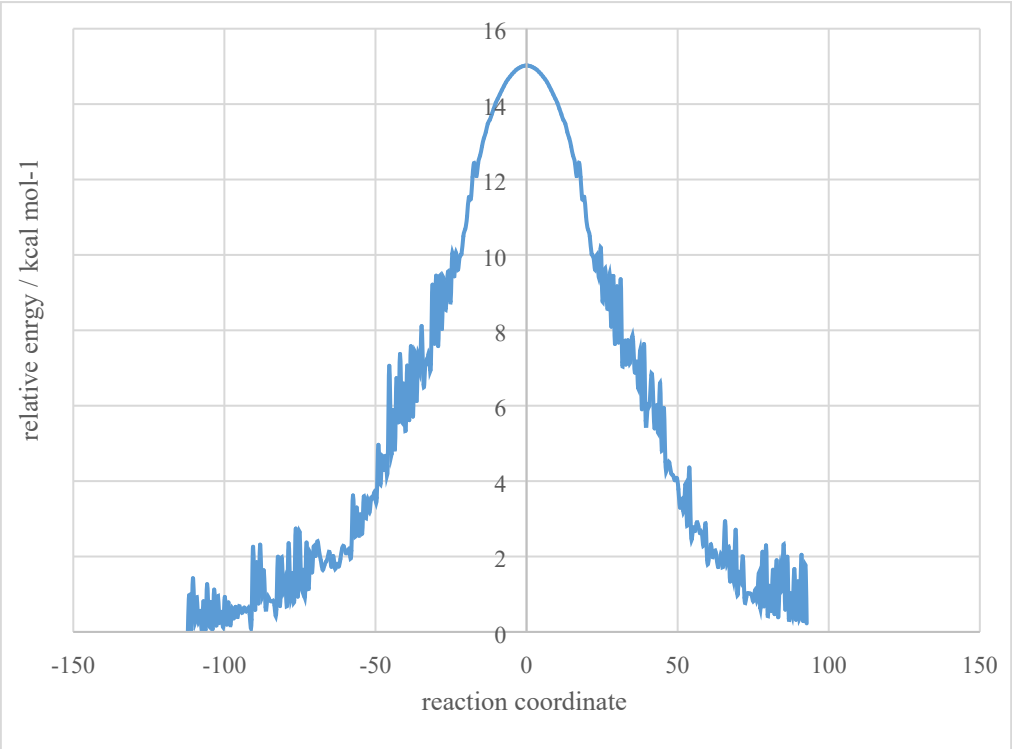

Fig. S32. Potential energies of gear slippage as a function of the reaction coordinate for **SnPh2** calculated at the IRC-B3LYP-D3/6-31G* level.

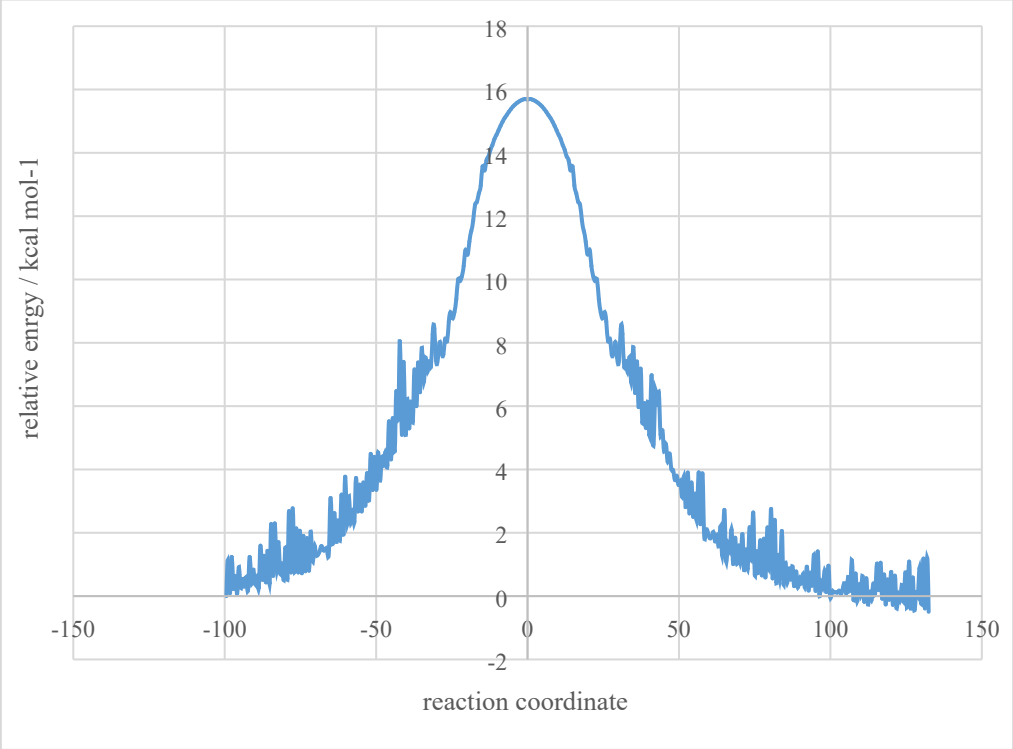

Fig. S33. Potential energies of gear slippage as a function of the reaction coordinate for **SnPh2** calculated at the IRC-ωB97XD/6-31G* level.

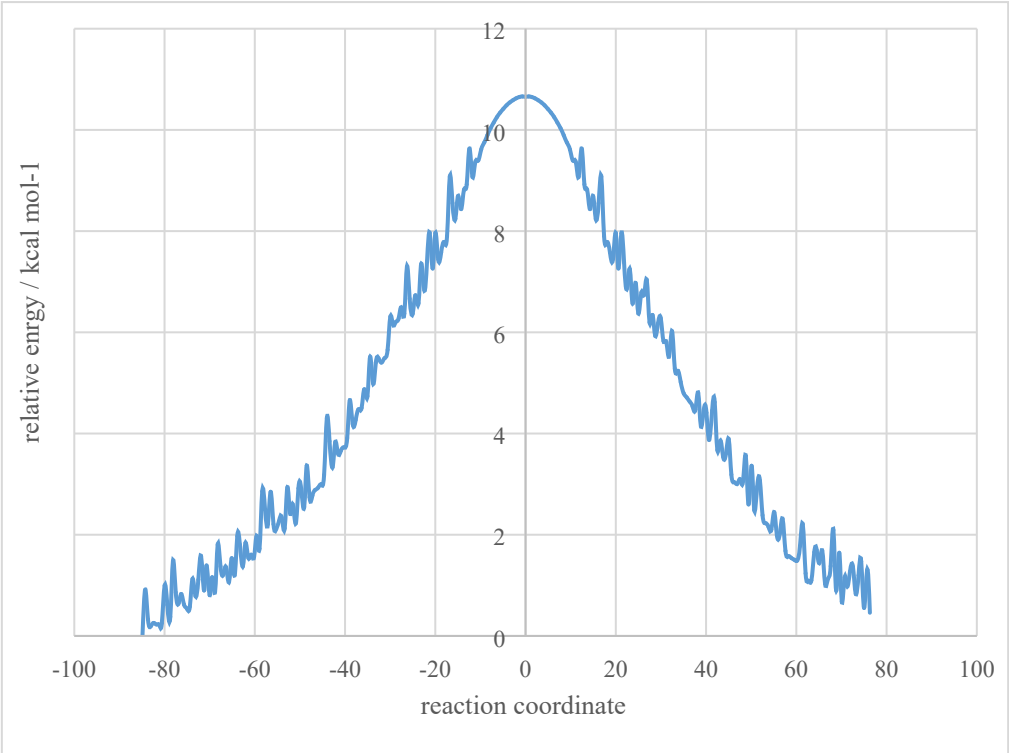

Fig. S34. Potential energies of gear slippage as a function of the reaction coordinate for **SnMe2** calculated at the IRC-B3LYP-D3/6-31G* level.

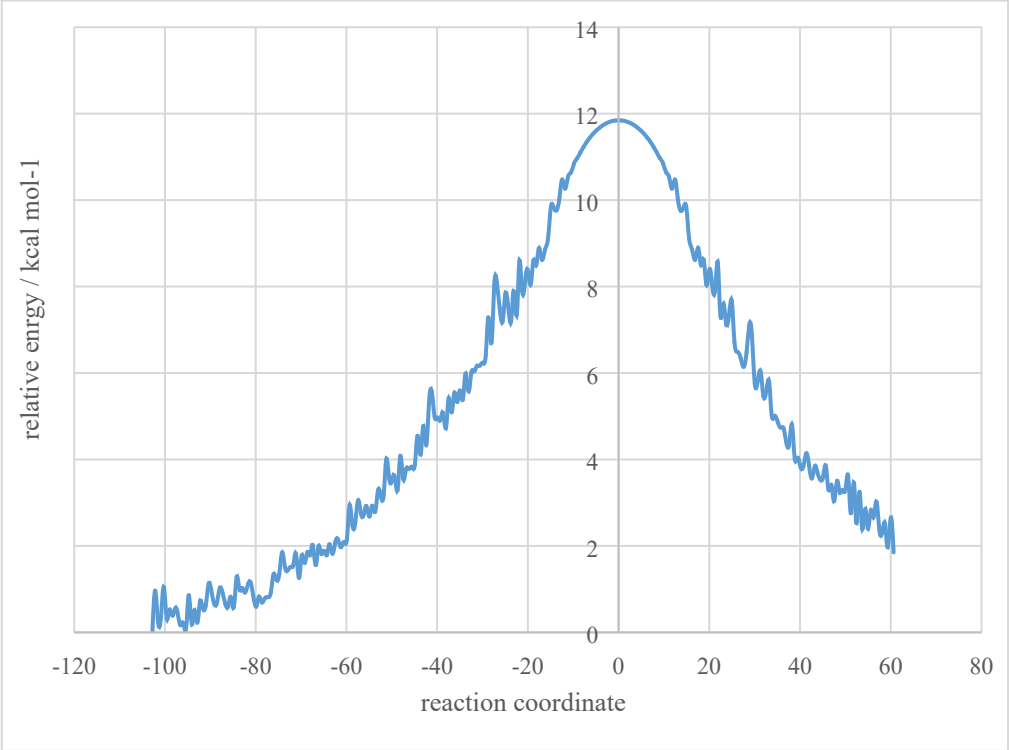

Fig. S35. Potential energies of gear slippage as a function of the reaction coordinate for **SnMe2** calculated at the IRC-ωB97XD/6-31G* level.