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Supporting Information

Reductive Dehydrocoupling of Diphenyltin Dihydride with $LiAlH_4$: Selective Synthesis and Structures of the First Bicyclo[2.2.1]heptastannane-1,4-diide and Bicyclo[2.2.2]octastannane-1,4-diide

Beate G. Steller,[a] Roland C. Fischer,[a*] Michaela Flock, Michael S. Hill,[b] David J. Liptrot,[b*] Claire L. M[c]Mullin,[b] Nasir A. Rajabi,[b] Kathrin Tiefling[a] and Andrew S. Wilson[b]

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1. Experimental Details

All manipulations involving air or moisture sensitive compounds were either performed under a nitrogen atmosphere using standard Schlenk tube techniques or were carried out in a nitrogen flushed Glovebox UNILAB supplied by M.Braun. The solvents dimethoxyethane and THF-d8 (both dried over potassium) and acetonitrile-d3 (dried over phosphorus pentoxide) were distilled prior to use. All other solvents were obtained from an Innovative Technology solvent drying system.
For the conversions with organotin hydrides, purchased $LiAlH_4$ was recrystallised from Et_2O. All other commercially available chemicals were used as received from chemical suppliers.
Elemental analysis was performed with an Elementar Vario MICRO cube. Melting point measurements were carried out by threefold determination with a Buechi 535 or a Electrothermal Mel-Temp instrument.

NMR Spectroscopy:

^{1}H (300.22 MHz), ^{13}C (75.5 MHz) as well as ^{119}Sn (111.92 MHz) NMR spectra were recorded on a Mercury 300 MHz spectrometer from Varian at 25°C if not otherwise stated. Chemical shifts are given in ppm relative to TMS regarding ^{1}H, ^{13}C and in case ^{119}Sn relative to Me_4Sn. Spectra were referenced to solvent residual signals. Coupling constants (^{n}J) are reported in Hertz (Hz).

UV/VIS:

All UV/VIS measurements were performed in quartz glass cuvettes with a thickness of 1 cm on a Cary 60 UV/VIS device from Agilent Technologies. If not otherwise stated, measurements were done in absorption mode. Analysis of measured results was done with Spekwin32. Dry acetonitrile was used as solvent in all cases.

Crystal Structure Determination:

For single crystal X-ray diffractometry all suitable crystals were covered with a layer of silicone oil. A single crystal was selected, mounted on a glass rod on a copper pin, and placed in the cold N_2 stream provided by an Oxford Cryosystems cryometer (T=100 K). XRD data collection was performed on a Bruker APEX II diffractometer with use of Mo Kα radiation (λ= 0.71073 Å) and a CCD area detector. Empirical absorption corrections were applied using SADABS.[1] The structures were solved with use of either direct methods or the Patterson option in SHELXS and refined by the full-matrix least-squares procedures in SHELXL.[2] The space group assignments and structural solutions were evaluated using PLATON.[3] For more refinement details on compounds **1-5** see below.

Syntheses:

Synthesis of [bicyclo[2.2.1]Sn_7Ph_{10}][$Li(12Cr4)_2$]$_2$ (1)

275 mg Ph_2SnH_2 (1.00 mmol, 3.5 eq) were slowly added to a solution of 10.9 mg $LiAlH_4$ (0.29 mmol, 1.0 eq) and 102 mg 12-crown-4 (0.58 mmol, 2.0 eq) in 10 mL THF. The solution slowly turned yellow and a slight evolution of dihydrogen was observed. After stirring the reaction mixture at room temperature overnight, the solution had turned orange. A colorless precipitate was removed *via* centrifugation. After concentration to about 5 ml and storage at -30°C the product was isolated as light orange crystals which were suitable for X-ray crystallography. Alternatively, the reaction can be carried out in DME, whereupon **1** crystallizes upon storage at room temperature as orange crystals.
Yield: 152 mg, 44.6 % (with respect to Ph_2SnH_2) yellow-orange crystals. M.p. 121-123°C (decomp)
NMR spectra for [bicyclo[2.2.1]Sn_7Ph_{10}][$Li(12cr4)_2$]·3dme.
^{1}H NMR (300.22 MHz, CD_3CN) δ 7.60 (2H, d, *ortho*-Ph), 7.44 (8H, m, *ortho*-Ph), 7.27-7.21 (12H, m, Ph), 6.96 (4H, m, Ph), 6.88 (12H, m, Ph), 6.77-6.69 (12H, m, Ph), 3.62 (64H, s, C*H*$_2$O, 12cr4), 3.49 (12H, C*H*$_2$O, dme), 3.32 (18 H, C*H*$_3$O, dme) ppm;
$^{13}C\{^{1}H\}$ NMR (75.51 MHz, CD_3CN): δ 140.7 (*C*-ipso, Ph), 140.4 (*C*-ipso, Ph), 139.4 (*C*-ipso, Ph), 139.2 (Ph), 129.3 (Ph), 128.8 (Ph), 128.7 (Ph), 128.5 (Ph), 128.3 (Ph), 127.4 (Ph), 127.2 (Ph), 126.0 (Ph), 72.4 (*C*H_2O, dme), 70.2 (*C*H_2O, 12Cr4), 58.9 (*C*H_3O, dme) ppm;
$^{119}Sn\{^{1}H\}$ NMR (111.92 MHz, CD_3CN): δ 200.3, 35.6, -857.3 ppm. For detailed analysis of Sn-Sn coupling pattern see below. Anal. Calcd for $C_{94}H_{118}Li_2O_{16}Sn_7$0.5($C_4H_8O$): C 47.90, H 5.05 Found: C 48.06, H 5.13.

Synthesis of [bicyclo[2.2.2]Sn_8Ph_{12}][$Li(12Cr4)_2$]$_2$ (2)
275 mg Ph_2SnH_2 (1.00 mmol, 4.0 eq) were slowly added to a solution of 9.5 mg $LiAlH_4$ (0.25 mmol, 1.0 eq) and 88.1 mg 12-crown-4 (0.50 mmol, 2.0 eq) in 10 mL THF. The solution turned orange red under concomitant formation of dihydrogen. After centrifugation and removal of a colorless precipitate, the product was isolated as orange-red crystals after cooling the solution to -30°C. Alternatively, the reaction can be carried out in DME, whereupon **2** crystallizes upon storage at room temperature as deep orange-red crystals.
Yield: 187 mg, 57.3 % (with respect to Ph_2SnH_2) orange-red crystals. M.p. 137-139°C (decomp.).Anal. Calcd for $C_{104}H_{124}Li_2O_{16}Sn_8$: C 48.16, H 4.82 Found: C 48.23, H 5.01.
^{1}H NMR (300.22 MHz, CD_3CN) δ 7.46 (24H, m, *ortho*-Ph), 6.91 (12H, *pseudo*-t, *para*-Ph), 6.82 (24H, *pseudo*-d, *meta*-Ph), 3.53 (64H, s, 12cr4) ppm;
^{13}C{^{1}H} NMR (75.5 MHz, CD_3CN): δ 140.5 (*C*-ipso, Ph), 129.3 (Ph), 127.8 (Ph), 126.1 (Ph), 70.3 (CH_2O, 12Cr4) ppm;
^{119}Sn{^{1}H} NMR (111.92 MHz, CD_3CN): δ -316.8, -585.0 ppm. For detailed analysis of Sn-Sn coupling pattern see below.

Synthesis of [bicyclo[2.2.2]Sn_8Ph_{13}][$Li(12Cr4)_2$] (3)
275 mg Ph_2SnH_2 (1.00 mmol, 8.0 eq) were slowly added to a solution of 4.8 mg $LiAlH_4$ (0.13 mmol, 1.0 eq) and 48 mg 12-crown-4 (0.27 mmol, 2.1 eq) in 10 mL dme. The solution slowly turned yellow and a slight evolution of dihydrogen was observed. After stirring the reaction mixture at room temperature overnight, the solution had turned orange. A colorless precipitate was removed *via* centrifugation. After concentration to about 5 ml and storage at -30°C, the product was isolated as orange crystals which are suitable for X-ray crystallography. Anal. Calcd for $C_{94}H_{90}LiO_8Sn_8$: C 48.99, H 3.94 Found: C 49.24, H 3.99.
Yield: 108 mg, 37.4% (with respect to Ph_2SnH_2) yellow crystals. M.p. 91-94 °C (decomp.). NMR spectra for [bicyclo[2.2.2]Sn_8Ph_{13}][$Li(12cr4)_2$]·dme.
^{1}H NMR (300.22 MHz, CD_3CN) δ 7.40 (t, 1H, Ph), 7.39 (8H, d, Ph), 7.06 (32H, m, Ph), 6.82 (24H, m, Ph), 3.64 (64H, s, CH_2O, 12cr4), 3.48 (8H, s, CH_2O, dme), 3.31 (12H, s, CH_3O, dme) ppm;
^{13}C{^{1}H} NMR (75.5 MHz, CD_3CN): δ 139.2 (*C*-ipso, Ph), 139.2 (*C*-ipso, Ph), 138.5 (*C*-ipso, Ph), 128.9 (Ph), 128.8 (Ph), 128.5 (Ph), 128.4 (Ph), 128.3 (Ph), 128.1 (Ph), 127.9 (Ph), 127.2 (Ph), 127.0 (Ph), 72.2 (CH_2O, dme), 70.1 (CH_2O, 12Cr4), 58.6 (CH_3O, dme) ppm;
^{119}Sn{^{1}H} NMR (111.92 MHz, CD_3CN): δ -183.1, -238.6, -470.8, -757.9 ppm. For detailed analysis of Sn-Sn coupling pattern see below.

Synthesis of [$PhAlH_3$][$Li(12Cr4)_2$] (4)
275 mg Ph_2SnH_2 (1.00 mmol, 2.0 eq) were slowly added to a solution of 19.0 mg $LiAlH_4$ (0.50 mmol, 1.0 eq) and 176 mg 12-crown-4 (1.00 mmol, 2.0 eq) in 10 mL DME. Evolution of hydrogen and the slow formation of elemental tin were observed. After storing the dark red-brown reaction mixture for 48 hours at room temperature, the elemental tin was removed *via* filtration The product was isolated as colourless crystals from the orange-brown reactions mixture. Yield: 55 mg, 23.4 % (with respect to $LiAlH_4$). M.p. 78-81°C (decomp.). Anal. Calcd for $C_{22}H_{40}AlLiO_8$: C 56.65, H 8.64 Found: C 56.17, H 8.53.
NMR spectra for [$PhAlH_3$][$Li(dme)_2$] (^{1}H) and [$PhAlH_3$][$Li(12cr4)_2$]·2dme (^{13}C).
^{1}H NMR (300.22 MHz, C_6D_6) δ 7.41 (2H, *pseudo*-t, Ph), 7.06 (3H, m, Ph), 3.28 (8H, s, CH_2O, dme), 3.16, (3H, b, AlH_3), 3.07 (12H, s, CH_3O, dme) ppm;
^{13}C{^{1}H} NMR (75.5 MHz, THF-d8): δ 140.1 (*C*-ipso, Ph), 139.5 (*C*-ortho, Ph), 126.4 (*C*-meta, Ph), 125.1 (*C*-para, Ph), 72.7 (CH_2O, dme), 69.1 (CH_2O, 12Cr4), 58.6 (CH_3O, dme) ppm.

Synthesis of [Ph_3AlH][$Li(12Cr4)_2$] (5)
275 mg Ph_2SnH_2 (1.00 mmol, 0.75 eq) were slowly added to a solution of 50.6 mg $LiAlH_4$ (1.33 mmol, 1.0 eq) and 470 mg 12-crown-4 (2.67 mmol, 2.0 eq) in 10 mL DME. Evolution of hydrogen and the slow formation of elemental tin were observed and a dark brown reactions mixture had formed. The elemental tin was removed *via* filtration from the red-brown solution. After careful layering the reactions mixture with n-heptane and storage at -30°C, the product crystallised from the solution as colourless crystals. Yield: 140 mg, 39.4% (with respect to Ph_2SnH_2). M.p. 107-109°C (decomp.). Anal. Calcd for $C_{30}H_{42}AlLiO_6$: C 67.66, H 7.95 Found: C 67.32, H 7.58.
NMR spectra for [$PhAlH_3$][$Li(12cr4)_2$]·6dme.
^{1}H NMR (300.22 MHz, THF-d8) δ 7.65 (6H, m, Ph), 6.78 (9H, m, Ph), 3.72 (64H, s, 12Cr4), 3.43 (24H, s, C*H*$_2$O, dme), 3.27 (36H, s, C*H*$_3$O, dme), 2.53 (1H, s, broad, Al*H*) ppm;
^{13}C{^{1}H} NMR (75.5 MHz, THF-d8): δ 140.5 (*C*-ipso, Ph), 139.4 (*C*-ortho, Ph), 126.2 (*C*-meta, Ph), 125.0 (*C*-para, Ph), 72.8 (*C*H_2O, dme), 69.1 (*C*H_2O, 12Cr4), 58.9 (*C*H_3O, dme) ppm.

2. Crystallographic Details

Refinement Details

Compound **1**

The asymmetric unit in this structure comprises one bicyclo[2.2.1]heptastannane-1,3-diide dianion, two $[Li(12Cr4)_2]^+$ cations, one molecule of THF with some disorder, and diffuse solvent which was treated with a solvent mask algorithm *via* the *OLEX2* software.[4] The phenyl rings based on C7 and C49 in the main feature were seen to exhibit disorder 50:50 and 65:35 disorder, respectively. The four arising fractional occupancy rings were ultimately refined as rigid hexagons. 60:40 disorder was accounted for in the 12Cr4 based on O5-O8, while 65:35 disorder was evident in the crown moiety that includes O9-O12. The methylenes based on C94 and C95 of the discernible solvent were also modelled subject to being disordered, over 2 sites, in a 75:25 ratio. O-C and C-C distance restraints were included in the latter refinement stages for metrics involving fractional occupancy atoms. ADP restraints were also employed, to assist convergence, in disordered regions. The diffuse solvent equates to approximately one molecule of THF per asymmetric unit, and an allowance has been made for same in the results as presented.

Compound **2**

The asymmetric unit in this structure comprises one bicyclo-2.2.2-octastannane-1,4-diide dianion, two $[Li(12Cr4)_2]^+$ cations, and diffuse solvent which was treated with a solvent mask algorithm *via* the *OLEX2* software. 65:35 disorder of the carbon atoms positions was accounted for in the 12Cr4 moieties containing O1-O4 and O5-O8 O-C and C-C distance restraints were included in the latter refinement stages for metrics involving fractional occupancy atoms. ADP restraints were also employed, to assist convergence, in disordered regions. The diffuse solvent equates to approximately two molecules of THF per asymmetric unit, and an allowance has been made for same in the results as presented.

Compound **3**

The model presented herein arises from integration of the data as a two component twin, by virtue of twinning about the reciprocal 1 -1 0 axis. This belies, however, the information in the diffraction pattern which indicated rising from three or four constituents. The model itself is heavily restrained, with only the tin centres being anisotropically refined freely. Oxygen atoms were also anisotropically refined but with restraints, while carbon atoms were treated isotropically. With focus on the structure itself, the elements of the asymmetric unit which were clear include one bicyclo[2.2.2]octastannane-1-ide anion, half of a $[Li(12Cr4)_2]^+$ cation (*i.e.* one lithium centre located at an inversion centre and one complete 12Cr4), half of a 12Cr4 (at full-occupancy, close to an inversion

centre and largely ordered), and a diffuse region of electron density for which occupation was treated using the *PLATON* SQUEEZE algorithm. The full occupancy 12Cr4 moiety was modelled for 50:50 disorder with distance and ADP restraints being included to assist convergence. Some carbons in two of the phenyl rings present in the anion were also modelled for 50:50 disorder as the data were reasonably well equipped to resolve the smearing of electron density in these cases.

There was no credible evidence (in the electron density) for half of the lithium proximate to the 12Cr4 fragment containing O5 and O6. The conformation of this crown almost suggests that there may be no alkali metal iron coordinated to it - not least on steric grounds given the proximity of both sides of this moiety to symmetry related phenyl groups in the anion. However, half of the lithium is not easy to locate using compromised X-ray, where the maximum assigned electron density peak is 8.4 electrons per cubic Ångstrom!

Analysis of the packing revealed voids in the structure, at unit cell intervals along the *c* axis, where one might expect to entertain some weaknesses in the crystals themselves. Indeed, the diffraction pattern very much resembled what one might expect to record from a sample comprised of slightly rotated plates along one axis. These voids did not, according to solvent masking algorithms, appear to contain a very high level of electron density. The electron density present appears to be very diffuse and it has been treated *via PLATON* squeeze in this case. Is quite plausible that the remaining alkali metal ion content is located in these voids, coordinated to some very diffuse THF solvent. The asymmetric unit formula presented here takes account of the electron density present in the lattice voids as one half of a lithium ion and one THF molecule. Obviously, the credibility of output from *PLATON* in assessing this electron density is to be viewed alongside the quality of the data themselves, particularly at lower Bragg angles.

Compound **4**

The refinement of the structural model for 4 proseeded normally. H1, H2 and H3 were located and refined without restraints. The highest residual electron density maximum is located at a chemically insignificant distance from Al1.

Compound **5**

The asymmetric unit in this structure comprises one $[Ph_3AlH]^-$ anion and $[Li(DME)(12Cr4)]^+$cation. 80:20 disorder was modelled for the atoms in the DME ligand and for C23, C24 and O4 in the 12Cr4 moiety. O-C and C-C distance restraints were included in the latter refinement stages for metrics involving fractional occupancy atoms. ADP restraints were also employed, to assist convergence, in disordered regions. H1 (attached to Al1) was located and refined without restraints.

Table 2.1: Selected crystallographic data for **1-5.**

Compound	**1**	**2**	**3**	**4**	**5**
Crystal data					
Chemical formula	$C_{60}H_{50}Sn_7$· 2($C_{16}H_{32}LiO_8$)· 0.5(C_4H_8O)	$C_{72}H_{60}Sn_8$· 2($C_{16}H_{32}LiO_8$)	$C_{94}H_{90}LiO_8Sn_8$	C_6H_8Al· $C_{16}H_{32}LiO_8$	$C_{18}H_{16}Al$ $C_{12}H_{26}LiO_6$·
M_r	2356.67	2593.52	2304.11	466.46	532.55
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$	Triclinic, $P\bar{1}$	Orthorhombic, *Pbca*	Monoclinic, $P2_1/c$
Temperature (K)	100	100	100	100	100
a, *b*, *c* (Å)	14.3301 (9), 15.1075 (10), 26.1181 (19)	29.253 (2), 14.3128 (9), 26.5807 (17)	14.2707 (6), 14.2569 (6), 31.4766 (13)	14.856 (11), 14.196 (10), 23.825 (16)	11.8667 (4), 20.5281 (8), 12.5639 (5)
α, β, γ (°)	82.634 (2), 76.623 (3), 70.379 (2)	90, 90.276 (3), 90	70.797 (2), 67.696 (2), 60.735 (2)	90, 90, 90	90, 106.359 (1), 90
V (Å^3)	5173.7 (6)	11128.9 (13)	5086.5 (4)	5024 (6)	2936.67 (19)
Z	2	4	2	8	4
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α
μ (mm^{-1})	1.72	1.83	1.98	0.12	0.11
Crystal size (mm)	0.35×0.21×0.14	0.23×0.20×0.15	0.36×0.24×0.01	0.21×0.19×0.16	0.20×0.18×0.14
Data collection					
Absorption correction	Multi-scan - Bruker software	Multi-scan - Bruker software	Multi-scan - Bruker software	Multi-scan - Bruker software	Multi-scan - Bruker software
T_{min}, T_{max}	0.581, 0.800	0.602, 0.746	0.515, 0.744	0.974/0.981	0.979/0.985
No. of measured, independent and observed [$I > 2s(I)$] reflections	145924, 30024, 23308	96591, 24221, 15488	23104, 23104, 15660	149530, 6067, 4602	14532, 5737, 4290
R_{int}	0.028	0.072	0.080	0.059	0.062
(sin q/l)$_{max}$ (Å^{-1})	0.704	0.639	0.649	0.661	0.617
Refinement					
No. of reflections	30024	24221	23104	6067	5737
No. of parameters	1399	1315	423	301	377
No. of restraints	833	626	167	0	20
H-atom treatment	Constr.	Constr.	Constr.	Mixed	Mixed
$R[F^2 > 2s(F^2)]$, $wR(F^2)$, S	0.037, 0.107, 1.04	0.058, 0.139, 1.01	0.129, 0.374, 1.03	0.070, 0.205, 1.14	0.054, 0.153, 1.05
D_{max}, D_{min} (e Å^{-3})	1.63, -1.39	3.12, -1.29	8.44, -4.22	1.46, -0.59	0.64, -0.42

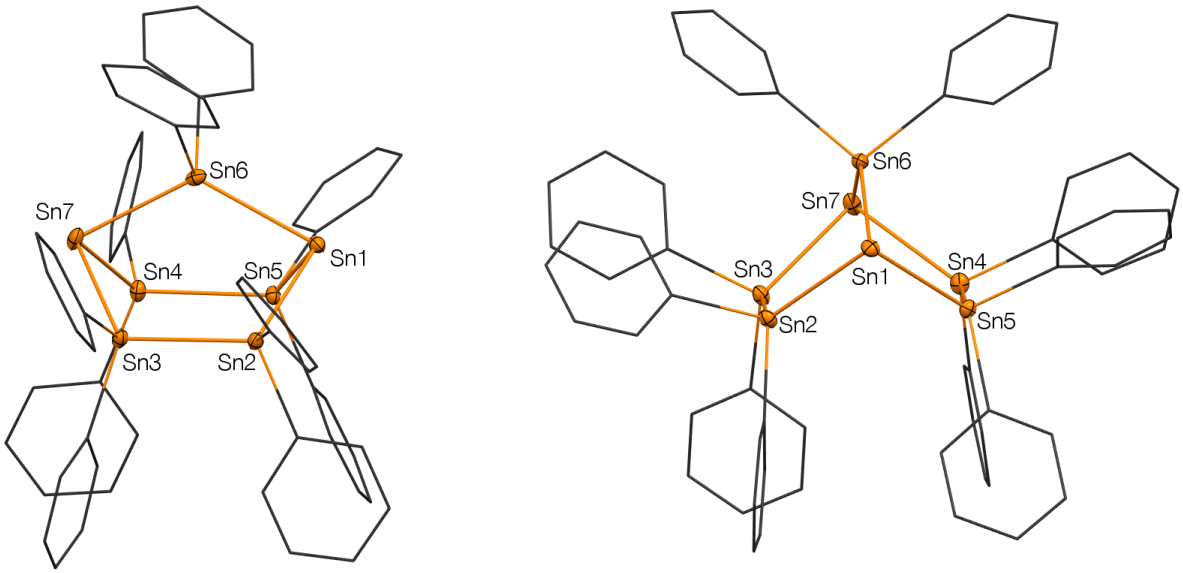


Figure S2.1 Solid state structure of **1**, side and front view, cationic fragments and hydrogens omitted for clarity, phenyl rings drawn as wireframe, metal atoms are drawn at 30% probability level. Bond distances [Å] and angles [°] in **1** are: Sn1-Sn2 2.8351(6), Sn1-Sn5 2.8378(5), Sn1-Sn6 2.8674(6), Sn2-Sn3 2.8383(7), Sn3-Sn7 2.8399(4), Sn4-Sn5 2.8206(7), Sn4-Sn7 2.8364(6), Sn6-Sn7 2.8618(7); Sn2-Sn1-Sn5 94.37(2), Sn2-Sn1-Sn6 86.75(1), Sn5-Sn1-Sn6 84.67(1), Sn1-Sn2-Sn3 111.10(2), Sn2-Sn3-Sn7 114.52(2), Sn5-Sn4-Sn7 111.83(2), Sn1-Sn5-Sn4 114.20(2), Sn1-Sn6-Sn7 123.18(2), Sn3-Sn7-Sn4 93.52(2), Sn3-Sn7-Sn6 85.41(1), Sn4-Sn7-Sn6 85.69(1).

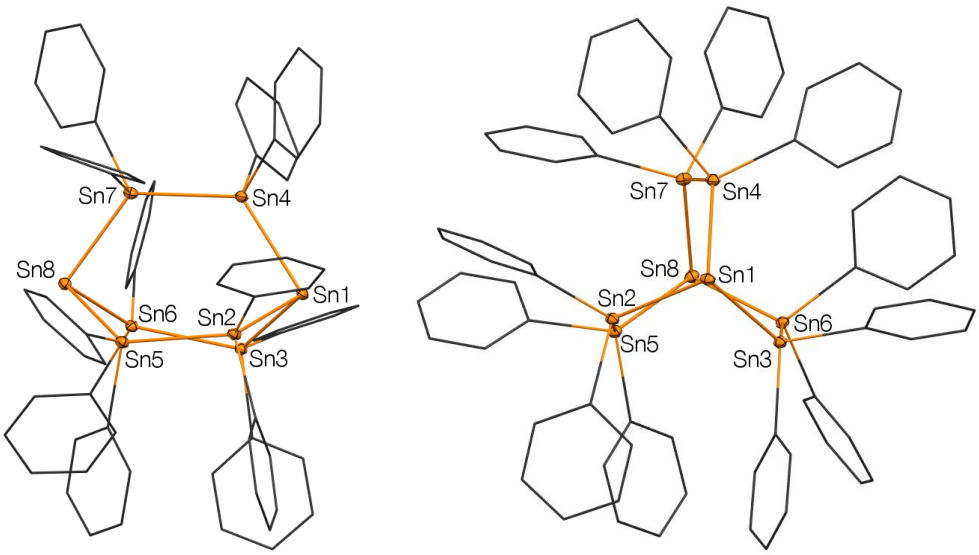


Figure S2.2 Solid state structure of **2**, side and front view, cationic fragments and hydrogens omitted for clarity, phenyl rings drawn as wireframe, metal atoms are drawn at 30% probability level. Bond distances [Å] and angles [°] in **2** are:Sn1-Sn2 2.8408(8), Sn1-Sn3 2.8533(8), Sn1-Sn4 2.8386(8), Sn2-Sn5 2.8318(8), Sn3-Sn6 2.8064(8), Sn4-Sn7 2.7884(8), Sn5-Sn8 2.8248(8), Sn6-Sn8 2.8242(8), Sn7-Sn8 2.8064(8); Sn2-Sn1-Sn3 91.29(2), Sn2-Sn1-Sn4 91.41(2), Sn3-Sn1-Sn4 93.35(2), Sn1-Sn2-Sn5 120.48(3), Sn1-Sn3-Sn6 121.19(3), Sn1-Sn4-Sn7 123.14(3), Sn2-Sn5-Sn8 124.58(3), Sn3-Sn6-Sn8 123.57(3), Sn4-Sn7-Sn8 122.11(3), Sn5-Sn8-Sn6 90.95(2), Sn5-Sn8-Sn7 89.00(2), Sn6-Sn8-Sn7 94.13(2).

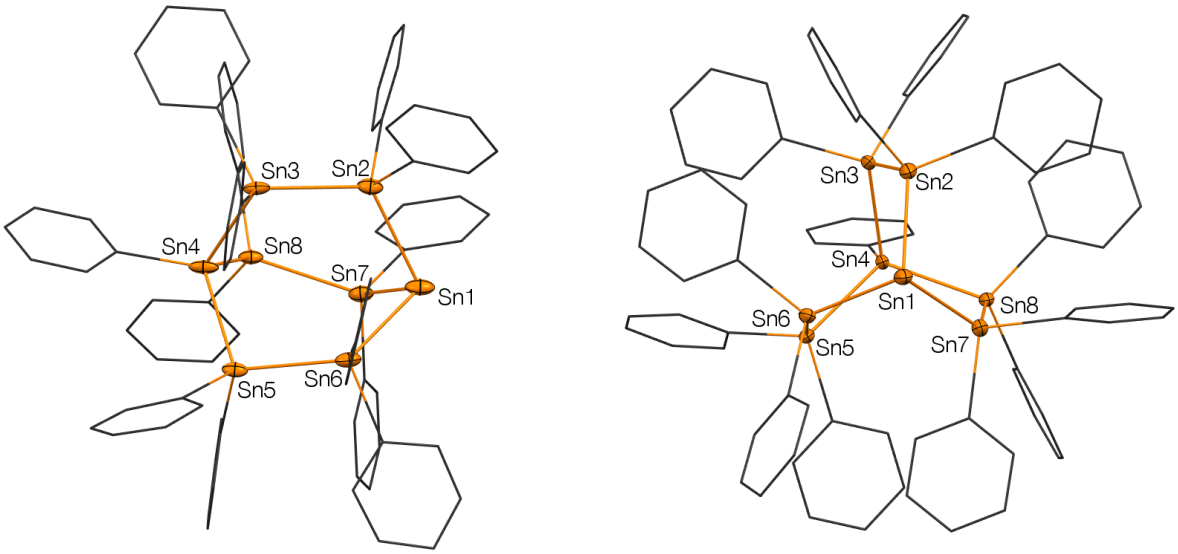


Figure S2.3 Solid state structure of **3**, side and front view, cationic fragments and hydrogens omitted for clarity, phenyl rings drawn as wireframe, metal atoms are drawn at 30% probability level. Bond distances [Å] and angles [°] in **3** are: Sn1-Sn2 2.852(3), Sn1-Sn6 2.861(2), Sn1-Sn7 2.838(2), Sn2-Sn3 2.811(2), Sn3-Sn4 2.788(2), Sn4-Sn5 2.778(3), Sn4-Sn8 2.787(2), Sn5-Sn6 2.826(2) Sn7-Sn8 2.829(3); Sn2-Sn1-Sn6 96.92(8), Sn2-Sn1-Sn7 95.47(8), Sn6-Sn1-Sn7 95.30(8), Sn1-Sn2-Sn3 117.45(8), Sn2-Sn3-Sn4 110.44(8), Sn3-Sn4-Sn5 106.93(8), Sn3-Sn4-Sn8-105.22(8), Sn5-Sn4-Sn8 106.47(8), Sn4-Sn5-Sn6 105.41(7), Sn1-Sn6-Sn5 122.24(8), Sn1-Sn7-Sn8 121.90(8), Sn4-Sn8-Sn7 106.58(7).

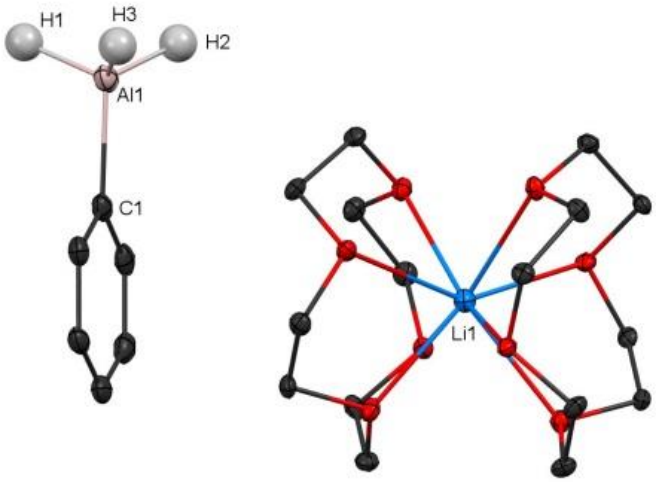


Figure S2.4 Molecular structure of **4**, only hydrogen atoms attached to Al are shown, all other H atoms are omitted for clarity. Bond distances [Å] and angles [°] in **4** are: Al1-H1 1.54(5), Al1-H2 1.52(5) , Al1-H3 1.45(4), Al1-C1 2.022(4); H1-Al1-H2 106(2), H1-Al1-H3 110(2), H1-Al1-C17 111(2), H2-Al1-H3 107(2), H2-Al1-C17-113(2), H3-Al1-C1 111(2). Hydrogen atoms at Al1 were located in the Fourier difference map.

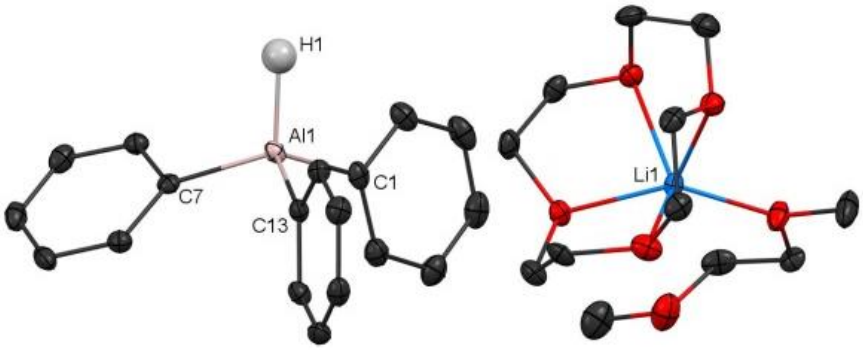


Figure S2.5 Molecular structure of **5**, only hydrogen atoms attached to Al are shown, all other H atoms are omitted for clarity. Bond distances [Å] and angles [°] in **5** are: Al1-C1 2.021(2), Al1-C7 2.010(2), Al1-C13 2.008(3), Al1-H1 1.65(2); C1-Al1-H1 105.4(8), C7-Al1-H1 110.5(8), C13-Al1-H1 110.7(8), C1-Al1-C7 110.92(9), C1-Al1-C13 109.69(9), C7-Al1-C13 109.55(9). The hydrogen atom at Al1 was located in the Fourier difference map.

3. UV-Vis Spectroscopy

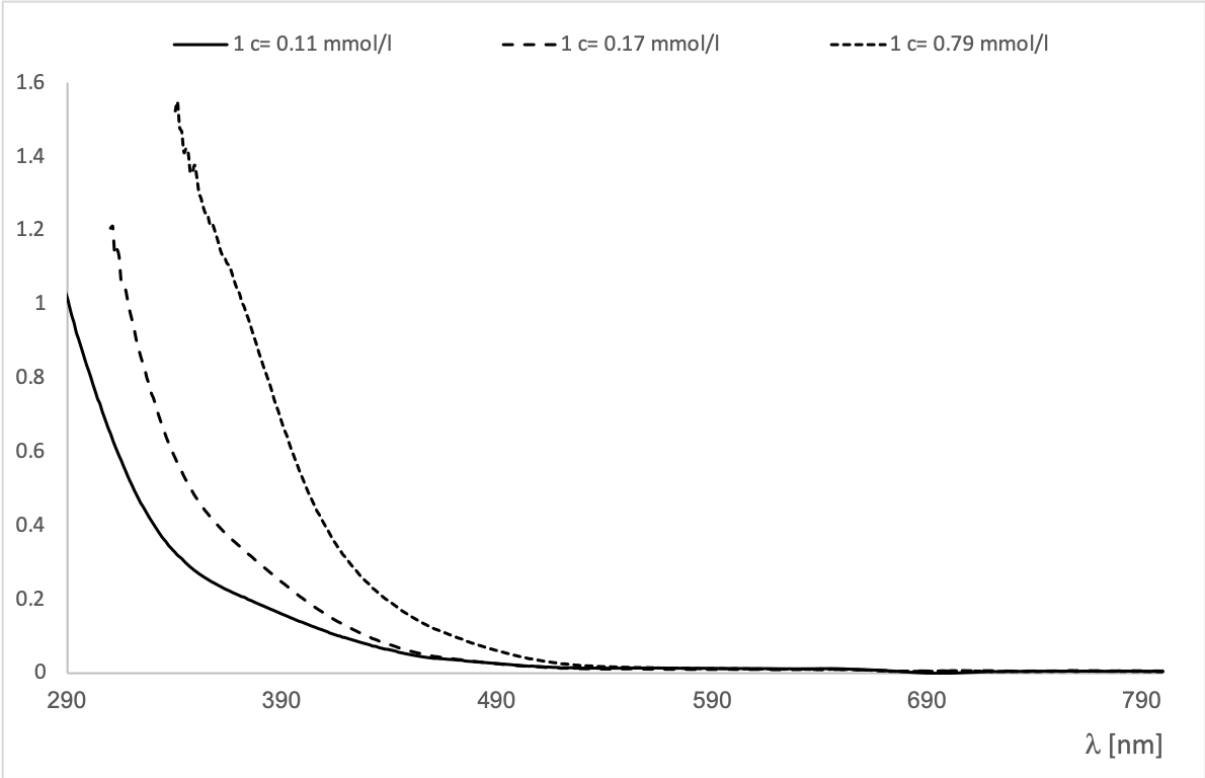


Figure S3.1 UV-Vis spectra of **1** in acetonitrile

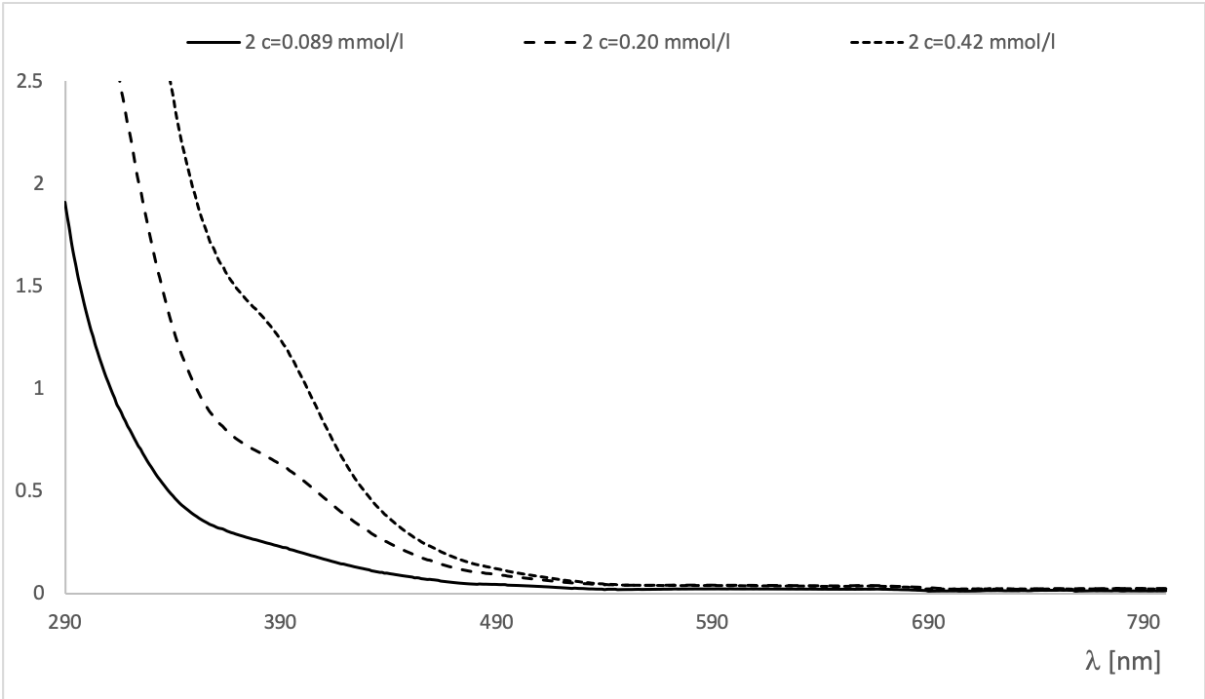


Figure S3.2 UV-Vis spectra of **2** in acetonitrile

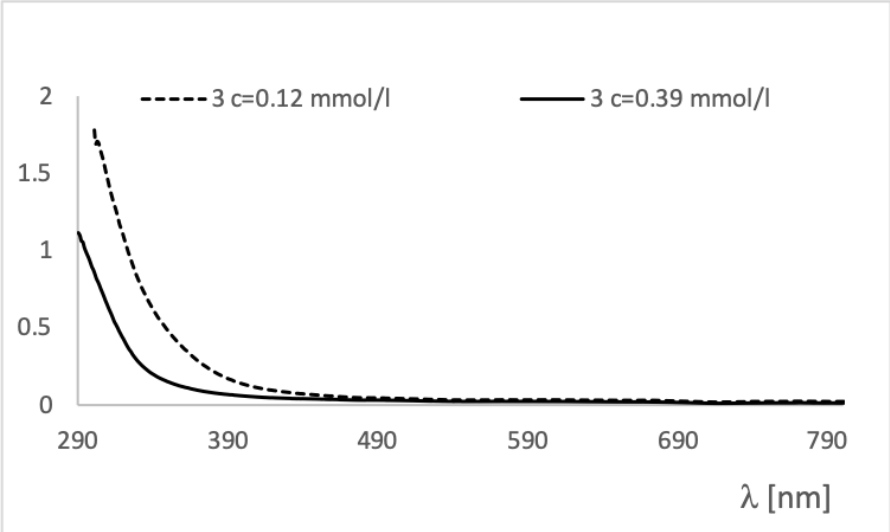


Figure S3.3 UV-Vis spectrum of **3** in acetonitrile

4. NMR Spectra

Compound **1**,
1,3-Dilithio-2,2,4,4,5,5,6,6,7,7-decaphenylbicyclo[2.2.1]heptastannane-1,3-diide

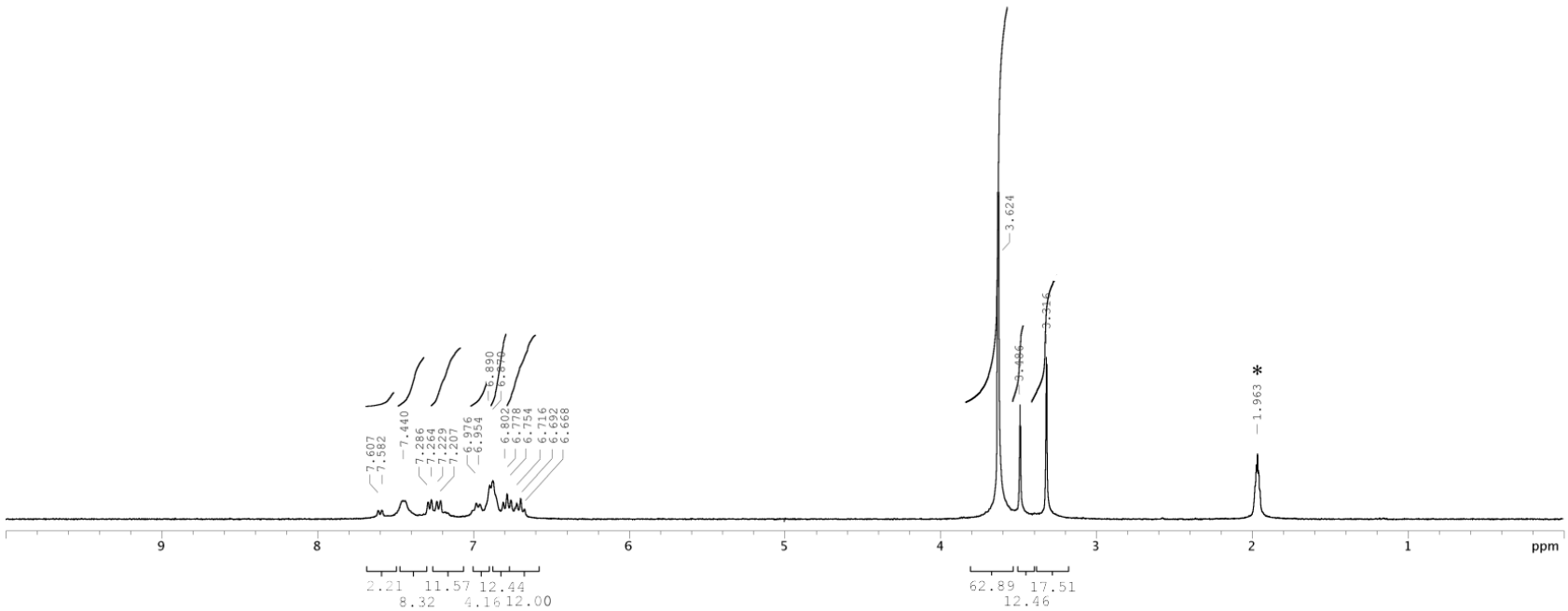


Figure S4.1 ^{1}H NMR spectrum of Compound **1**, CD_3CN, (* solvent residual signal, CD_3CN).

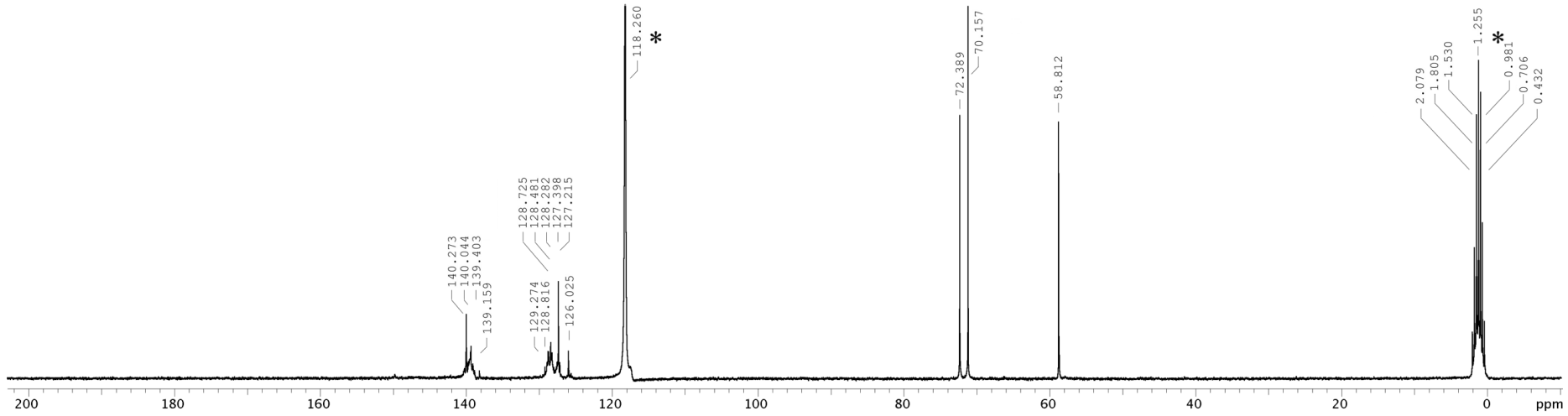


Figure S4.2 $^{13}C\{^{1}H\}$ NMR spectrum of Compound **1**, CD_3CN, (* solvent signals, CD_3CN).

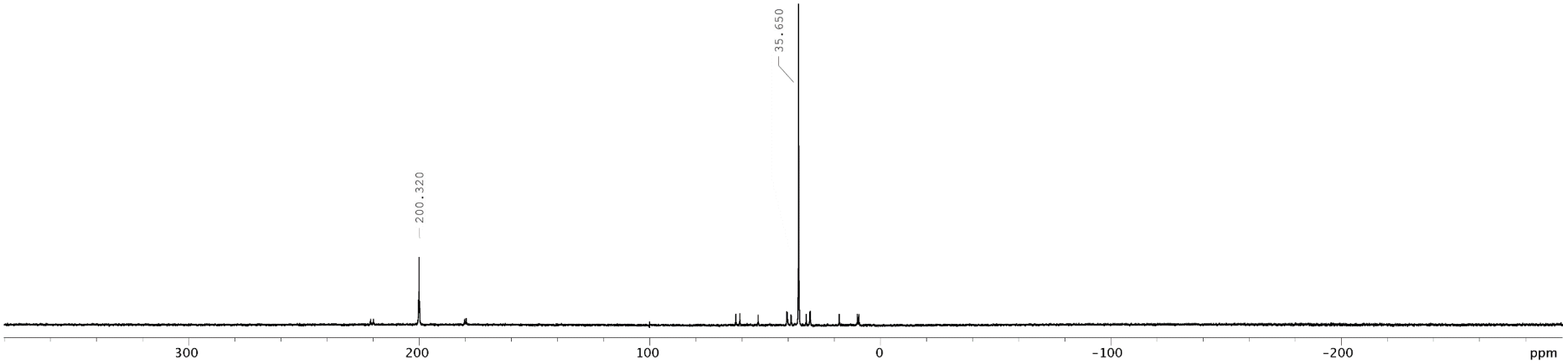


Figure S4.3 $^{119}Sn\{^{1}H\}$NMR spectrum of Compound **1**, 400 – -400 ppm, CD_3CN.

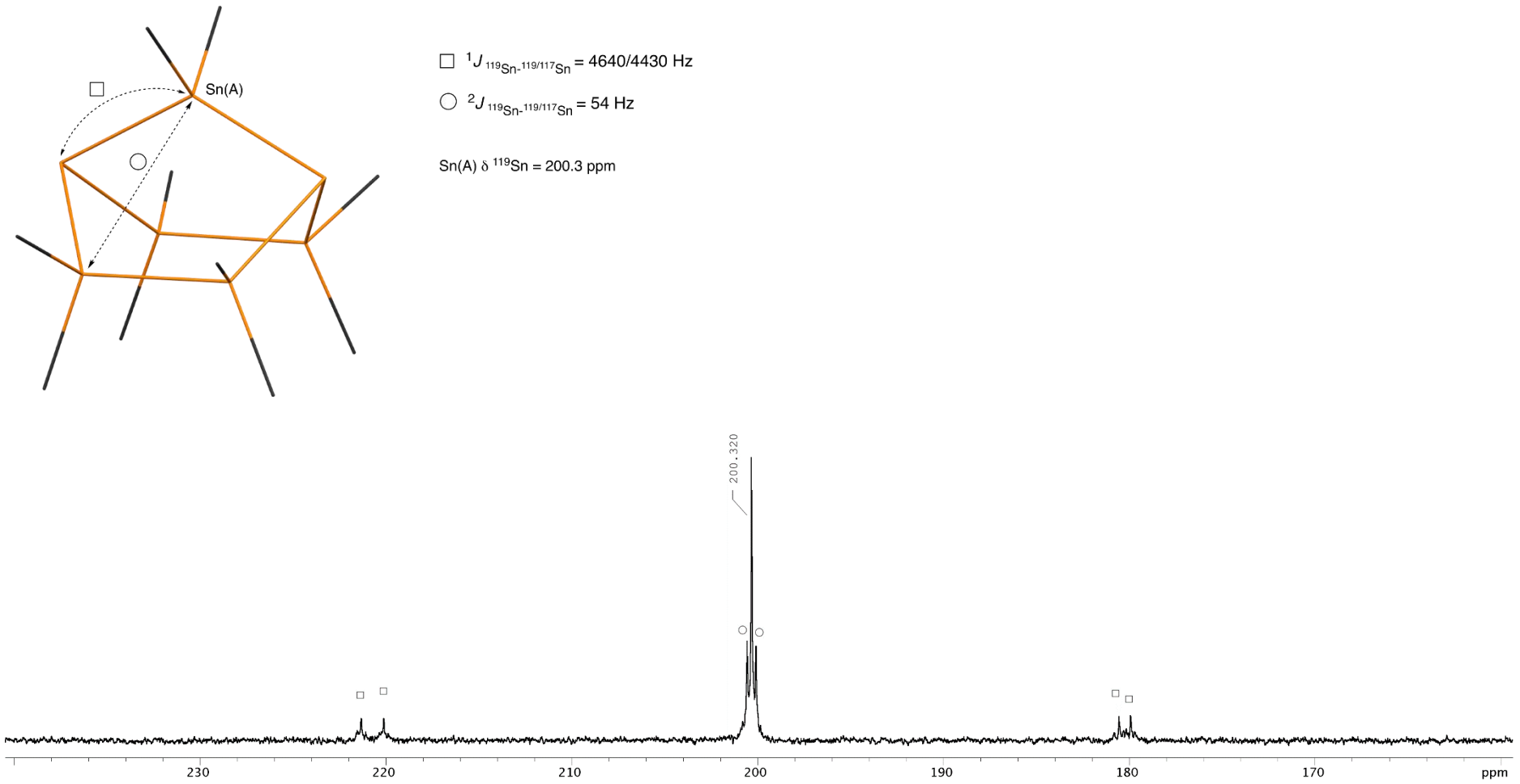


Figure S4.4 Detail of ^{119}Sn{^{1}H}NMR spectrum of Compound **1**, signal assigned to Sn(A) including coupling pattern, CD_3CN. $^{2}J_{119Sn-117/119Sn}$ coupling constant at 54 Hz not resolved.

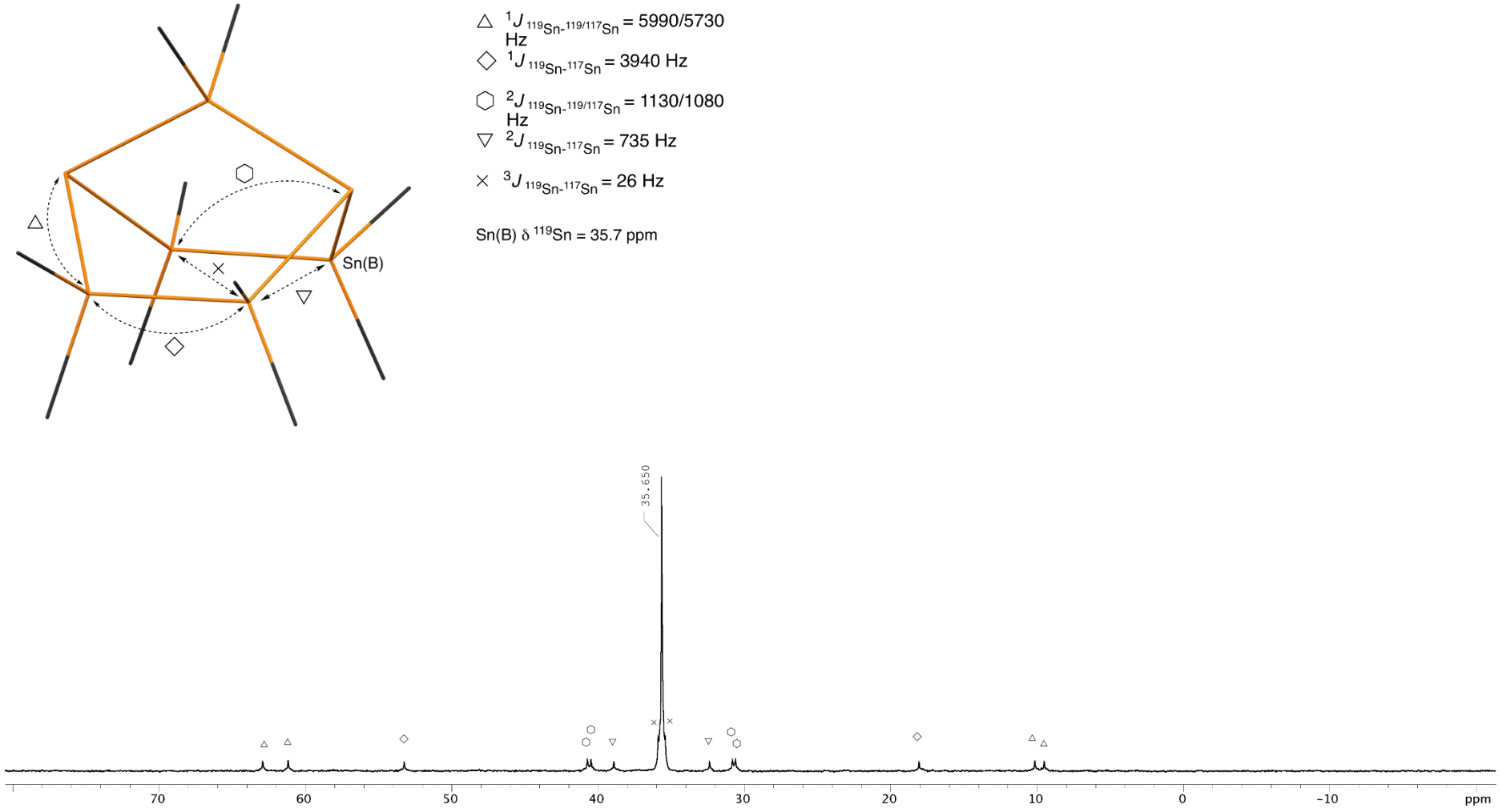


Figure S4.5 Detail of $^{119}Sn\{^{1}H\}$NMR spectrum of Compound **1**, signal assigned to Sn(B) including coupling pattern, CD_3CN.

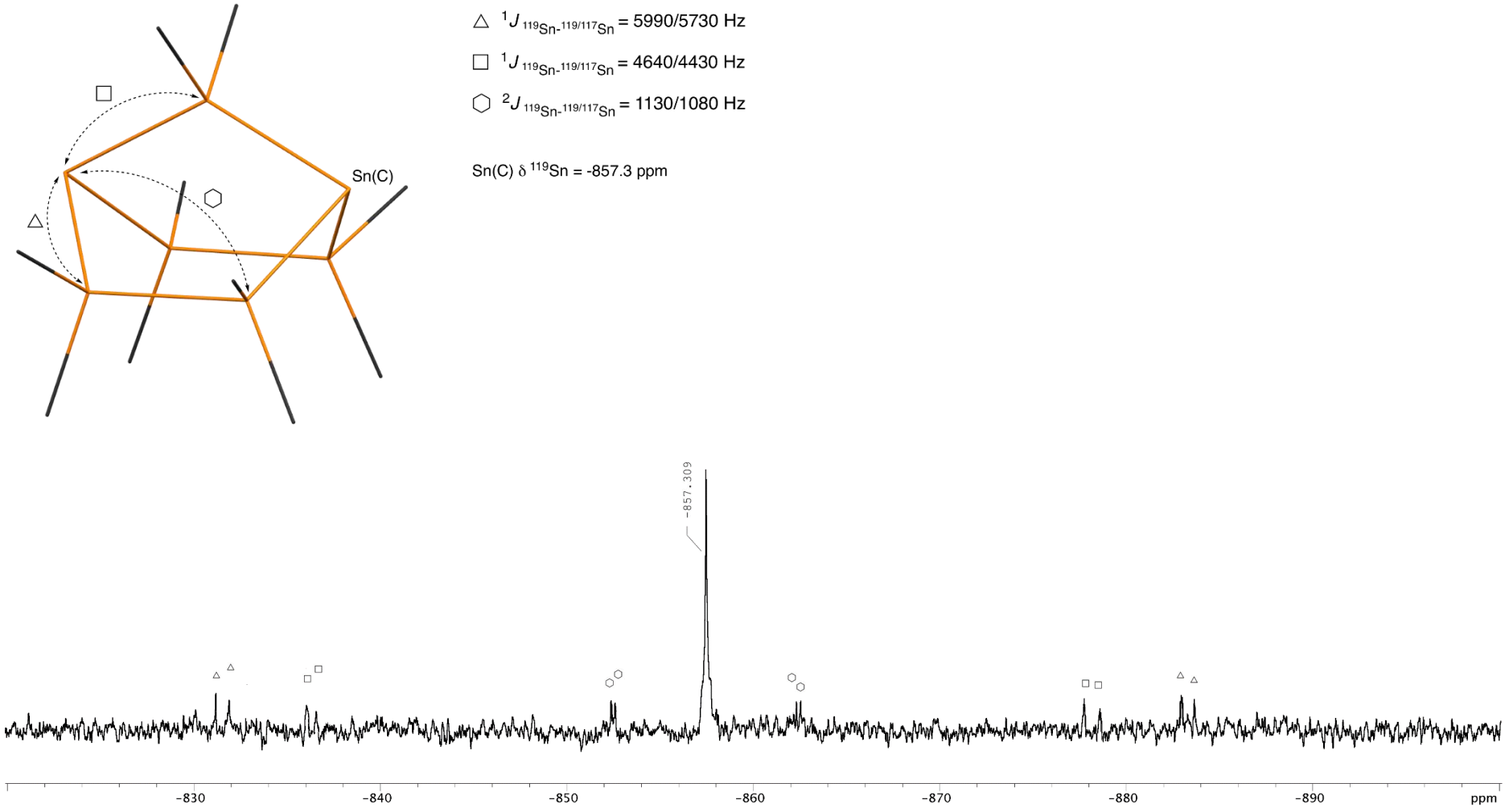
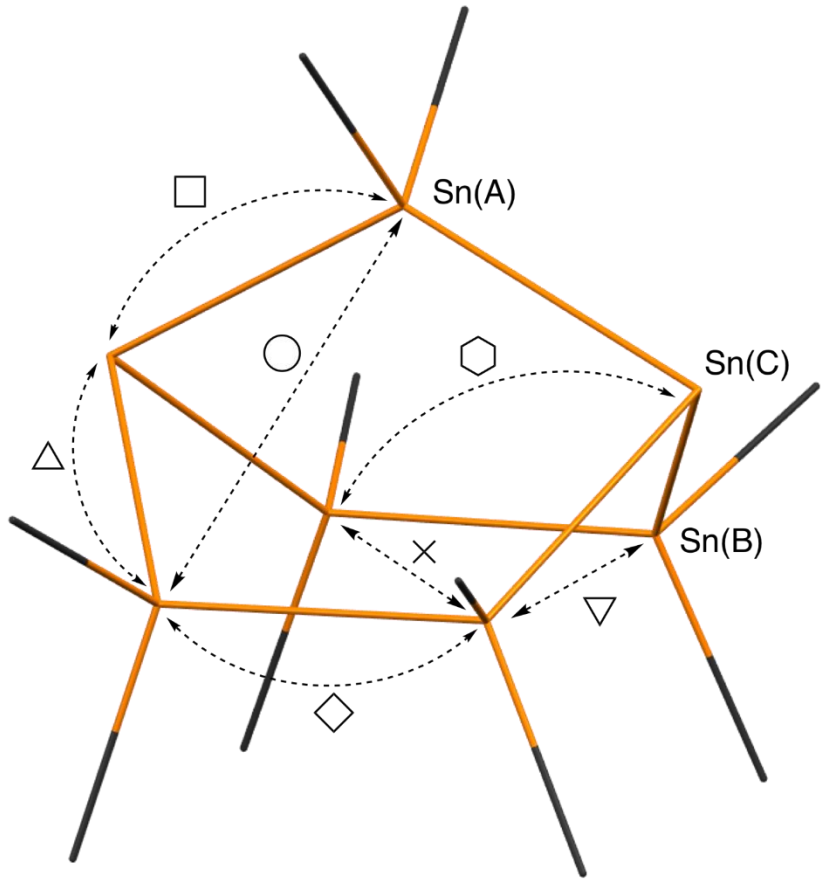


Figure S4.6 Detail of $^{119}Sn\{^{1}H\}$NMR spectrum of Compound **1**, signal assigned to Sn(C) including coupling pattern, CD_3CN.



△ $^{1}J_{^{119}Sn-^{119/117}Sn}$ = 5990/5730 Hz

□ $^{1}J_{^{119}Sn-^{119/117}Sn}$ = 4640/4430 Hz

◇ $^{1}J_{^{119}Sn-^{117}Sn}$ = 3940 Hz

⬡ $^{2}J_{^{119}Sn-^{119/117}Sn}$ = 1130/1080 Hz

▽ $^{2}J_{^{119}Sn-^{117}Sn}$ = 735 Hz

○ $^{2}J_{^{119}Sn-^{119/117}Sn}$ = 54 Hz

× $^{3}J_{^{119}Sn-^{117}Sn}$ = 26 Hz

Sn(A) δ ^{119}Sn = 200.3 ppm
Sn(B) δ ^{119}Sn = 35.7 ppm
Sn(C) δ ^{119}Sn = -857.3 ppm

Figure S4.7 Assignment of coupling constants and ^{119}Sn shifts for compound **1**.

Compound 2,
1,4-Dilithio-2,2,3,3,5,5,6,6,7,7,8,8-dodecaphenylbicyclo[2.2.2]octastannane-1,4-diide
[^{1}H, ^{13}C, ^{119}Sn]

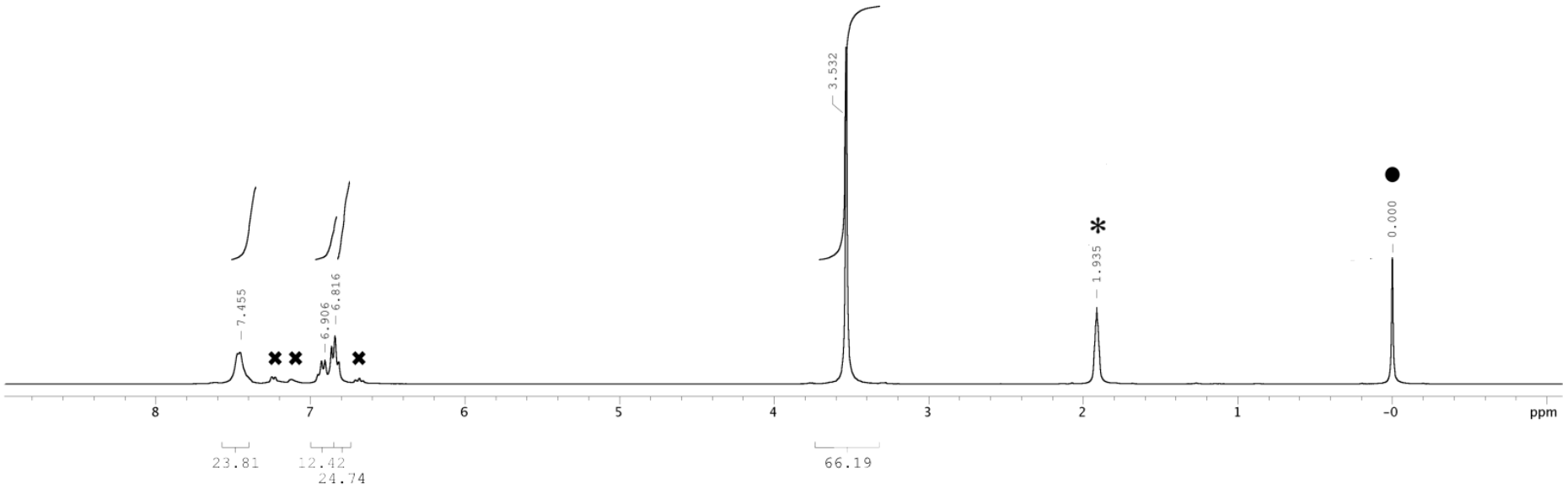


Figure S4.8 ^{1}H NMR spectrum of Compound **2**, CD_3CN, (* solvent residual signal, CD_3CN; ● $SiMe_4$ reference; ✖ impurity).

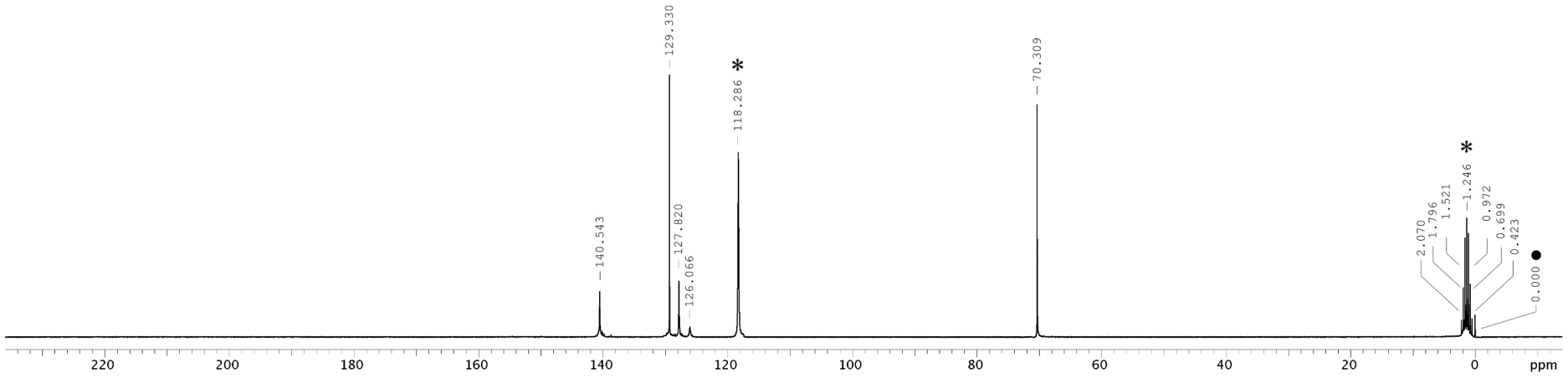


Figure S4.9 $^{13}C\{^{1}H\}$NMR spectrum of Compound **2**, CD_3CN, (* solvent signals, CD_3CN; ● $SiMe_4$ reference).

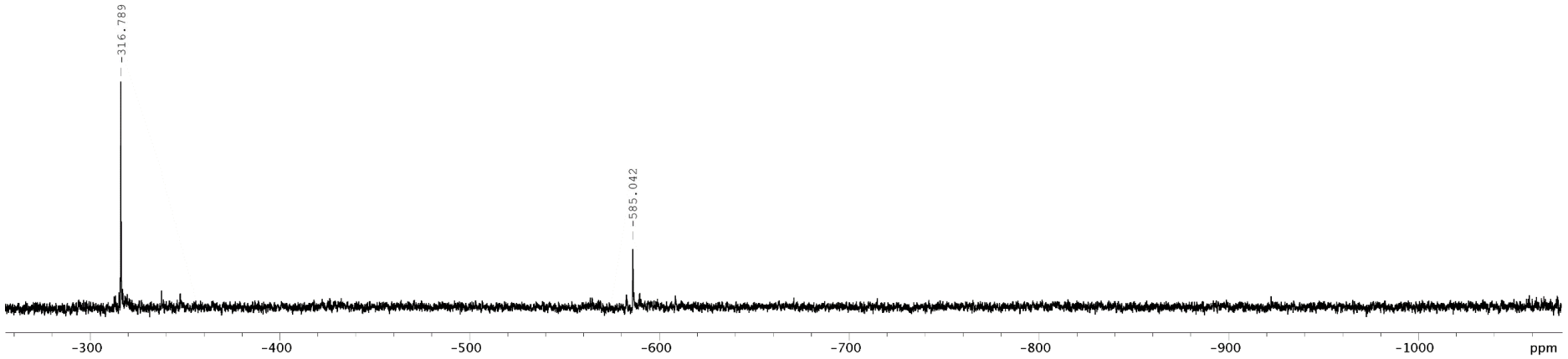


Figure S4.10 $^{119}Sn\{^{1}H\}$NMR spectrum of Compound **2**, CD_3CN.

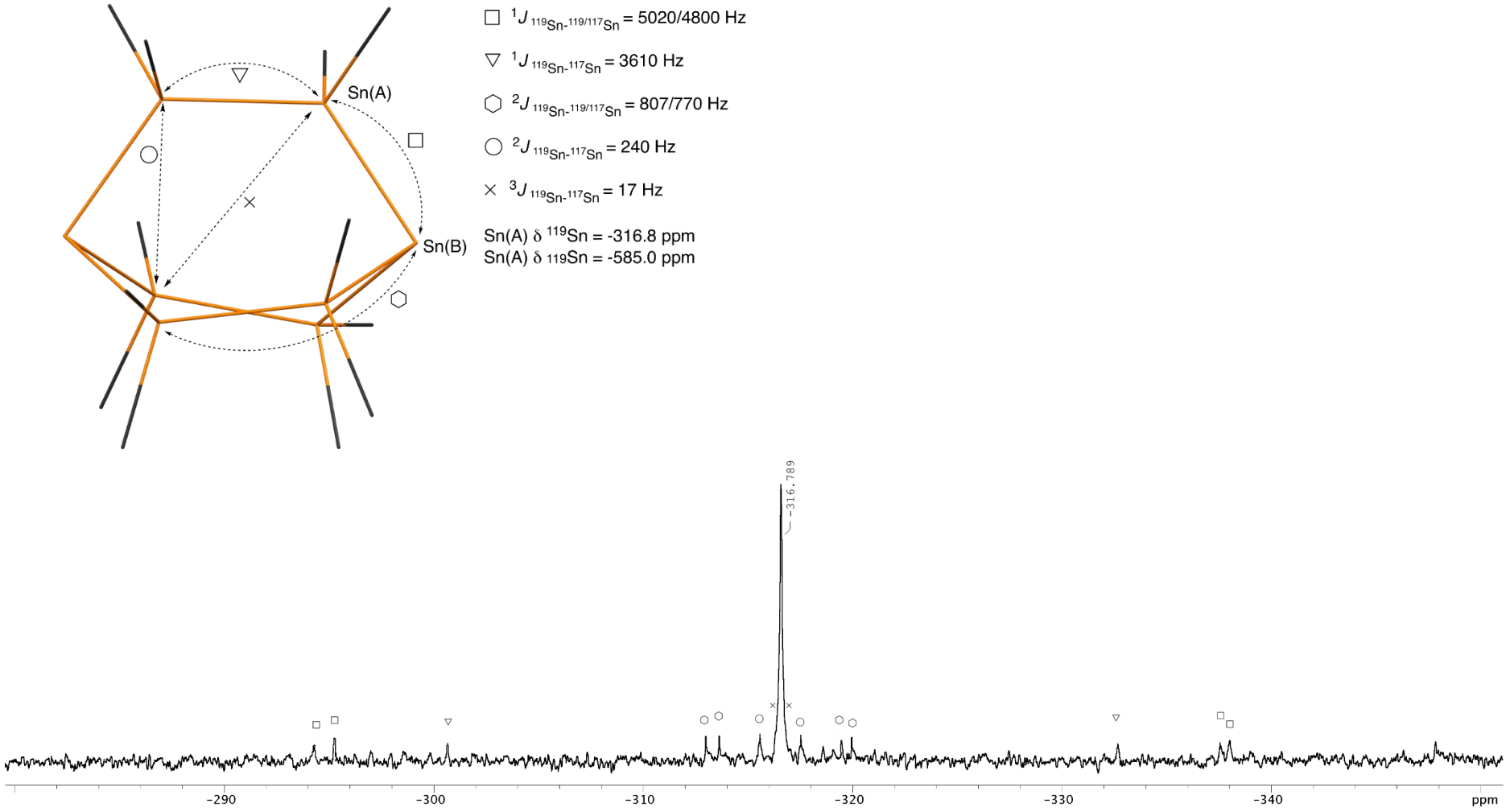


Figure S4.11 Detail of $^{119}Sn\{^{1}H\}$NMR spectrum of Compound **2**, signal assigned to Sn(A) including coupling pattern, CD_3CN.

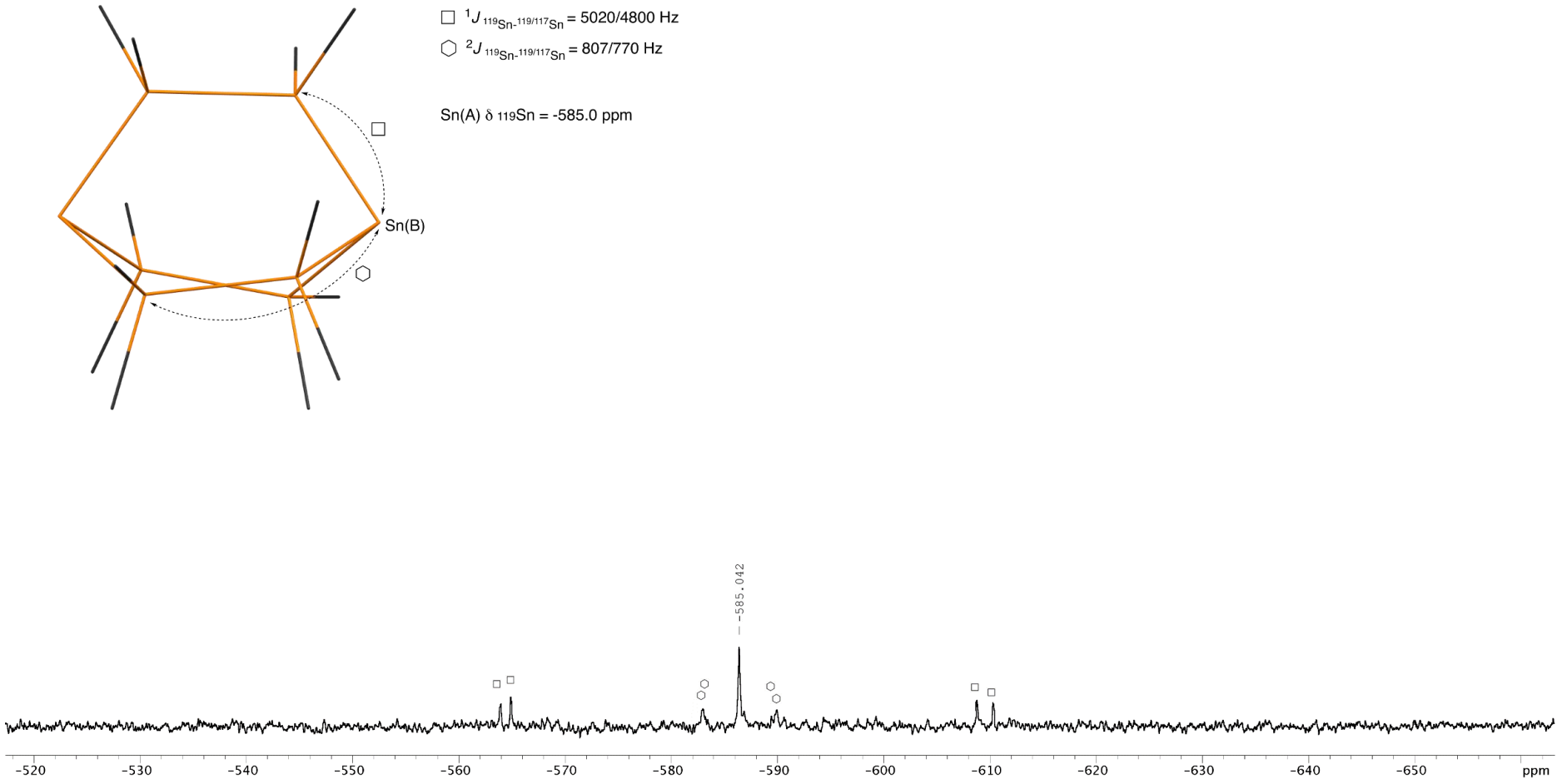


Figure S4.12 Detail of $^{119}Sn\{^{1}H\}$NMR spectrum of Compound **2**, signal assigned to Sn(B) including coupling pattern, CD_3CN.

Compound 3,
1-Lithio-2,2,3,3,4,5,5,6,6,7,7,8,8-tridecaphenylbicyclo[2.2.2]octastannide
[^{1}H, ^{13}C, ^{119}Sn]

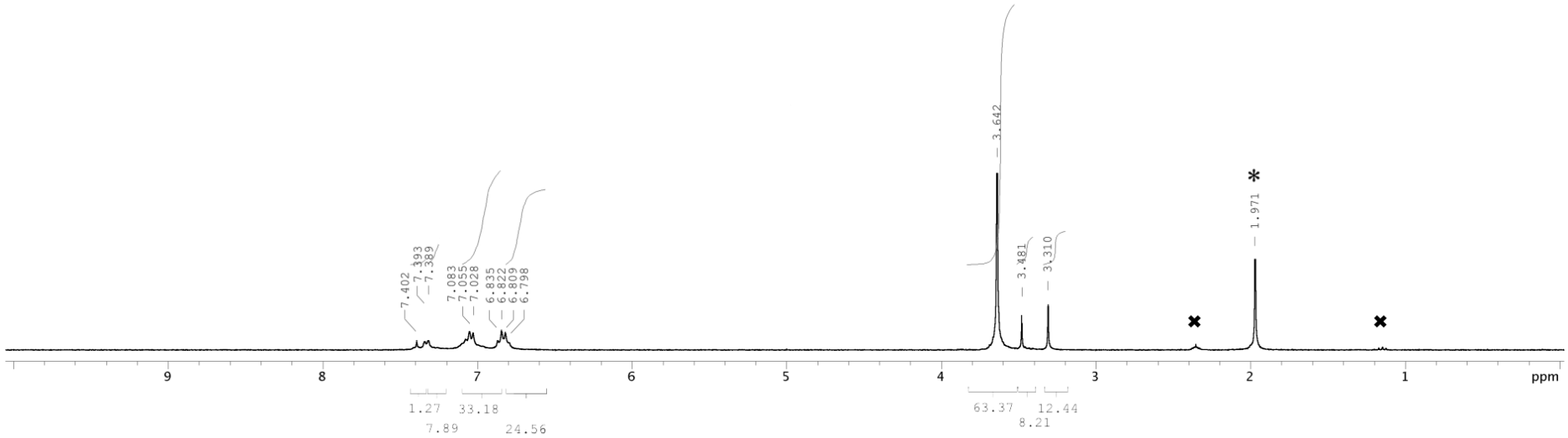


Figure S4.13 ^{1}H NMR spectrum of Compound **3**, CD_3CN, (* solvent residual signal, CD_3CN; ✖ impurity).

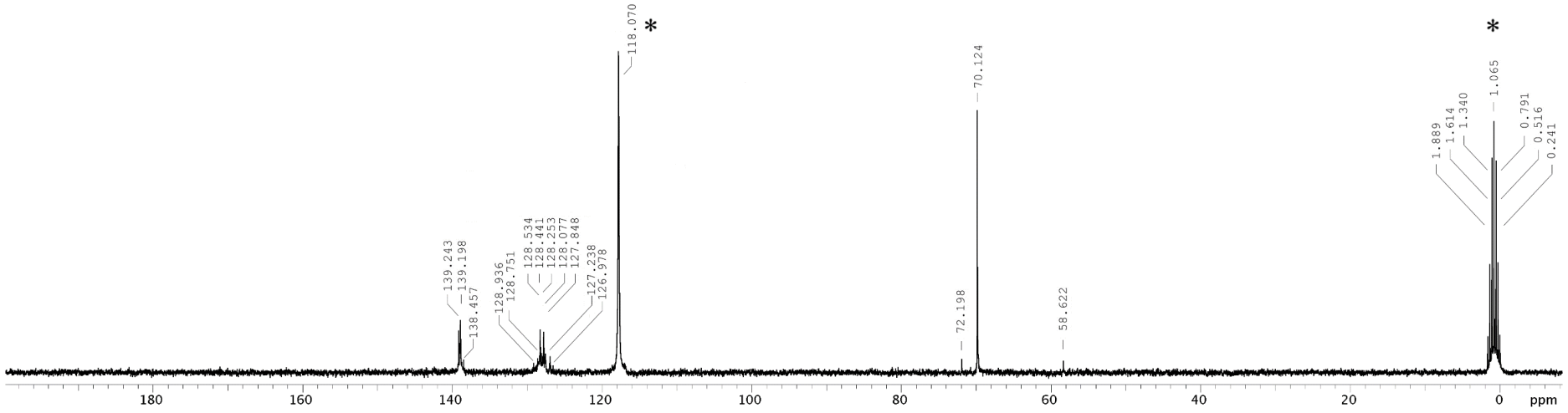


Figure S4.14 $^{13}C\{^{1}H\}$NMR spectrum of Compound **3**, CD_3CN, (* solvent signals, CD_3CN).

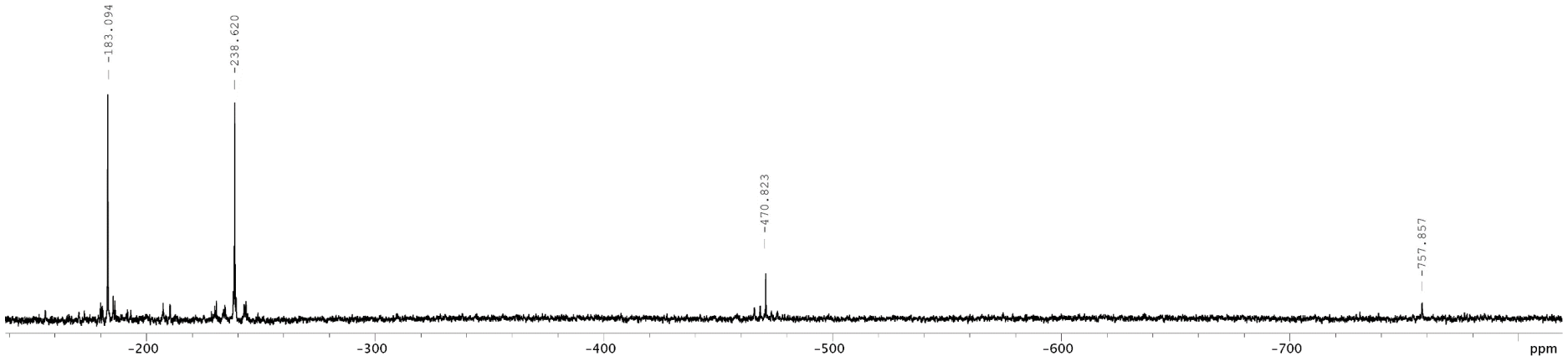


Figure S4.15 $^{119}Sn\{^{1}H\}$NMR spectrum of Compound **3**, CD_3CN.

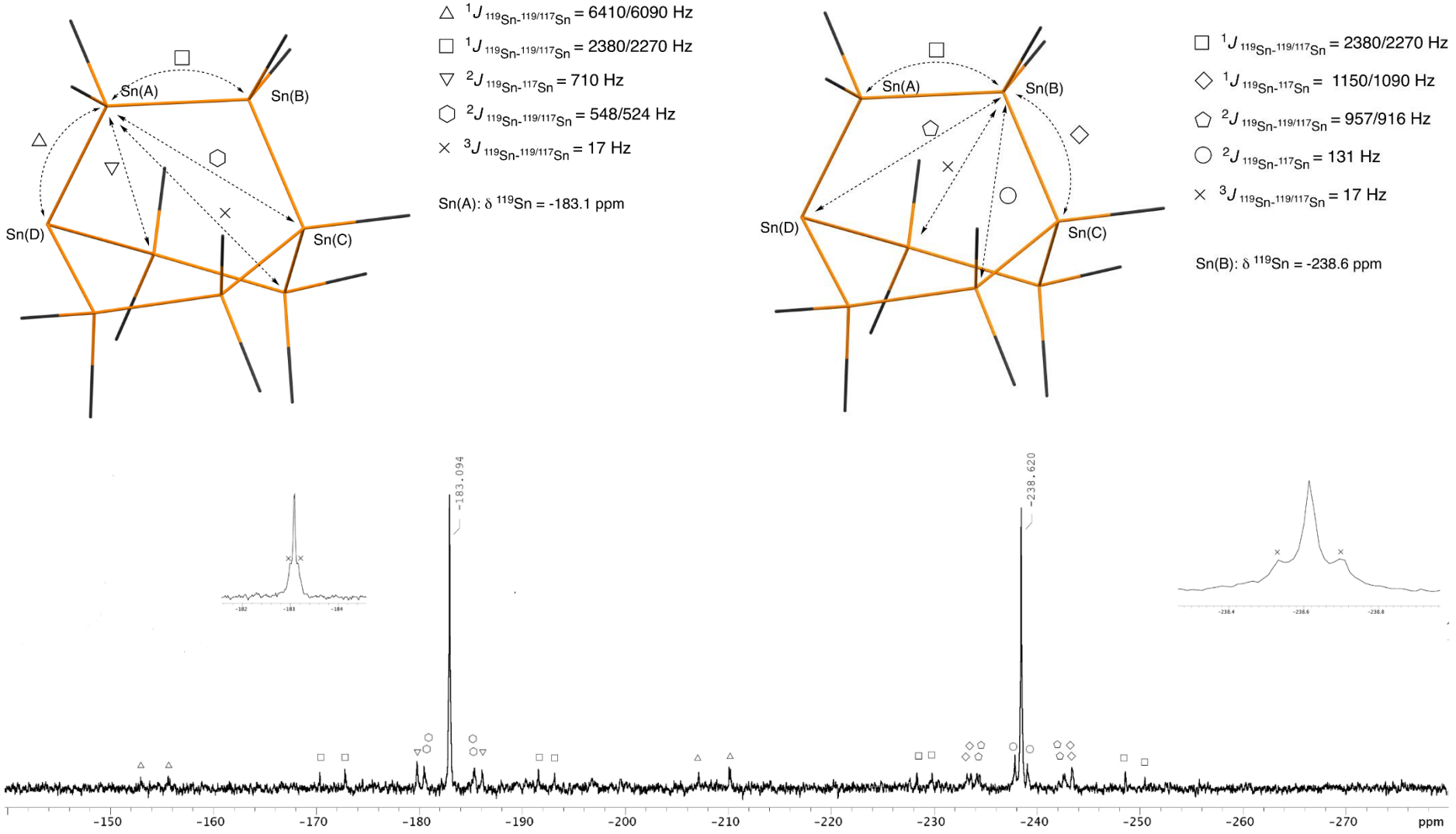


Figure S4.16 Detail of ^{119}Sn{^{1}H}NMR spectrum of Compound **1**, signals assigned to Sn(A) and Sn(B) including coupling pattern, CD_3CN. $^{2}J_{^{119}Sn-^{117/119}Sn}$ coupling constant at 17 Hz not resolved.

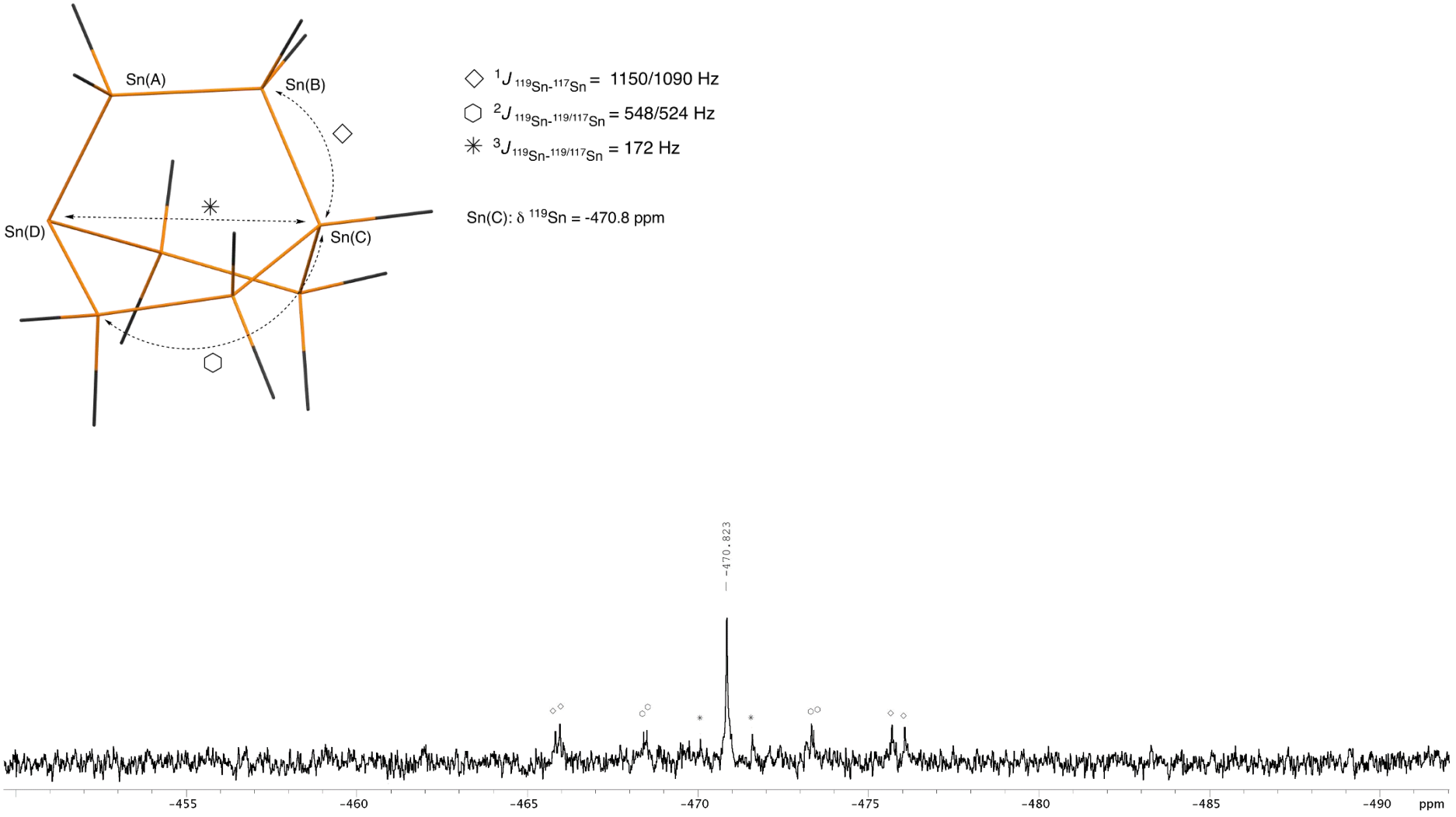
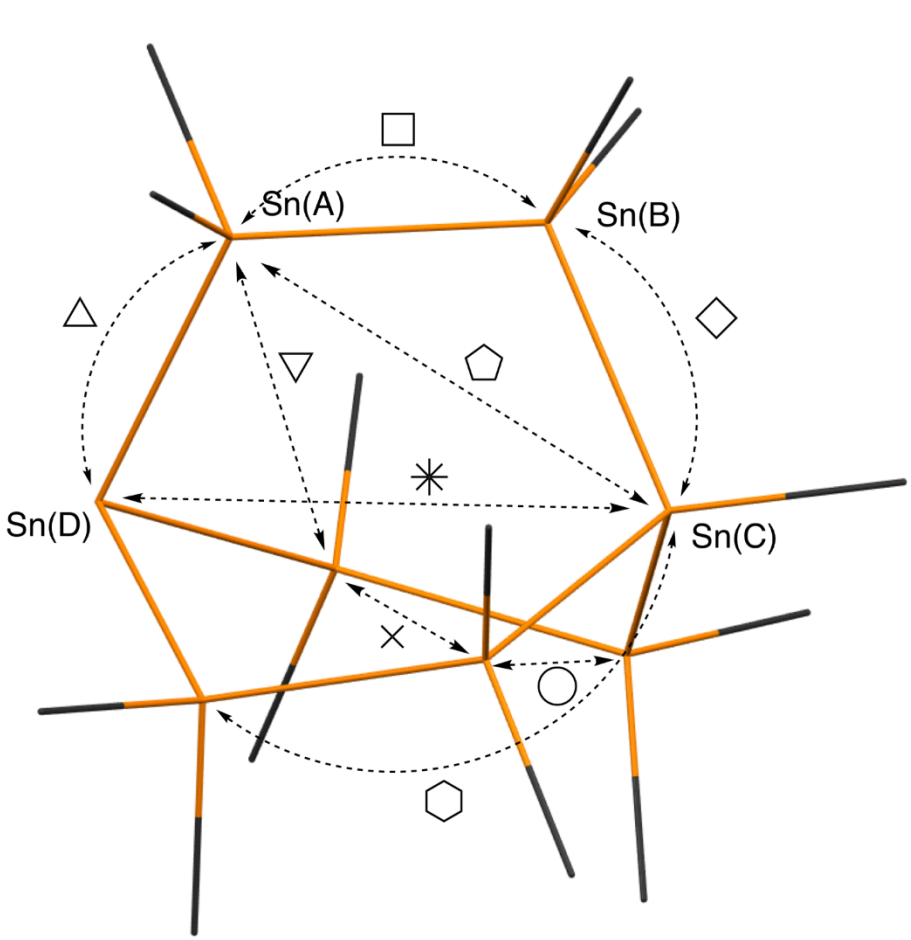


Figure S4.17 Detail of $^{119}Sn\{^{1}H\}$NMR spectrum of Compound **3**, signal assigned to Sn(C) including coupling pattern, CD_3CN. $^{3}J_{119Sn-117/119Sn}$ coupling constant at 172 Hz not resolved.



△ $^{1}J_{^{119}Sn\text{-}^{119/117}Sn}$ = 6410/6090 Hz

□ $^{1}J_{^{119}Sn\text{-}^{119/117}Sn}$ = 2380/2270 Hz

◇ $^{1}J_{^{119}Sn\text{-}^{117}Sn}$ = 1150/1090 Hz

⬠ $^{2}J_{^{119}Sn\text{-}^{119/117}Sn}$ = 957/916 Hz

▽ $^{2}J_{^{119}Sn\text{-}^{117}Sn}$ = 710 Hz

⬡ $^{2}J_{^{119}Sn\text{-}^{119/117}Sn}$ = 548/524 Hz

✳ $^{3}J_{^{119}Sn\text{-}^{119/117}Sn}$ = 172 Hz

◯ $^{2}J_{^{119}Sn\text{-}^{117}Sn}$ = 131 Hz

× $^{3}J_{^{119}Sn\text{-}^{119/117}Sn}$ = 17 Hz

Sn(A): δ ^{119}Sn = -183.1 ppm
Sn(B): δ ^{119}Sn = -238.6 ppm
Sn(C): δ ^{119}Sn = -470.8 ppm
Sn(D): δ ^{119}Sn = -757.9 ppm

Figure S4.18 Assignment of coupling constants and ^{119}Sn shifts for compound **3**.

Compound 4, Lithiumphenylaluminumtrihydride [^{1}H, ^{13}C]

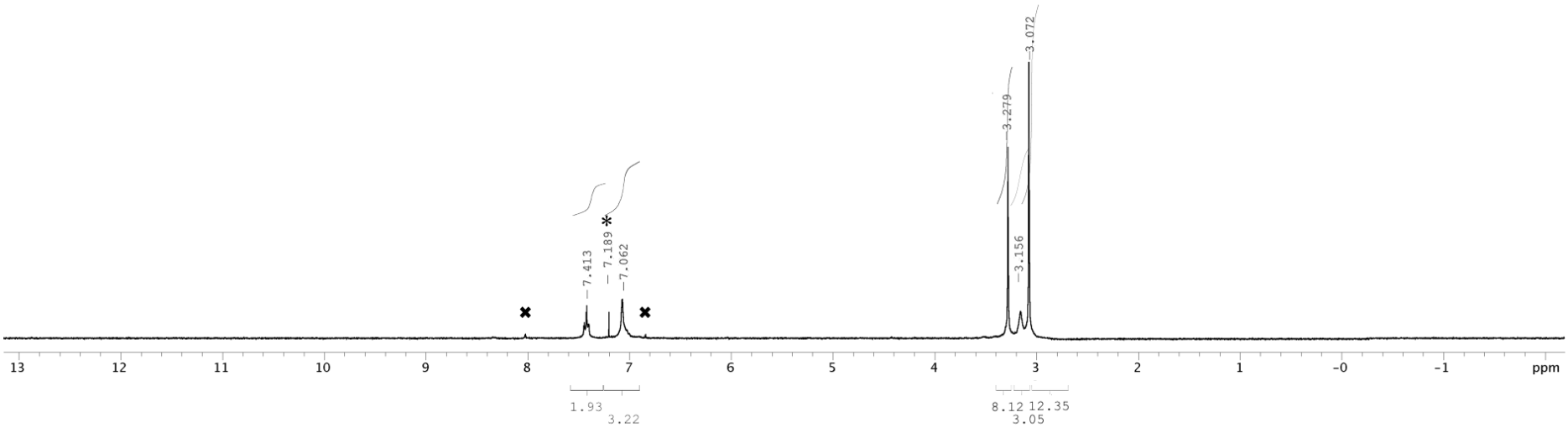


Figure S4.19 ^{1}H NMR spectrum of Compound **4**, C_6D_6, (* solvent residual signal, C_6D_6; ✖ impurity).

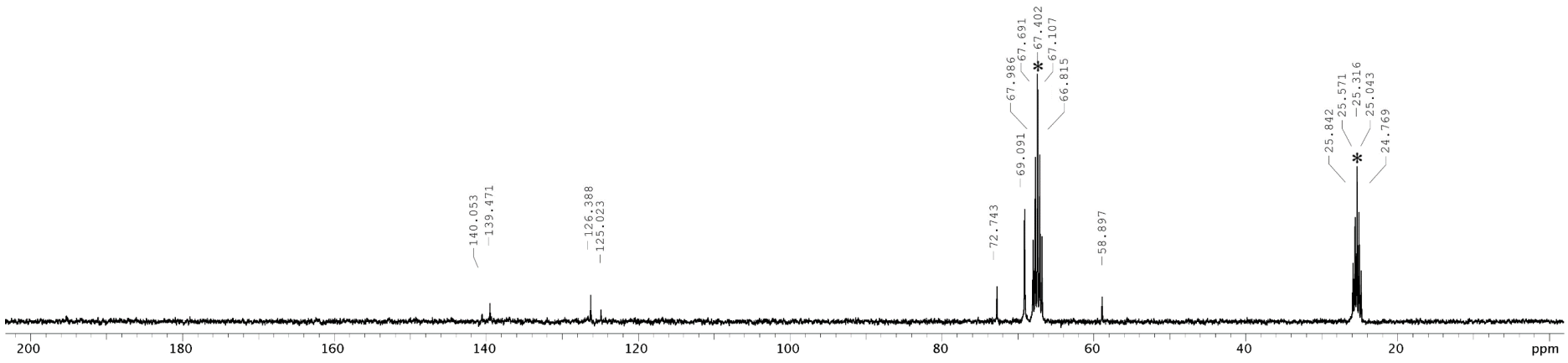


Figure S4.20 $^{13}C\{^{1}H\}$NMR spectrum of Compound **4**, THF-d8, (* solvent signals, THF-d8).

Compound 5, Lithiumtriphenylaluminumhydride [^{1}H, ^{13}C]

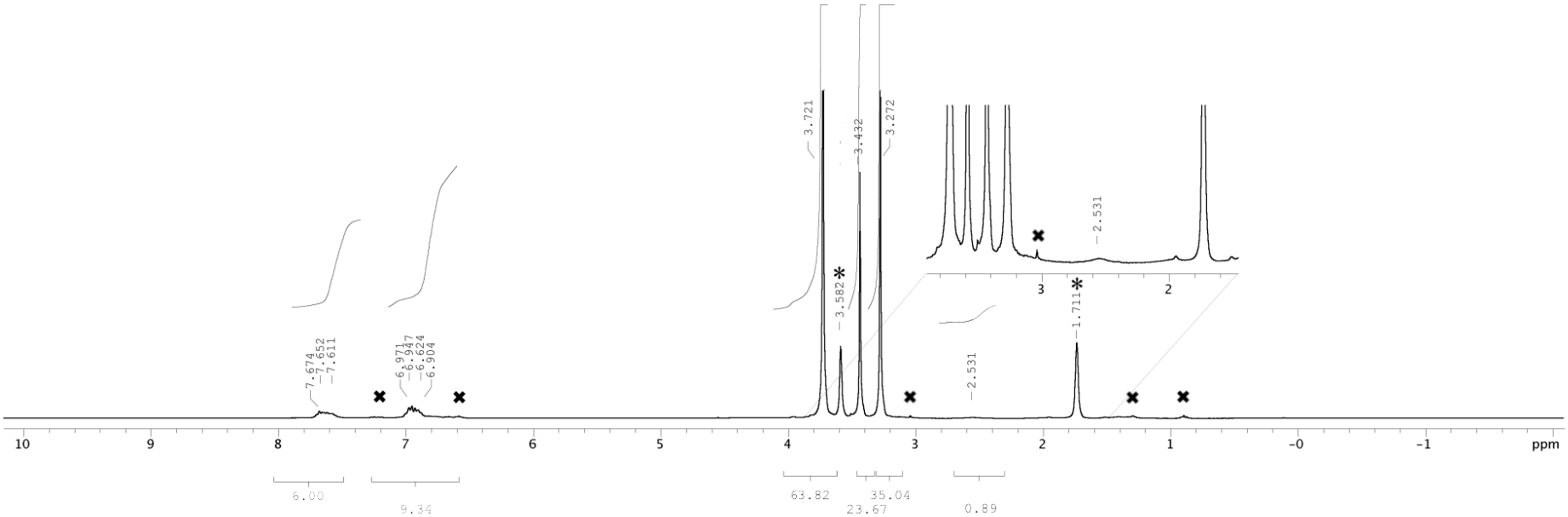


Figure S4.21 ^{1}H NMR spectrum of Compound **5**, THF-d8, (* solvent residual signal, THF-d8; ✖ impurity).

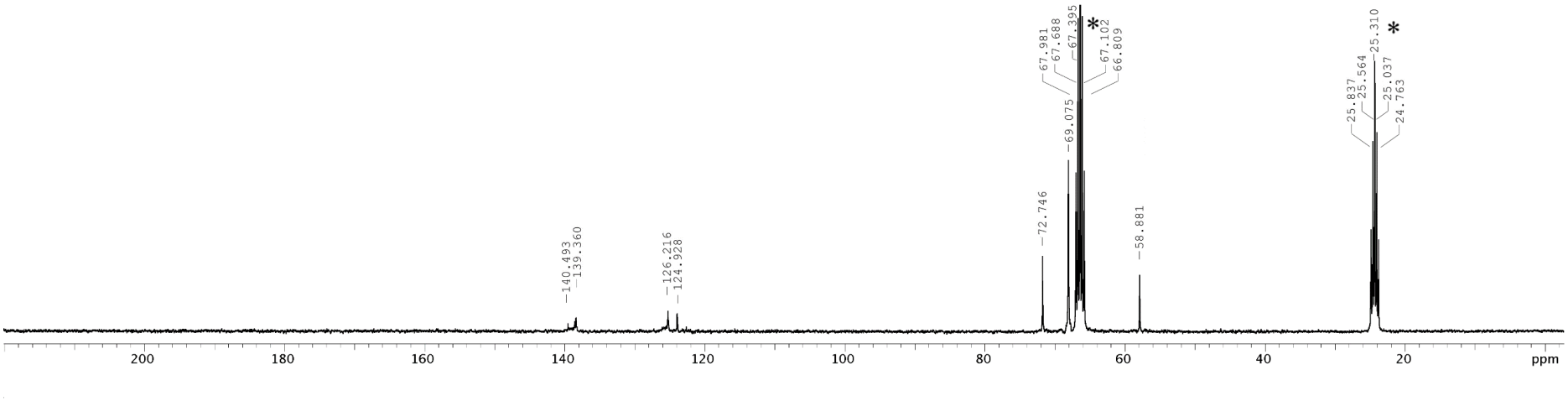


Figure S4.22 $^{13}C\{^{1}H\}$NMR spectrum of Compound **5**, THF-d8, (* solvent signal, THF-d8)

Isotopic labelling experiments

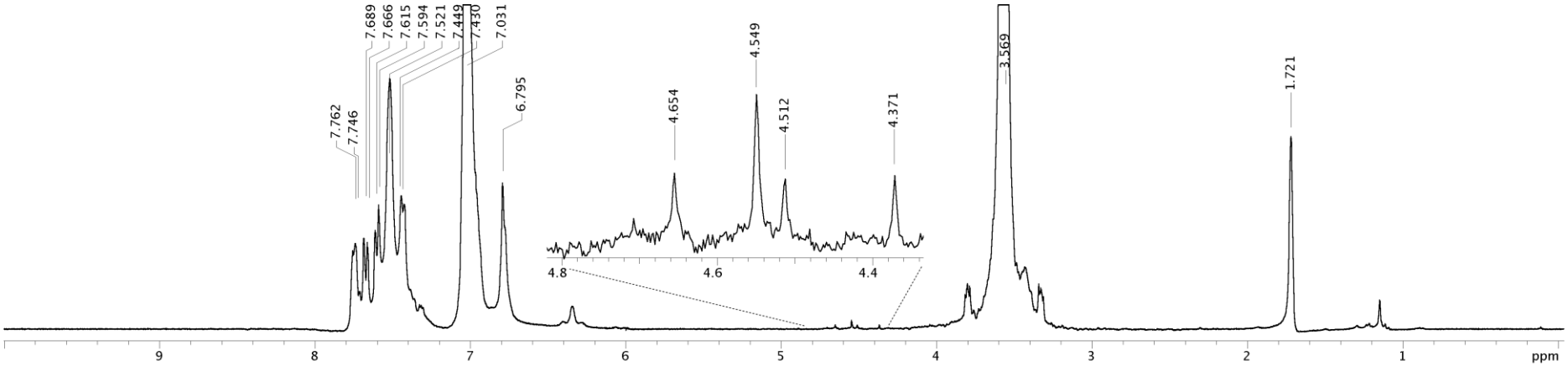


Figure S4.23 ^{1}H NMR spectrum: Reaction of Ph_2SnD_2 with $LiAlH_4$, THF-d8. Formation of trace amounts of H_2 and HD.

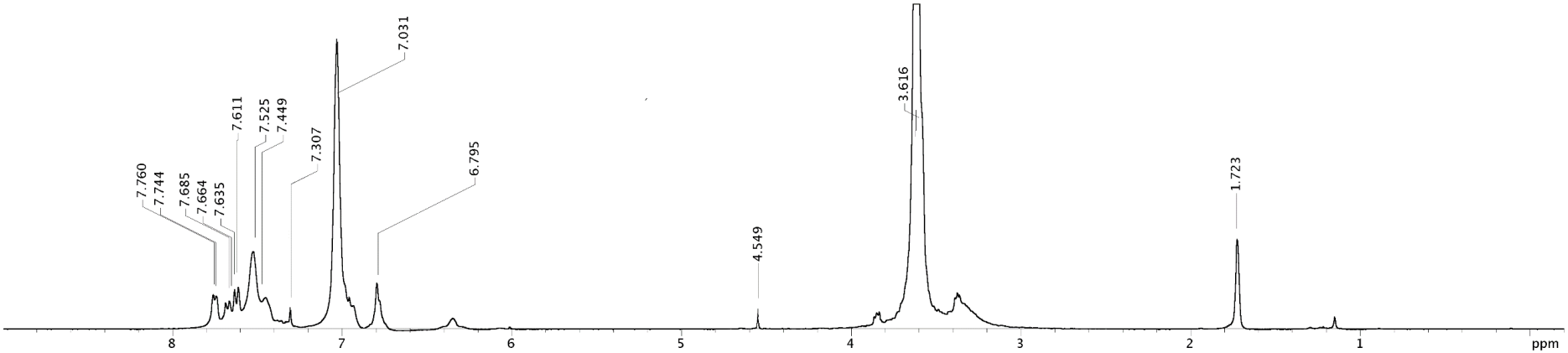


Figure S4.24 ^{1}H NMR spectrum: Reaction of Ph_2SnH_2 with $LiAlD_4$, THF-d8. Formation of H_2.

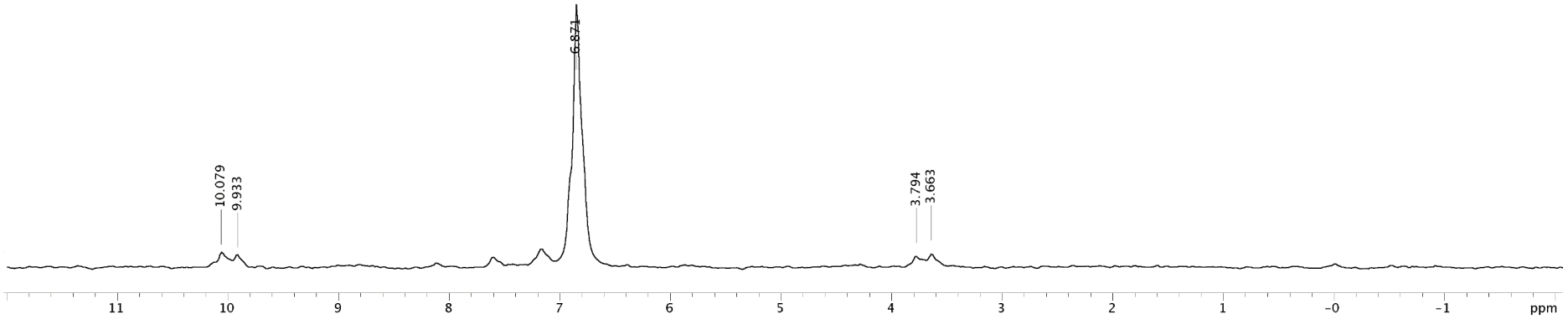


Figure S4.25 ^{2}H NMR spectrum Ph_2SnD_2 in THF.

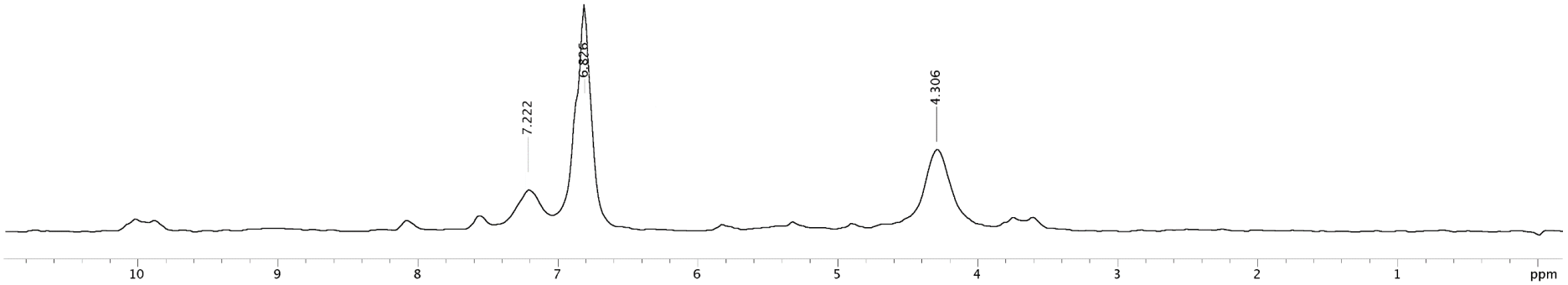


Figure S4.26 ^{2}H NMR spectrum: Reaction of Ph_2SnD_2 with $LiAlH_4$, THF. Formation of D_2.

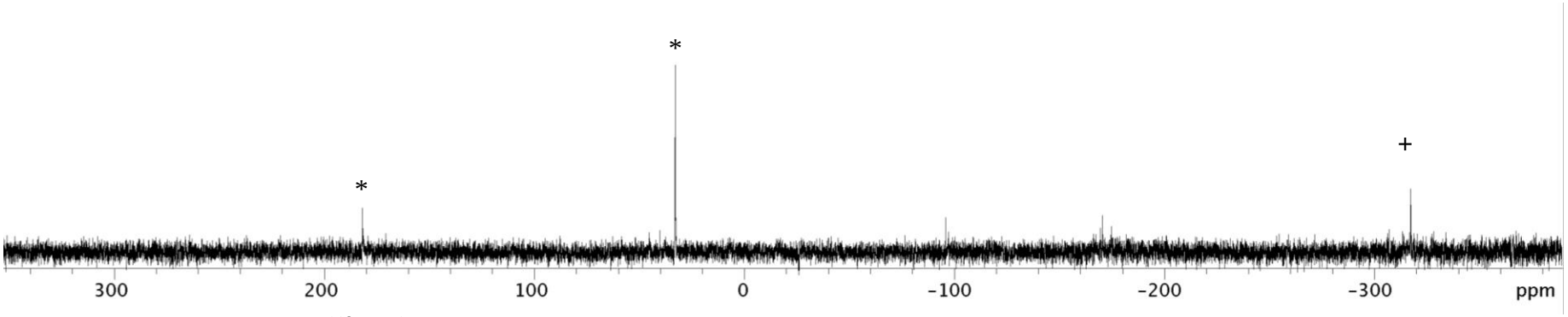


Figure S4.27 Representative $^{119}Sn\{^{1}H\}$ NMR spectra of reaction solutions using a $Ph_2SnH_2/LiAlH_4$ ratio of 3.5:1. Increased formation of compound 1 (signals marked with *) is observed compared to compound 2 (marked with +). Other shifts belong to unidentified byproducts.

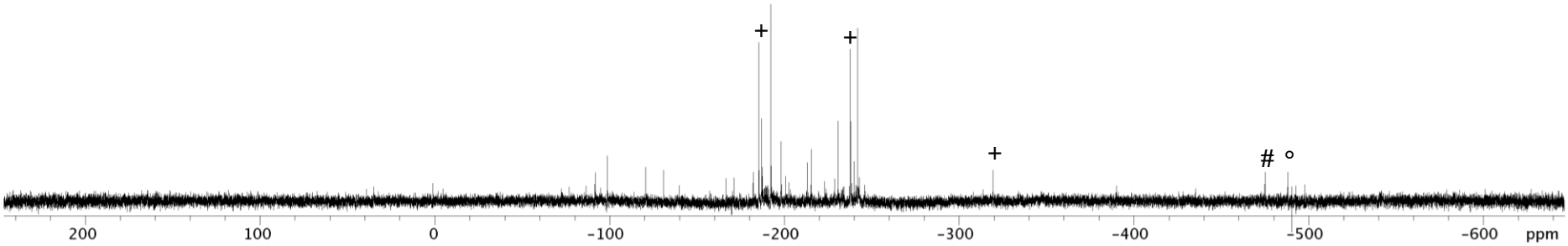


Figure S4.28 Representative $^{119}Sn\{^{1}H\}$ NMR spectra of reaction solutions using a $Ph_2SnH_2/LiAlH_4$ ratio of 4:1. Increased formation of compound 2 (signals marked with +) is observed compared to compound 1 (no signals found). Shifts assigned to compound 3 are observed as well (marked with #). Other shifts belong to unidentified byproducts. Artefacts are denoted with °.

5. Computational Details

DFT calculations were run with Gaussian 09 (Revision D.01).[5] The Sn centres were described with the Stuttgart RECPs and associated basis sets,[6] and 6-31G** basis sets were used for all other atoms (BS1).[7] An additional d-function was used to describe polarization for the Sn atoms (ζ = 0.180).[8] Initial BP86[9] optimizations were performed using the 'grid = ultrafine' option and being fully characterized via analytical frequency calculations as minima (all positive eigenvalues). The agreement of the bridgehead $Sn_{br}\cdots Sn_{br}$ (**1**: Sn1-Sn7; **2**: Sn1-Sn8; **3**: Sn1-Sn4) distance in the three BP86 computed structures to the crystallographic data (see Fig 2-4) was ~ 0.2 Å. Attempts to improve this agreement through optimising with cations present to balance the overall charge of the calculation had no effect.

Functional testing was performed using other GGA functionals (PBE[5b] and BLYP[10]), hybrid-GGA functionals (B3LYP[11] and ωB97xD[12]) and a Minnesota functional (M06[13]), to identify if this discrepancy was unique to the BP86 functional. Dispersion corrections were applied using Grimme's D3 parameter set[15] for separate BP86, PBE, BLYP and B3LYP functional optimisations (i.e. for calculations that did not already include a treatment of dispersion effects). As Table S5.1 shows, there was a small reduction in the $Sn_{br}\cdots Sn_{br}$ distance error when B3LYP was the chosen functional, whilst dispersion corrections and M06 made these distance errors larger.

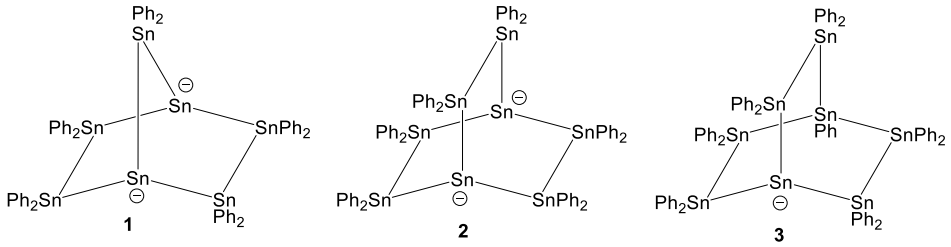
To ensure a good reproduction of the Sn cluster geometry, BP86 optimisations on the crystal structures were computed when freezing the positions of the Sn atoms, thereby only allowing the carbon and hydrogen atoms to move during the optimisation process (**b**). This naturally reproduced the crystal structure Sn-Sn and $Sn_{br}\cdots Sn_{br}$ distances exactly, but also as shown in Table S5.2 saw minimal difference in the Frontier Orbital energies. The difference in relative energies between these optimisation strategies is also shown in the final row of Table S2, with these additional constraints on the Sn atom positions only raising the energy of the structures by 5.3 – 10.6 kcal/mol.

Natural Bond Orbital (NBO) analysis calculations were viewed in GaussView (v5.0.8) to generate orbital pictures shown in the manuscript and in Figures S5.1.

Table S5.1. Computed $Sn_{br}\cdots Sn_{br}$ distances (in Å) for **1**, **2** and **3** with different DFT functionals and their associated deviation from the crystallographic distance

Structure	DFT Functional	$Sn_{br}\cdots Sn_{br}$ [Å]	Deviation [Å]
1		*5.0393(7)*	--
1	BP86	5.259	0.220
1	BP86/D3	5.327	0.288
1	PBE	5.275	0.236
1	PBE/D3	5.319	0.280
1	BLYP	5.263	0.224
1	BLYP/D3	5.326	0.287
1	B3LYP	5.211	0.172
1	B3LYP/D3	5.256	0.217
1	□B97xD	5.203	0.164
1	M06	5.341	0.302
2		*5.9374(9)*	--
2	BP86	6.165	0.228
2	BP86/D3	6.350	0.413
2	PBE	6.198	0.261
2	PBE/D3	6.314	0.377
2	BLYP	6.137	0.200
2	BLYP/D3	6.281	0.344
2	B3LYP	6.082	0.145
2	B3LYP/D3	6.201	0.264
2	□B97xD	6.219	0.282
2	M06	6.406	0.469
3		*5.269(3)*	--
3	BP86	5.476	0.207
3	BP86/D3	5.622	0.353
3	PBE	5.494	0.225
3	PBE/D3	5.558	0.289
3	BLYP	5.502	0.233
3	BLYP/D3	5.582	0.313
3	B3LYP	5.452	0.183
3	B3LYP/D3	5.494	0.225
3	□B97xD	5.551	0.282
3	M06	5.776	0.507

Table S5.2. Computed HOMO and LUMO energies, and energy difference ($E_{LUMO-HOMO}$) (in eV) of structures **1**, **2** and **3** using BP86/BS1 for (**a**) full optimisation and (**b**) constraining the Sn atom positions to coordinates obtained from X-ray structures (C and H atoms free to optimise). The Constraint Energy (in kcal/mol) shows the energy difference between the computed (**b**) and (**a**) geometries.



(**a**) Fully Optimised Geometries			
HOMO	0.65	0.64	-2.10
LUMO	3.05	2.73	0.44
$E_{LUMO-HOMO}$	*2.40*	*2.09*	*2.54*
(b) C and H Optimised Geometries			
HOMO	0.71	0.68	-1.99
LUMO	3.04	2.83	0.48
$E_{LUMO-HOMO}$	*2.33*	*2.15*	*2.47*
Constraint Energy Difference [in kcal/mol]	+ 5.3	+ 9.2	+ 10.6

Figure S5.1. Natural Bond Orbitals for the HOMO-1, HOMO and LUMO frontier orbitals of structures **1**, **2** and **3**, all carbon and hydrogen atoms shown as wireframe, Sn atoms as grey balls.

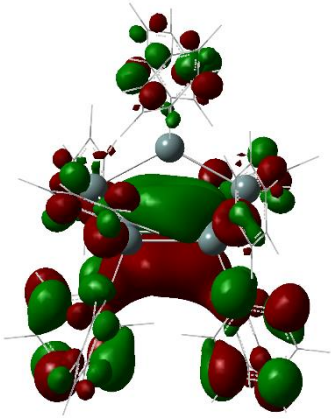
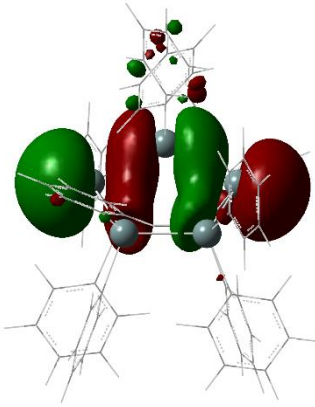
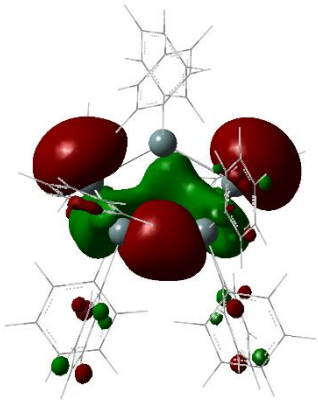
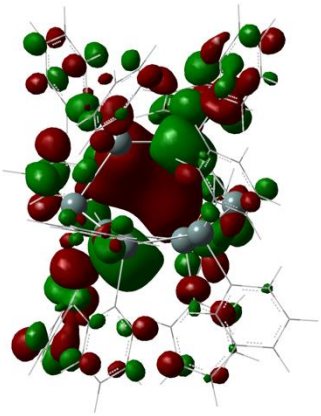
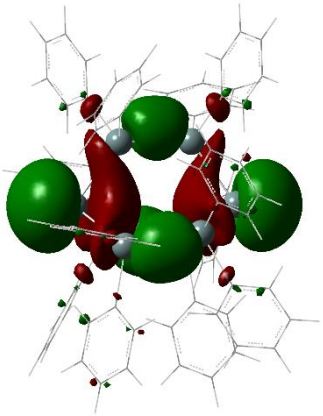
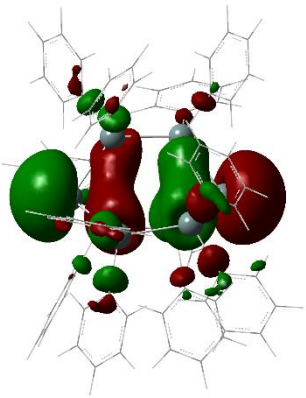
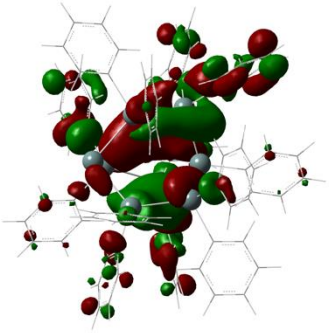
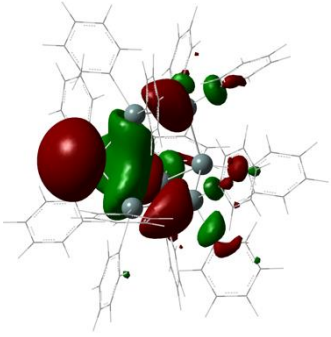
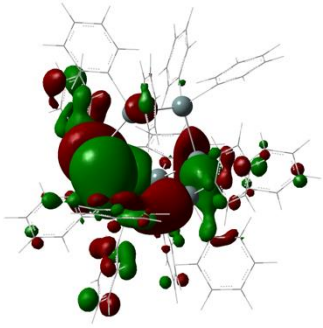
	LUMO	HOMO	HOMO-1
1			
2			
3			

Figure S5.1. Natural Bond Orbitals for the HOMO-X frontier orbitals of structures **1**, **2** and **3**, all carbon and hydrogen atoms shown as wireframe, Sn atoms as grey balls.

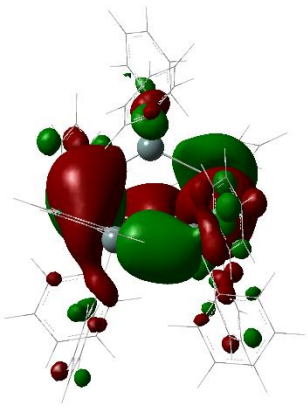
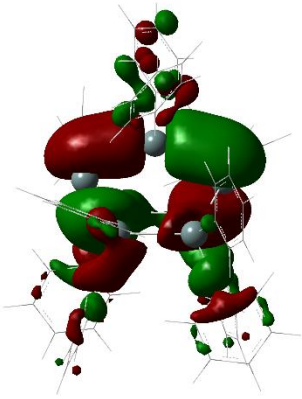
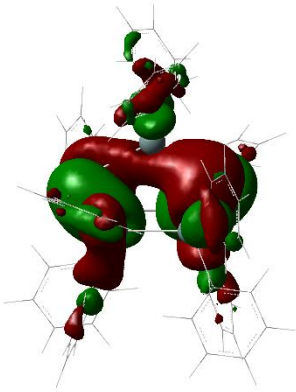
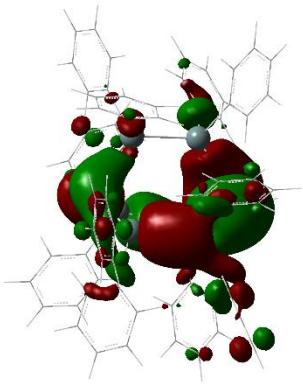
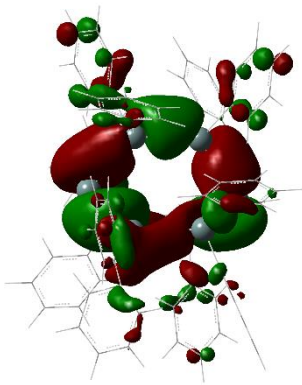
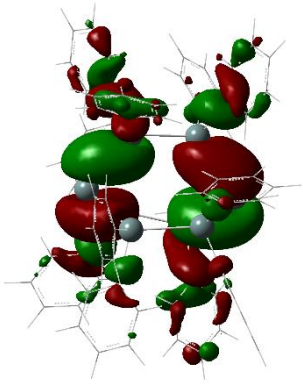
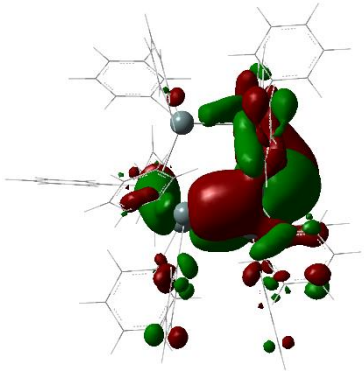
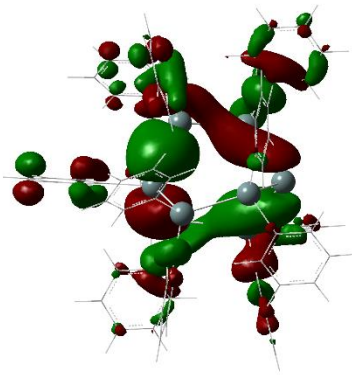
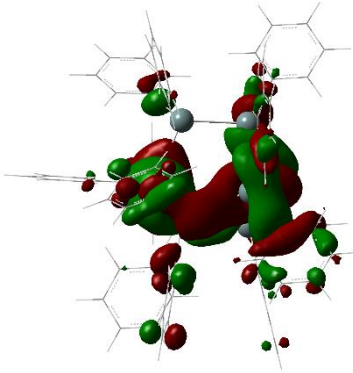
	HOMO-2	HOMO-3	HOMO-4
1			
2			
3			

Figure S5.1. Natural Bond Orbitals for the HOMO-X frontier orbitals of structures **1**, **2** and **3**, all carbon and hydrogen atoms shown as wireframe, Sn atoms as grey balls.

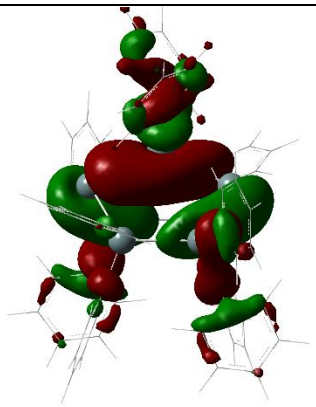
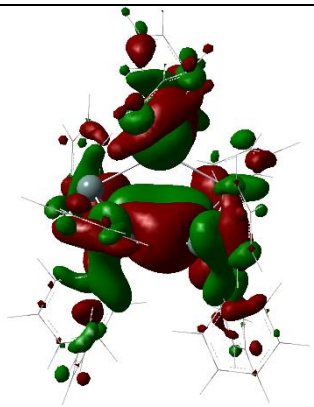
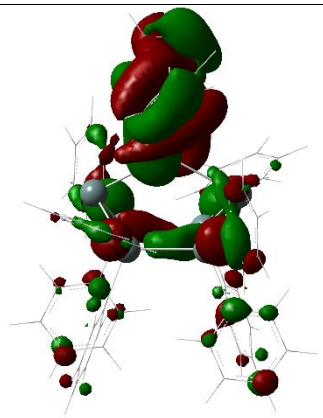
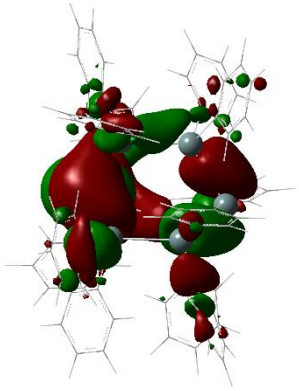
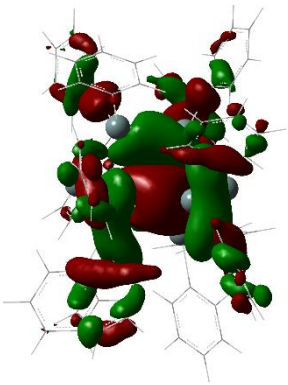
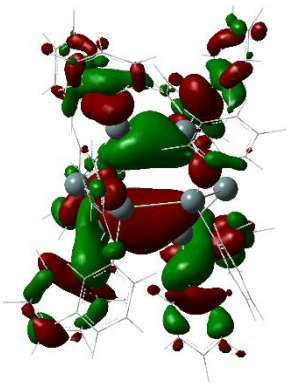
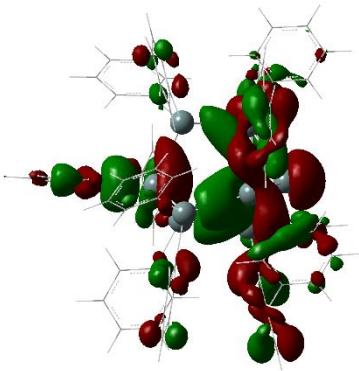
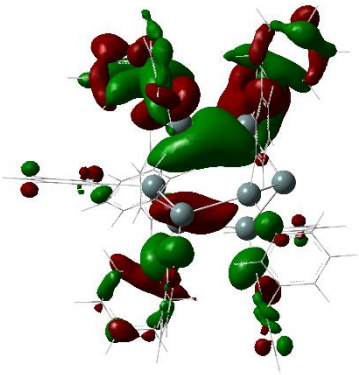
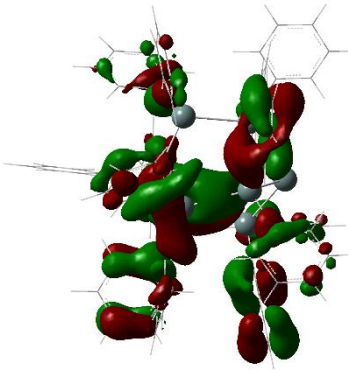
	HOMO-5	HOMO-6	HOMO-7
1			
2			
3			

Figure S5.1. Natural Bond Orbitals for the HOMO-X frontier orbitals of structures **1**, **2** and **3**, all carbon and hydrogen atoms shown as wireframe, Sn atoms as grey balls.

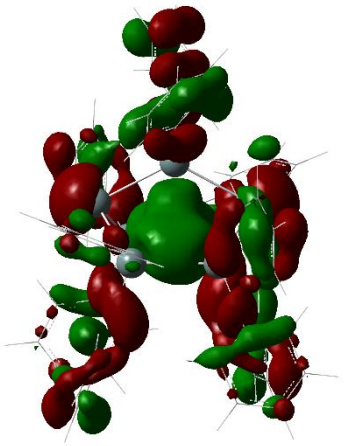
	HOMO-8
1	

Table S5.3. Calculated and experimental ^{119}Sn NMR shifts for compounds **1**, **2** and **3**. (BPBE-GD3/IGLOII//BPBE-GD3/SDD level of theory). [5b,14,15]

Sn atom	Calcd. Shift, [ppm]	Avg. Calcd. Shift, [ppm]	Exp. Shift, [ppm]	Shift difference Calc.-Exp.[ppm]
$[Ph_{10}Sn_7]^{2-}$ **1**				
1	-1043,55	-1082,64	-857,30	-225,34
2	-61,32	-43,80	35,65	-79,45
3	-22,59	-43,80	35,65	-79,45
4	-55,62	-43,80	35,65	-79,45
5	-35,65	-43,80	35,65	-79,45
6	147,83	147,83	200,35	-52,52
7	-1121,72	-1082,64	-857,30	-225,34
$[Ph_{12}Sn_8]^{2-}$ **2**				
1	-808,19	-811,42	*-585,00*	-226,42
2	-193,57	-199,96	-316,80	116,84
3	-204,17	-199,96	-316,80	116,84
4	-200,12	-199,96	-316,80	116,84
5	-213,11	-199,96	-316,80	116,84
6	-200,70	-199,96	-316,80	116,84
7	-188,08	-199,96	-316,80	116,84
8	-814,66	-811,42	-585,00	-226,42
$[Ph_{13}Sn_8]^{2-}$ **3**				
1	-843,84	-843,84	-757,90	-85,94
2	-139,86	-151,79	-183,50	31,71
3	-283,22	-218,68	-238,60	19,92
4	-424,86	-424,86	-470,80	45,94
5	-196,79	-218,68	-238,60	19,92
6	-154,30	-151,79	-183,50	31,71
7	-161,22	-151,79	-183,50	31,71
8	-176,02	-218,68	-238,60	19,92

Table S5.4. Mulliken charges of Sn atoms in **1**, **2** and **3**.

Sn atom	1	2	3
1	-0.356	-0.343	-0.236
2	0.279	0.272	0.268
3	0.280	0.275	0.291
4	0.284	0.288	0.130
5	0.277	0.295	0.276
6	0.328	0.282	0.276
7	-0.358	0.287	0.282
8		-0.340	0.277

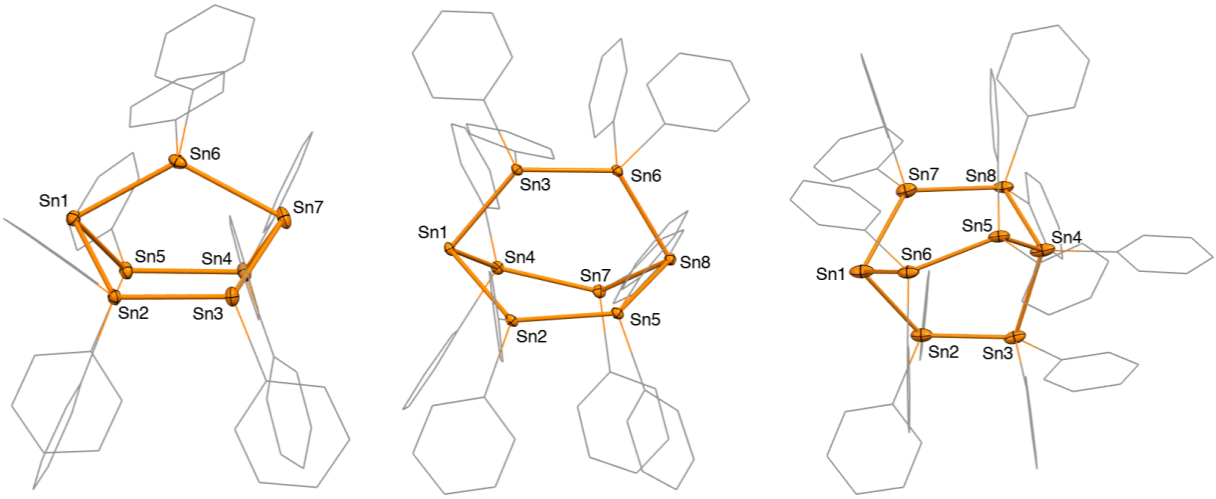


Figure S5.2 Numbering scheme of tin atoms in **1-3** for Tables S5.3 and S5.4.

Cartesian Coordinates and Computed Energies (in Hartrees)

1-BP86

SCF Energy = -2803.73707091
Enthalpy 0K = -2802.683513
Enthalpy 298K = -2802.598027
Free Energy 298K = -2802.831873
Lowest Frequency = 9.5049 cm^{-1}
Second Frequency = 12.3383 cm^{-1}

Sn	-0.05663	2.15544	-0.43177
Sn	-2.49544	1.27266	0.86675
Sn	-2.40146	-1.61751	0.70031
Sn	2.35833	-1.42578	0.89637
Sn	2.33800	1.47019	1.01424
Sn	0.08843	0.20142	-2.54541
Sn	0.05402	-2.06975	-0.74425
C	-2.73258	1.97233	2.93858
C	-3.36785	3.20855	3.18974
H	-3.74543	3.81335	2.35660
C	-3.53760	3.67450	4.50450
H	-4.03373	4.63530	4.68195
C	-3.07703	2.90908	5.58859
H	-3.21414	3.27000	6.61378
C	-2.44952	1.67479	5.35345
H	-2.10137	1.06461	6.19424
C	-2.27813	1.20940	4.03693
H	-1.80262	0.23445	3.87846
C	-4.12190	-2.44788	-0.39465
C	-4.40503	-2.06213	-1.72402
H	-3.78225	-1.31892	-2.23571
C	-5.48908	-2.62455	-2.41931
H	-5.69035	-2.31278	-3.45005
C	-6.30767	-3.58030	-1.79547
H	-7.15270	-4.01887	-2.33736
C	-6.03637	-3.97343	-0.47513
H	-6.66889	-4.72096	0.01691

C	-4.95022	-3.41298	0.22005
H	-4.75041	-3.73521	1.24864
C	-2.52780	-2.49445	2.70934
C	-1.46325	-3.22708	3.27632
H	-0.52751	-3.36903	2.72396
C	-1.57780	-3.78388	4.56227
H	-0.73419	-4.34013	4.98411
C	-2.76136	-3.61916	5.29892
H	-2.85134	-4.05419	6.30030
C	-3.82913	-2.89070	4.74960
H	-4.75426	-2.75386	5.32062
C	-3.71064	-2.32848	3.46691
H	-4.55344	-1.75619	3.06054
C	2.33685	-2.36916	2.88071
C	2.40107	-3.77787	2.98888
H	2.43881	-4.40094	2.08692
C	2.42622	-4.40351	4.24808
H	2.48355	-5.49595	4.31268
C	2.38315	-3.62820	5.41910
H	2.40692	-4.11384	6.40077
C	2.31345	-2.22886	5.32605
H	2.27996	-1.61858	6.23527
C	2.29082	-1.60409	4.06682
H	2.24201	-0.50999	4.01928
C	4.19444	-2.19812	-0.04409
C	4.46425	-1.99147	-1.41572
H	3.75778	-1.44137	-2.04836
C	5.64582	-2.48394	-1.99616
H	5.83419	-2.31148	-3.06129
C	6.57668	-3.18732	-1.21421
H	7.49752	-3.57118	-1.66687
C	6.32227	-3.39615	0.15088
H	7.04439	-3.94351	0.76732
C	5.13980	-2.90496	0.73211
H	4.95555	-3.08065	1.79842
C	2.44878	2.32638	3.03574
C	3.68675	2.80734	3.51698
H	4.58135	2.75473	2.88519
C	3.78615	3.36785	4.80211
H	4.75318	3.73835	5.16060
C	2.64982	3.45634	5.62298
H	2.72778	3.89623	6.62326
C	1.41298	2.98383	5.15483
H	0.51715	3.05425	5.78144
C	1.31391	2.42243	3.87004
H	0.33387	2.06994	3.52712
C	4.08033	2.29376	-0.04286
C	4.01705	3.58912	-0.60571
H	3.09180	4.17513	-0.54717
C	5.13466	4.14827	-1.24947
H	5.06806	5.15424	-1.67886
C	6.33286	3.42058	-1.33915
H	7.20467	3.85669	-1.83915
C	6.40854	2.13224	-0.78672
H	7.33805	1.55665	-0.85761
C	5.28951	1.57151	-0.14563
H	5.36679	0.55821	0.26431
C	2.84210	1.24831	-3.74421
H	2.63819	2.14702	-3.15134
C	4.01283	1.20152	-4.52095
H	4.69824	2.05564	-4.51829
C	4.30470	0.06298	-5.28921
H	5.21475	0.02906	-5.89805
C	3.42789	-1.03424	-5.27082
H	3.65087	-1.92785	-5.86455
C	2.26233	-0.99054	-4.48467
H	1.60215	-1.86654	-4.46876
C	1.94810	0.15553	-3.71693
C	-1.53529	0.34898	-4.02104
C	-1.31296	-0.05115	-5.35692
C	-2.80493	0.85948	-3.67169
H	-0.33213	-0.43392	-5.66258
H	-3.01082	1.20181	-2.65006
C	-2.33603	0.04864	-6.31548
C	-3.82920	0.95989	-4.63033
H	-2.14565	-0.26507	-7.34807
H	-4.80368	1.36493	-4.33709
C	-3.59641	0.55186	-5.95358
H	-4.39218	0.63149	-6.70221
C	-4.18368	2.15976	-0.23276
C	-5.40298	1.45867	-0.37061
C	-4.08788	3.45969	-0.78042
H	-5.50575	0.44319	0.02895
H	-3.15103	4.02478	-0.70771
C	-6.49871	2.04406	-1.02856
C	-5.18489	4.04655	-1.43620
H	-7.43593	1.48496	-1.12623
H	-5.09250	5.05557	-1.85311
C	-6.39184	3.33986	-1.56010
H	-7.24631	3.79641	-2.07152
C	-0.09255	4.27563	-1.03962
C	-0.48311	4.65464	-2.34295
C	0.27286	5.28575	-0.12110
H	-0.77649	3.89368	-3.07562
H	0.57556	5.02338	0.89999
C	-0.50321	6.00919	-2.71953
C	0.25385	6.63981	-0.49904
H	-0.80612	6.28586	-3.73558
H	0.54160	7.41031	0.22493
C	-0.13346	7.00321	-1.79917
H	-0.14711	8.05801	-2.09395
C	0.16588	-4.07812	-1.63867
C	-1.01281	-4.77533	-1.98297
C	1.41611	-4.68672	-1.88594
H	-1.99673	-4.32650	-1.80315
H	2.34786	-4.16837	-1.63000
C	-0.94158	-6.05463	-2.56082
C	1.48424	-5.96644	-2.46415
H	-1.86476	-6.58430	-2.82112
H	2.46131	-6.42701	-2.64864
C	0.30628	-6.65217	-2.80171
H	0.36040	-7.64992	-3.25064

1-BP86(C/H-optimised)

SCF Energy = -2340.54549166
Enthalpy 0K = -2339.677118
Enthalpy 298K = -2339.612855
Free Energy 298K = -2339.798623
Lowest Frequency = 10.4686 cm^{-1}
Second Frequency = 13.3584 cm^{-1}

Sn	0.03757	-1.00874	2.52402
Sn	2.14591	0.53477	1.42396
Sn	2.03372	0.54356	-1.41212
Sn	-2.10130	0.56262	-1.41638
Sn	-2.01502	0.59832	1.40266
Sn	-0.04169	-2.39164	0.01335
Sn	-0.04246	-1.04998	-2.51448
C	2.47636	2.58204	2.26544
C	2.40649	2.78204	3.66511
H	2.16300	1.93667	4.32114
C	2.63413	4.04434	4.24037
H	2.57055	4.16924	5.32889
C	2.93193	5.14721	3.42168
H	3.10557	6.13516	3.86633

C	3.00034	4.97418	2.02951
H	3.22743	5.82774	1.37884
C	2.77746	3.70565	1.46102
H	2.83379	3.59897	0.37143
C	3.94938	-0.33546	-2.19714
C	5.16806	-0.30870	-1.47983
H	5.19563	0.10945	-0.46670
C	6.35529	-0.82858	-2.02885
H	7.28306	-0.79971	-1.44379
C	6.35083	-1.39379	-3.31456
H	7.27462	-1.80303	-3.74282
C	5.15069	-1.43873	-4.04374
H	5.13323	-1.88399	-5.04699
C	3.96903	-0.91636	-3.48754
H	3.03833	-0.96956	-4.06827
C	2.35929	2.62371	-2.19058
C	1.30858	3.56802	-2.24898
H	0.29972	3.29115	-1.92241
C	1.51822	4.87102	-2.73514
H	0.67649	5.57248	-2.77309
C	2.79310	5.26311	-3.17611
H	2.95972	6.27860	-3.55730
C	3.85228	4.34104	-3.12700
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H	-3.11126	5.87174	-1.42824
C	-2.68369	3.74400	-1.48501
H	-2.79144	3.64084	-0.39898
C	-4.05936	-0.27937	-2.11251
C	-4.30153	-1.67261	-2.08580
H	-3.53436	-2.35645	-1.70257
C	-5.51719	-2.21339	-2.54018
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C	-6.52484	-1.36970	-3.03740
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C	-6.30514	0.01749	-3.07399
H	-7.08429	0.68734	-3.46163
C	-5.08712	0.55205	-2.61529
H	-4.93322	1.63751	-2.65725
C	-2.27909	2.69693	2.15413
C	-3.55291	3.17343	2.54449
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H	-4.73248	4.82909	3.31058
C	-2.63444	5.35991	3.10641
H	-2.77105	6.38468	3.47445
C	-1.36043	4.90662	2.72570
H	-0.48988	5.56927	2.79718
C	-1.18967	3.59199	2.25604
H	-0.18105	3.26613	1.97725
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C	-3.98845	-0.71910	3.52998
H	-3.06420	-0.75183	4.12228
C	-5.18183	-1.19594	4.10175
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H	-7.30748	-1.54937	3.79965
C	-6.35956	-0.68062	2.04489
H	-7.28151	-0.67129	1.45008
C	-5.16069	-0.20619	1.48010
H	-5.17322	0.15712	0.44580
C	-2.83109	-3.71257	0.99236
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C	-3.90826	-4.61837	1.00124
H	-4.72195	-4.48526	1.72444
C	-3.94279	-5.68097	0.08384
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C	3.72332	-4.83568	-0.84322
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C	3.57934	-5.98947	-0.05552
H	4.35509	-6.76578	-0.06196
C	4.07461	-0.37508	2.11073
C	5.13338	0.41577	2.61435
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H	5.01839	1.50567	2.66468
H	3.47384	-2.42848	1.68795
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1-BLYP

SCF Energy = -2339.16383976

Sn	0.03215	-1.10189	2.60558
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Sn	-2.21000	0.69928	-1.43145
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Sn	-0.05513	-1.00284	-2.65589
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C	3.45919	2.75132	3.41271
H	3.88465	1.87712	3.91616
C	3.71284	4.02906	3.94674
H	4.31939	4.13034	4.85439
C	3.19113	5.17484	3.31823
H	3.38791	6.17068	3.73009
C	2.41801	5.02772	2.15244
H	2.01394	5.91021	1.64516
C	2.16821	3.74479	1.62516
H	1.57348	3.66513	0.71061
C	4.15254	-0.25285	-2.34047
C	4.47659	-1.61550	-2.12016
H	3.80858	-2.25147	-1.53133
C	5.65017	-2.18974	-2.64396
H	5.86795	-3.24534	-2.44943
C	6.53784	-1.41209	-3.41010
H	7.45209	-1.85598	-3.81956
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H    4.85107   1.56424  -3.31780
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C    2.74215   5.44754  -3.02611
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C    3.73471   4.83848  -2.23688
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H   -2.43286   6.09696  -1.07076
C   -2.35635   3.93809  -1.28378
H   -2.27889   3.78615  -0.20353
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C   -4.48648  -1.43114  -2.20115
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H   -7.65337  -1.42086  -3.53167
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H   -5.02310   1.90954  -2.68743
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C    2.38447  -6.36860  -0.74995
C    3.81818  -4.91906   0.56607
H    2.20916  -7.31740  -1.27123
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C    3.61220  -6.13970  -0.10136
H    4.39710  -6.90416  -0.11445
C    4.17428  -0.45248   2.15789
C    5.39604  -0.34430   1.44771
C    4.19816  -1.17783   3.37558
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C    6.58534  -0.92328   1.93127
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1-B3LYP

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H    3.87804   1.76764   3.87609
C    3.72520   3.90602   3.93189
H    4.33354   3.99124   4.83103
C    3.21285   5.05466   3.32377
H    3.41859   6.03761   3.74294
C    2.43796   4.92801   2.16913
H    2.04022   5.81303   1.67712
C    2.17682   3.66230   1.63296
H    1.57991   3.59872   0.72665
C    4.11144  -0.28865  -2.30021
C    4.39512  -1.65649  -2.12861
H    3.69564  -2.29709  -1.59659
C    5.56663  -2.23152  -2.62795
H    5.75229  -3.29203  -2.47107
C    6.49312  -1.44889  -3.32100
H    7.40670  -1.89334  -3.71144
C    6.23262  -0.09006  -3.50848
H    6.94447   0.53147  -4.05003
C    5.05766   0.47782  -3.00415
H    4.87886   1.53797  -3.16725
C    2.44862   2.68298  -2.15206
C    1.50532   3.31744  -2.97869
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C    1.65401   4.65149  -3.37222
H    0.89316   5.11381  -3.99644
C    2.76367   5.38628  -2.95126
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C	-2.77596	5.16721	3.58726
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C	-1.49218	4.66693	3.36083
H	-0.61587	5.25775	3.61876
C	-1.32342	3.39667	2.80050
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C	-4.07002	-0.33222	2.20033
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H	-3.23087	-1.11343	4.03397
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H	-7.41856	-1.91568	3.50291
C	-6.45569	-0.80672	1.91830
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H	-5.26079	0.25201	0.48989
C	-2.80246	-3.97419	0.89910
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H	-4.61717	-4.84740	1.66778
C	-4.26038	-5.42409	-0.38143
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1-PBE

SCF Energy = -2337.48260943

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H	2.00448	5.81109	1.63509
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C	4.36200	-1.66875	-2.11338
H	3.62820	-2.32332	-1.62864
C	5.56536	-2.23378	-2.56367
H	5.74591	-3.30506	-2.41744
C	6.53079	-1.43061	-3.19050
H	7.47222	-1.86847	-3.54267
C	6.27784	-0.06127	-3.36315
H	7.02268	0.57624	-3.85584
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H	4.89527	1.57043	-3.05386
C	2.39701	2.68332	-2.14007
C	1.45288	3.32370	-2.97035
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C	-3.66051	3.11139	2.67319
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C	-2.72296	5.17561	3.56086
H	-2.86022	6.17751	3.98433
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H	-0.54900	5.25828	3.61436
C	-1.26378	3.37850	2.81380
H	-0.24517	2.99876	2.67621
C	-4.03680	-0.35925	2.17970
C	-4.10106	-1.10241	3.37924
H	-3.19304	-1.23270	3.98224
C	-5.29956	-1.69137	3.81551
H	-5.31911	-2.26424	4.75065
C	-6.46974	-1.54964	3.05317
H	-7.40598	-2.01273	3.38648
C	-6.42841	-0.81786	1.85739
H	-7.33085	-0.71273	1.24397
C	-5.22511	-0.23143	1.42822
H	-5.21560	0.31432	0.47849
C	-2.90148	-3.80565	0.82342
H	-2.71258	-3.26223	1.75643
C	-4.09856	-4.52977	0.69627
H	-4.82143	-4.52999	1.52014
C	-4.37441	-5.23070	-0.48759
H	-5.30793	-5.79614	-0.59128
C	-3.45078	-5.18991	-1.54387
H	-3.66032	-5.72560	-2.47792
C	-2.26537	-4.44536	-1.41309
H	-1.57565	-4.39512	-2.26538
C	-1.95764	-3.74376	-0.22440
C	1.44091	-4.13416	-0.08245
C	1.18431	-5.41691	-0.61392
C	2.72742	-3.90227	0.45269
H	0.19298	-5.64698	-1.02264
H	2.96977	-2.92982	0.89802
C	2.16845	-6.41948	-0.62002
C	3.72046	-4.89662	0.44679
H	1.93809	-7.40755	-1.03828
H	4.70657	-4.67606	0.87185
C	3.44379	-6.16197	-0.09295
H	4.21356	-6.94272	-0.09895
C	4.10417	-0.57125	2.04241
C	5.30381	-0.46019	1.30503
C	4.13391	-1.34940	3.22088
H	5.31870	0.11456	0.37220
H	3.21418	-1.47477	3.80693
C	6.48382	-1.09457	1.72721
C	5.31180	-1.98271	3.65372
H	7.39583	-1.00133	1.12603
H	5.30448	-2.58229	4.57196
C	6.49201	-1.85664	2.90573
H	7.41103	-2.35564	3.23498

1-M06

SCF Energy = -2338.55202081

Sn	0.10332	-1.20499	2.65582
Sn	2.04231	0.56234	1.34180
Sn	2.14432	0.50306	-1.55980
Sn	-1.96505	0.55986	-1.36681
Sn	-2.10361	0.31422	1.52382
Sn	0.09203	-2.49146	-0.01984
Sn	0.03118	-1.15312	-2.68406
C	1.90278	2.70125	1.89250
C	2.43191	3.19802	3.09036
H	2.97068	2.52484	3.76136
C	2.28817	4.53773	3.44767
H	2.70895	4.89886	4.38671
C	1.61315	5.41742	2.60352
H	1.50422	6.46662	2.87794
C	1.07603	4.94421	1.40953
H	0.54333	5.61318	0.73284
C	1.21679	3.60209	1.06710
H	0.78115	3.26523	0.12269
C	4.17960	-0.22708	-2.04121
C	4.50201	-1.56833	-1.79267
H	3.73581	-2.25701	-1.42849
C	5.79477	-2.05140	-1.97618
H	6.00957	-3.09591	-1.75061
C	6.80047	-1.20063	-2.42858
H	7.81536	-1.57312	-2.56722
C	6.49752	0.13006	-2.70480
H	7.27580	0.80279	-3.06699
C	5.20116	0.60677	-2.51343
H	4.98617	1.65578	-2.72671
C	2.31487	2.64355	-2.08634
C	1.32412	3.28040	-2.84249
H	0.50506	2.69642	-3.26765
C	1.33153	4.66046	-3.03950
H	0.52346	5.12551	-3.60388
C	2.35066	5.43524	-2.49397
H	2.35581	6.51539	-2.63799
C	3.35674	4.82314	-1.75060
H	4.15027	5.42342	-1.30601
C	3.32861	3.44640	-1.54385
H	4.10244	2.99287	-0.91937
C	-2.10161	2.71224	-1.89014
C	-2.37472	3.10098	-3.20958
H	-2.52665	2.33549	-3.97482
C	-2.45862	4.44386	-3.57427
H	-2.67522	4.71512	-4.60793
C	-2.26676	5.43854	-2.61746
H	-2.33272	6.48960	-2.89768
C	-1.98777	5.07731	-1.30278
H	-1.84272	5.83969	-0.53697
C	-1.90645	3.73184	-0.94829
H	-1.69179	3.48560	0.09312
C	-3.95666	-0.13520	-2.04601
C	-4.22882	-1.51035	-2.04321
H	-3.43788	-2.22498	-1.79774
C	-5.50265	-1.99962	-2.31934
H	-5.68092	-3.07454	-2.28618
C	-6.53946	-1.11756	-2.61556
H	-7.53950	-1.49561	-2.82777
C	-6.28914	0.25264	-2.63467
H	-7.09511	0.95053	-2.86469
C	-5.01151	0.73412	-2.35038
H	-4.83611	1.81237	-2.35449
C	-2.63478	2.34168	2.23619
C	-3.89040	2.88197	1.92512
H	-4.63615	2.25980	1.42373
C	-4.20393	4.20585	2.21845
H	-5.18392	4.60475	1.95620
C	-3.25755	5.02610	2.82999
H	-3.49396	6.06741	3.04819
C	-2.00764	4.50832	3.15466

H	-1.25095	5.13984	3.61991
C	-1.70485	3.17793	2.86370
H	-0.70908	2.80080	3.10894
C	-3.98981	-0.77236	1.99482
C	-4.04162	-1.58567	3.13562
H	-3.16496	-1.65603	3.78488
C	-5.17733	-2.32579	3.45918
H	-5.18398	-2.94982	4.35316
C	-6.30003	-2.27208	2.63601
H	-7.18762	-2.85639	2.87847
C	-6.27422	-1.47147	1.49830
H	-7.13635	-1.42928	0.83285
C	-5.13437	-0.73079	1.18818
H	-5.14058	-0.12859	0.27882
C	-2.66174	-3.86844	0.72829
H	-2.52062	-3.31755	1.66036
C	-3.87477	-4.52494	0.52777
H	-4.65170	-4.45967	1.29022
C	-4.09241	-5.23231	-0.65102
H	-5.03980	-5.74477	-0.81854
C	-3.09604	-5.26433	-1.62489
H	-3.26096	-5.80778	-2.55576
C	-1.89890	-4.57972	-1.42204
H	-1.15356	-4.57969	-2.22098
C	-1.64832	-3.86981	-0.23857
C	1.92399	-3.76475	-0.01180
C	2.18056	-4.76047	-0.96417
C	2.95628	-3.46021	0.88586
H	1.41185	-5.01877	-1.69627
H	2.80883	-2.68534	1.64287
C	3.40382	-5.42631	-1.01264
C	4.19171	-4.10307	0.83601
H	3.57395	-6.19828	-1.76386
H	4.97734	-3.81017	1.53297
C	4.41682	-5.09582	-0.11364
H	5.38005	-5.60391	-0.16138
C	4.02415	-0.05007	2.15223
C	5.18877	-0.04833	1.37211
C	4.12346	-0.57435	3.44878
H	5.16099	0.33167	0.34946
H	3.23223	-0.61522	4.08024
C	6.39453	-0.54962	1.85946
C	5.32685	-1.06765	3.95041
H	7.27391	-0.55080	1.21552
H	5.37058	-1.46961	4.96288
C	6.46799	-1.05977	3.15278
H	7.40826	-1.45684	3.53511

1-ωB97xD

SCF Energy = -2339.77499646

Sn	0.04334	-1.20306	2.58470
Sn	2.02742	0.51488	1.36099
Sn	2.10335	0.48219	-1.49934
Sn	-1.97702	0.55060	-1.37792
Sn	-2.10222	0.34940	1.47702
Sn	0.05536	-2.52679	-0.02850
Sn	0.01837	-1.15522	-2.61763
C	2.04887	2.63793	1.94313
C	2.68745	3.08605	3.10695
H	3.21987	2.37405	3.73504
C	2.65984	4.42968	3.47907
H	3.16176	4.75081	4.38944
C	1.99444	5.36164	2.68431
H	1.97433	6.41071	2.97039
C	1.35639	4.93816	1.52153
H	0.83465	5.64885	0.88642
C	1.38322	3.59295	1.16343
H	0.87863	3.29581	0.24787
C	4.14667	-0.20209	-1.96235
C	4.52105	-1.51924	-1.66243
H	3.78776	-2.22053	-1.27328
C	5.83195	-1.95816	-1.82921
H	6.08451	-2.98216	-1.56783
C	6.80641	-1.08544	-2.30772
H	7.83338	-1.42231	-2.43047
C	6.45332	0.22319	-2.62873
H	7.20447	0.91264	-3.00913
C	5.13756	0.65484	-2.45930
H	4.88466	1.68281	-2.71026
C	2.19477	2.59041	-2.11820
C	1.23418	3.13193	-2.98060
H	0.46212	2.49110	-3.39928
C	1.22089	4.48997	-3.29552
H	0.44040	4.88222	-3.94102
C	2.18302	5.33907	-2.75632
H	2.16867	6.40100	-2.99045
C	3.15444	4.82273	-1.90176
H	3.89949	5.48010	-1.46005
C	3.15165	3.46629	-1.58504
H	3.89383	3.09128	-0.88286
C	-2.07532	2.69048	-1.89705
C	-2.43474	3.10411	-3.18798
H	-2.68138	2.35840	-3.94202
C	-2.48937	4.45402	-3.53345
H	-2.77440	4.74473	-4.54240
C	-2.17579	5.42878	-2.58842
H	-2.21230	6.48232	-2.85510
C	-1.81097	5.04131	-1.30240
H	-1.56804	5.78733	-0.55036
C	-1.76554	3.69019	-0.96503
H	-1.49289	3.42380	0.05196
C	-3.96895	-0.13320	-2.02815
C	-4.26270	-1.50366	-1.98881
H	-3.48581	-2.22348	-1.73921
C	-5.54930	-1.97762	-2.23190
H	-5.74226	-3.04506	-2.16719
C	-6.57745	-1.08656	-2.53173
H	-7.58526	-1.45259	-2.71468
C	-6.30480	0.27848	-2.59206
H	-7.10070	0.98293	-2.82550
C	-5.01435	0.74553	-2.34113
H	-4.82440	1.81683	-2.37302
C	-2.46036	2.37175	2.26878
C	-3.67435	3.02603	2.01415
H	-4.47125	2.49832	1.49325
C	-3.88135	4.34762	2.40022
H	-4.82878	4.83491	2.18111
C	-2.86829	5.05089	3.05077
H	-3.02106	6.08817	3.33995
C	-1.65933	4.41776	3.32250
H	-0.85221	4.95448	3.81373
C	-1.46435	3.09034	2.93913
H	-0.50597	2.62305	3.15068
C	-4.02008	-0.62898	1.98744
C	-4.10274	-1.43887	3.12932
H	-3.22520	-1.56337	3.76221
C	-5.27602	-2.11187	3.46669
H	-5.30540	-2.73735	4.35614
C	-6.40540	-1.99135	2.65888
H	-7.31937	-2.52447	2.91087
C	-6.34899	-1.18924	1.52285
H	-7.21324	-1.09647	0.87006
C	-5.17204	-0.51547	1.19836
H	-5.15677	0.08617	0.29478

C	-2.74310	-3.73266	0.75283
H	-2.57995	-3.15359	1.65776
C	-3.99169	-4.32289	0.56307
H	-4.77146	-4.17388	1.30550
C	-4.23633	-5.06803	-0.58699
H	-5.20952	-5.52678	-0.74696
C	-3.22994	-5.20608	-1.54236
H	-3.41587	-5.77720	-2.44949
C	-1.99580	-4.58591	-1.35246
H	-1.24444	-4.66440	-2.13617
C	-1.72103	-3.83574	-0.19931
C	1.88330	-3.77679	-0.07122
C	2.22154	-4.59729	-1.15721
C	2.85700	-3.59917	0.92122
H	1.50893	-4.73845	-1.96780
H	2.64812	-2.96005	1.77573
C	3.46734	-5.21658	-1.24416
C	4.11526	-4.19332	0.83548
H	3.70310	-5.84287	-2.10179
H	4.85569	-3.99050	1.60516
C	4.42169	-5.01157	-0.24842
H	5.40274	-5.47469	-0.32688
C	3.99085	-0.21205	2.07381
C	5.17067	0.01951	1.35347
C	4.08403	-1.02397	3.21267
H	5.14632	0.62454	0.45125
H	3.18659	-1.24031	3.79056
C	6.38493	-0.54539	1.73867
C	5.29573	-1.58723	3.61305
H	7.27219	-0.36929	1.13596
H	5.33378	-2.21803	4.49848
C	6.45130	-1.35295	2.87121
H	7.39537	-1.80303	3.16990

1-BP86(D3)

SCF (BP86) Energy = -2340.53078650
Enthalpy 0K = -2339.654778
Enthalpy 298K = -2339.582430
Free Energy 298K = -2339.774788
Lowest Frequency = 10.5196 cm^{-1}
Second Frequency = 14.0570 cm^{-1}

Sn	0.01572	-1.34038	2.62750
Sn	2.07311	0.36925	1.40867
Sn	2.06338	0.48868	-1.48955
Sn	-1.95354	0.71524	-1.32502
Sn	-2.05389	0.41385	1.56656
Sn	-0.13768	-2.55695	-0.09917
Sn	-0.07308	-1.07532	-2.69241
C	2.53141	2.46417	1.98528
C	3.57467	2.78404	2.88416
H	4.15978	1.97608	3.34183
C	3.89168	4.12025	3.18832
H	4.70730	4.34346	3.88877
C	3.16848	5.17054	2.59484
H	3.41671	6.21350	2.82814
C	2.13604	4.87294	1.68958
H	1.57742	5.67634	1.19600
C	1.82872	3.53586	1.38946
H	1.04160	3.33639	0.65401
C	4.08217	-0.33868	-1.90641
C	4.28770	-1.72403	-1.71762
H	3.44052	-2.37647	-1.47581
C	5.56496	-2.29796	-1.80978
H	5.68562	-3.37246	-1.62619
C	6.67586	-1.49291	-2.11452
H	7.67897	-1.93290	-2.17753
C	6.49125	-0.11656	-2.33243
H	7.35225	0.51982	-2.57728
C	5.20820	0.45188	-2.22725
H	5.08788	1.53097	-2.38754
C	2.32930	2.62920	-1.98802
C	1.42938	3.30227	-2.84350
H	0.59759	2.75493	-3.30155
C	1.55021	4.68009	-3.09350
H	0.81247	5.17799	-3.73208
C	2.58493	5.41632	-2.49250
H	2.67371	6.49458	-2.67579
C	3.49135	4.76797	-1.63731
H	4.28419	5.33757	-1.13721
C	3.35631	3.39176	-1.38472
H	4.04052	2.91766	-0.67037
C	-1.85979	2.89408	-1.75379
C	-2.22120	3.40065	-3.02424
H	-2.57099	2.71150	-3.80419
C	-2.14671	4.77552	-3.31402
H	-2.43453	5.14202	-4.30812
C	-1.70104	5.67902	-2.33326
H	-1.63516	6.75049	-2.55884
C	-1.33209	5.19607	-1.06752
H	-0.98482	5.88270	-0.28692
C	-1.41402	3.82258	-0.78646
H	-1.13869	3.48339	0.21620
C	-4.04224	0.28334	-1.93800
C	-4.50461	-1.05296	-1.91182
H	-3.80834	-1.87447	-1.70730
C	-5.86181	-1.35843	-2.10352
H	-6.18544	-2.40404	-2.04674
C	-6.79202	-0.33028	-2.33447
H	-7.85485	-0.56541	-2.47368
C	-6.35012	1.00394	-2.38040
H	-7.06921	1.81449	-2.55906
C	-4.98954	1.30403	-2.18305
H	-4.66456	2.35230	-2.19926
C	-2.21525	2.49012	2.33047
C	-3.39176	3.24342	2.11239
H	-4.28430	2.75093	1.70515
C	-3.43406	4.62118	2.38317
H	-4.35340	5.18889	2.19044
C	-2.29135	5.27975	2.87254
H	-2.31561	6.36038	3.06035
C	-1.11806	4.54563	3.11202
H	-0.21067	5.04373	3.47309
C	-1.08951	3.16314	2.85286
H	-0.15669	2.61449	3.02851
C	-4.08160	-0.36893	2.06527
C	-4.24960	-1.24107	3.16568
H	-3.38264	-1.49532	3.79080
C	-5.49749	-1.81616	3.46541
H	-5.59586	-2.49621	4.32136
C	-6.61491	-1.53018	2.66039
H	-7.58657	-1.99011	2.88046
C	-6.47216	-0.66088	1.56699
H	-7.32425	-0.44380	0.91201
C	-5.22114	-0.08586	1.27939
H	-5.13943	0.56543	0.40369
C	-3.10788	-3.43180	0.66201
H	-2.87640	-2.91652	1.60030
C	-4.42673	-3.87133	0.45394
H	-5.18882	-3.66291	1.21381
C	-4.75946	-4.53744	-0.73737
H	-5.78722	-4.88016	-0.91120
C	-3.77072	-4.74200	-1.71671
H	-4.02603	-5.24901	-2.65626
C	-2.46338	-4.26389	-1.51002

H -1.72284 -4.38274 -2.31202
C -2.09956 -3.60060 -0.31317
C 1.33416 -4.22888 -0.17235
C 1.05750 -5.50445 -0.71401
C 2.64257 -3.99878 0.31132
H 0.04908 -5.72913 -1.08609
H 2.90316 -3.02962 0.75211
C 2.04898 -6.50097 -0.77979
C 3.64298 -4.98340 0.24480
H 1.80829 -7.48439 -1.20570
H 4.64515 -4.75372 0.62801
C 3.34797 -6.24276 -0.30584
H 4.12163 -7.01887 -0.36339
C 4.04149 -0.57856 1.84115
C 5.21776 -0.07815 1.23728
C 4.14815 -1.78037 2.57556
H 5.17382 0.83991 0.63996
H 3.25538 -2.20238 3.05686
C 6.44265 -0.75744 1.33785
C 5.37030 -2.47055 2.68262
H 7.32448 -0.36523 0.81847
H 5.41865 -3.41118 3.24580
C 6.52079 -1.96241 2.05681
H 7.47085 -2.50752 2.11989

1-BLYP(D3)
SCF Energy = -2339.37649636
Sn 0.01419 -1.30245 2.64392
Sn 2.14067 0.37588 1.41938
Sn 2.10982 0.49220 -1.49908
Sn -1.99646 0.73511 -1.33741
Sn -2.08689 0.46583 1.57974
Sn -0.15924 -2.60877 -0.07568
Sn -0.07312 -1.08203 -2.67631
C 2.61417 2.46533 2.03103
C 3.66263 2.76525 2.93529
H 4.25313 1.95035 3.36731
C 3.97781 4.09434 3.27907
H 4.79522 4.29803 3.98079
C 3.24706 5.16143 2.72231
H 3.49134 6.19599 2.98695
C 2.20853 4.88672 1.81378
H 1.64168 5.70295 1.35545
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1-B3LYP(D3)
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1-PBE(D3)
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2-BP86

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Enthalpy 298K = -2806.141142
Free Energy 298K = -2806.379172
Lowest Frequency = 4.8512 cm^{-1}
Second Frequency = 16.0502 cm^{-1}

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H	4.70193	-2.60435	-0.66202
C	5.35450	-3.67571	-2.42065
H	6.05399	-4.30473	-1.85620
C	5.22051	-3.84401	-3.80889
H	5.81703	-4.59992	-4.33473
C	4.31104	-3.04107	-4.51701
H	4.19489	-3.16546	-5.60132
C	3.54454	-2.07798	-3.83452
H	2.83058	-1.46622	-4.40330
C	-3.14569	2.57129	-1.84649
C	-3.55480	2.84555	-3.17406
H	-2.80002	2.95291	-3.96354
C	-4.91267	2.98740	-3.51090
H	-5.19931	3.20162	-4.54847
C	-5.90090	2.85006	-2.52067
H	-6.96163	2.95702	-2.77935
C	-5.51815	2.57382	-1.19814
H	-6.27639	2.45887	-0.41477
C	-4.15705	2.43892	-0.86857
H	-3.89051	2.23353	0.17390
C	-0.26185	4.24589	-2.30947
C	1.05975	4.38610	-2.79132
H	1.76172	3.54648	-2.72002
C	1.50842	5.59082	-3.36117
H	2.54200	5.66791	-3.71984
C	0.63877	6.68917	-3.46586
H	0.98575	7.63007	-3.91109
C	-0.67973	6.57195	-2.99440
H	-1.36857	7.42336	-3.07120
C	-1.12041	5.36448	-2.42265
H	-2.15552	5.29159	-2.06717

2-BP86(C/H-optimised)

SCF (BP86) Energy = -2807.27831874

Enthalpy 0K = -2806.229195

Enthalpy 298K = -2806.141142
Free Energy 298K = -2806.379172
Lowest Frequency = 4.8512 cm^{-1}
Second Frequency = 16.0502 cm^{-1}

Sn	-0.02531	-0.08662	3.08050
Sn	-1.87796	-1.67058	1.41137
Sn	2.34540	-0.78689	1.44364
Sn	-0.53327	2.36323	1.48884
Sn	-1.50761	-1.88444	-1.49570
Sn	2.46571	-0.28301	-1.43673
Sn	-0.96884	2.31833	-1.41488
Sn	0.02879	0.09554	-3.08131
C	-3.96786	-1.02750	1.88990
C	-4.97548	-0.83213	0.91838
H	-4.74879	-0.97331	-0.14432
C	-6.28398	-0.46385	1.28480
H	-7.04302	-0.32012	0.50629
C	-6.61613	-0.28296	2.63704
H	-7.63546	0.00410	2.92352
C	-5.63036	-0.47180	3.62091
H	-5.87718	-0.33378	4.68126
C	-4.32467	-0.83726	3.24680
H	-3.56887	-0.97551	4.03111
C	-2.04214	-3.73187	2.27516
C	-3.30009	-4.36234	2.41965
H	-4.20908	-3.83694	2.10177
C	-3.41494	-5.65040	2.97332
H	-4.40448	-6.11503	3.07479
C	-2.26680	-6.34115	3.39657
H	-2.35318	-7.34614	3.82843
C	-1.00772	-5.73290	3.26139
H	-0.10121	-6.26021	3.58248
C	-0.90087	-4.44438	2.70838
H	0.09576	-3.99729	2.61241
C	2.93379	-2.92779	1.72368
C	2.33738	-3.96755	0.97302
H	1.57799	-3.73997	0.21515
C	2.69952	-5.31306	1.16649
H	2.21621	-6.08978	0.56316
C	3.67359	-5.65034	2.12082
H	3.95919	-6.69865	2.27339
C	4.28067	-4.63293	2.87627
H	5.04457	-4.88469	3.62372
C	3.91399	-3.28985	2.67717
H	4.40435	-2.51029	3.27328
C	4.10437	0.15475	2.46254
C	4.07299	0.35674	3.86217
H	3.17050	0.08680	4.42797
C	5.17068	0.90432	4.55219
H	5.11835	1.04699	5.63921
C	6.32956	1.27142	3.84825
H	7.18633	1.70355	4.38019
C	6.37925	1.08738	2.45643
H	7.27503	1.38092	1.89523
C	5.27961	0.53451	1.77564
H	5.33800	0.41311	0.68765
C	-2.19663	3.52007	2.44649
C	-2.11285	4.91494	2.65798
H	-1.21501	5.45984	2.34087
C	-3.15520	5.62467	3.28073
H	-3.06235	6.70793	3.43352
C	-4.31281	4.95185	3.70694
H	-5.12787	5.50446	4.19089
C	-4.41473	3.56502	3.50953
H	-5.30902	3.02125	3.83730
C	-3.36648	2.86135	2.88980
H	-3.47115	1.77660	2.76103
C	1.13192	3.82531	1.77991
C	2.14067	3.57310	2.73742
H	2.13037	2.63523	3.30634
C	3.17780	4.49296	2.97321
H	3.95489	4.25656	3.70953
C	3.22417	5.69887	2.25442
H	4.03213	6.41891	2.43450
C	2.23564	5.96985	1.29342
H	2.26869	6.90182	0.71569
C	1.20667	5.03908	1.05596
H	0.46376	5.26211	0.28114
C	-3.50085	-2.19380	-2.47495
C	-4.29055	-1.08836	-2.86973
H	-3.94084	-0.06510	-2.68454
C	-5.53191	-1.26588	-3.50747
H	-6.11850	-0.38559	-3.79630
C	-6.01121	-2.55945	-3.77196
H	-6.97828	-2.70109	-4.27067
C	-5.23892	-3.67069	-3.39390
H	-5.60154	-4.68662	-3.59844
C	-4.00078	-3.48653	-2.75280
H	-3.41146	-4.36840	-2.47254
C	-0.63983	-3.92388	-1.78855
C	-1.11571	-5.05657	-1.08600
H	-1.90128	-4.94302	-0.32977
C	-0.58404	-6.33866	-1.31997
H	-0.97098	-7.19760	-0.75796
C	0.44893	-6.51419	-2.25609
H	0.87061	-7.51141	-2.43345
C	0.94680	-5.40109	-2.95347
H	1.76813	-5.51798	-3.67018
C	0.40327	-4.12505	-2.72115
H	0.81431	-3.27045	-3.27285
C	3.90987	1.40383	-1.71899
C	4.96489	1.30060	-2.65581
H	5.08872	0.37586	-3.23292
C	5.86685	2.35975	-2.86247
H	6.67627	2.25139	-3.59645
C	5.73484	3.55266	-2.13184
H	6.43814	4.37973	-2.29035
C	4.69562	3.67592	-1.19476
H	4.57640	4.59542	-0.61064
C	3.79685	2.61268	-0.99341
H	3.00204	2.74211	-0.24879
C	3.66857	-1.88605	-2.43864
C	4.58795	-2.70738	-1.74751
H	4.70193	-2.60435	-0.66202
C	5.35450	-3.67571	-2.42065
H	6.05399	-4.30473	-1.85620
C	5.22051	-3.84401	-3.80889
H	5.81703	-4.59992	-4.33473
C	4.31104	-3.04107	-4.51701
H	4.19489	-3.16546	-5.60132
C	3.54454	-2.07798	-3.83452
H	2.83058	-1.46622	-4.40330
C	-3.14569	2.57129	-1.84649
C	-3.55480	2.84555	-3.17406
H	-2.80002	2.95291	-3.96354
C	-4.91267	2.98740	-3.51090
H	-5.19931	3.20162	-4.54847
C	-5.90090	2.85006	-2.52067
H	-6.96163	2.95702	-2.77935
C	-5.51815	2.57382	-1.19814
H	-6.27639	2.45887	-0.41477
C	-4.15705	2.43892	-0.86857
H	-3.89051	2.23353	0.17390
C	-0.26185	4.24589	-2.30947

C	1.05975	4.38610	-2.79132
H	1.76172	3.54648	-2.72002
C	1.50842	5.59082	-3.36117
H	2.54200	5.66791	-3.71984
C	0.63877	6.68917	-3.46586
H	0.98575	7.63007	-3.91109
C	-0.67973	6.57195	-2.99440
H	-1.36857	7.42336	-3.07120
C	-1.12041	5.36448	-2.42265
H	-2.15552	5.29159	-2.06717

2-BP86(D3)

SCF (BP86) Energy = -2807.25351603
Enthalpy 0K = -2806.200162
Enthalpy 298K = -2806.114563
Free Energy 298K = -2806.333986
Lowest Frequency = 16.4780 cm^{-1}
Second Frequency = 18.2741 cm^{-1}

Sn	-0.06982	-0.01012	3.17468
Sn	1.21348	-2.00385	1.47477
Sn	1.04388	2.04088	1.38753
Sn	-2.41612	-0.12618	1.39829
Sn	1.69201	-1.70706	-1.37237
Sn	0.72093	2.19319	-1.46901
Sn	-2.25084	-0.66470	-1.43819
Sn	0.02883	-0.09434	-3.17365
C	0.08468	-3.91264	1.67948
C	0.45013	-5.10283	1.00615
H	1.32562	-5.12267	0.35078
C	-0.31778	-6.27499	1.12164
H	-0.01164	-7.17081	0.56808
C	-1.48574	-6.28119	1.90300
H	-2.09946	-7.18754	1.97470
C	-1.87487	-5.10865	2.57090
H	-2.80129	-5.08344	3.15652
C	-1.09229	-3.94515	2.46179
H	-1.42967	-3.03867	2.98144
C	3.26070	-2.56400	2.12334
C	3.77562	-3.86881	1.93955
H	3.11235	-4.67822	1.61319
C	5.13827	-4.15026	2.14474
H	5.51613	-5.16791	1.98185
C	6.01847	-3.12713	2.54116
H	7.08495	-3.34118	2.68452
C	5.52113	-1.82969	2.74813
H	6.19003	-1.01284	3.04177
C	4.15768	-1.55567	2.54423
H	3.80663	-0.52731	2.68653
C	3.21826	2.02597	1.85042
C	4.21670	1.58852	0.95215
H	3.95920	1.28835	-0.06877
C	5.56613	1.51789	1.34324
H	6.30829	1.16281	0.62223
C	5.94390	1.87327	2.64773
H	6.99509	1.80846	2.95549
C	4.96486	2.30653	3.55923
H	5.24860	2.58393	4.58256
C	3.62007	2.38373	3.15888
H	2.87106	2.72896	3.88338
C	0.50652	4.04409	2.20556
C	0.29944	4.20478	3.59470
H	0.40958	3.33937	4.26322
C	-0.08379	5.44206	4.14295
H	-0.24184	5.53684	5.22481
C	-0.28019	6.55121	3.30181
H	-0.59314	7.51494	3.72221
C	-0.08561	6.41075	1.91750
H	-0.25270	7.26337	1.24828
C	0.30767	5.17243	1.37976
H	0.43431	5.08763	0.29474
C	-4.18151	-1.34508	1.98948
C	-5.27432	-0.75016	2.66054
H	-5.24753	0.32167	2.89330
C	-6.40737	-1.50187	3.02084
H	-7.24359	-1.01444	3.53902
C	-6.47315	-2.87215	2.71545
H	-7.35718	-3.45949	2.99379
C	-5.39952	-3.47992	2.04240
H	-5.43756	-4.54525	1.78339
C	-4.27147	-2.72223	1.68393
H	-3.45952	-3.22220	1.14829
C	-3.35311	1.88699	1.53581
C	-2.72837	2.90264	2.29135
H	-1.80925	2.68515	2.84513
C	-3.23665	4.21223	2.33950
H	-2.69143	4.98005	2.90016
C	-4.41668	4.52376	1.64504
H	-4.81480	5.54598	1.66468
C	-5.07344	3.52282	0.90687
H	-5.98663	3.75410	0.34509
C	-4.54375	2.22174	0.84908
H	-5.06554	1.46977	0.24958
C	1.81166	-3.85342	-1.92727
C	0.65313	-4.52211	-2.38060
H	-0.25724	-3.95322	-2.60094
C	0.61741	-5.92031	-2.51555
H	-0.31361	-6.40564	-2.83196
C	1.75688	-6.68477	-2.21336
H	1.73135	-7.77775	-2.30427
C	2.93186	-6.03655	-1.79034
H	3.82822	-6.62451	-1.55449
C	2.95601	-4.63727	-1.64836
H	3.87562	-4.15638	-1.29473
C	3.80539	-1.05519	-1.56874
C	4.86818	-1.60487	-0.81482
H	4.68161	-2.40132	-0.08874
C	6.18109	-1.12083	-0.94853
H	6.97709	-1.55991	-0.33511
C	6.45789	-0.05346	-1.82043
H	7.47743	0.34411	-1.90126
C	5.41502	0.51750	-2.56918
H	5.59817	1.37437	-3.22752
C	4.11143	0.00454	-2.45129
H	3.31649	0.46596	-3.04745
C	-0.64867	3.90688	-1.83048
C	-0.28979	4.90757	-2.76339
H	0.67957	4.85078	-3.27455
C	-1.14896	5.98431	-3.04537
H	-0.84611	6.74850	-3.77319
C	-2.39225	6.08143	-2.39721
H	-3.06619	6.91919	-2.61613
C	-2.76316	5.10057	-1.46290
H	-3.72307	5.15499	-0.94032
C	-1.89745	4.02930	-1.18000
H	-2.21806	3.28990	-0.43837
C	2.57902	3.12515	-2.27514
C	3.50947	3.80137	-1.45605
H	3.32930	3.88460	-0.37802
C	4.68914	4.35079	-1.98847
H	5.40478	4.84916	-1.32339
C	4.95531	4.25345	-3.36430
H	5.87692	4.67802	-3.78101
C	4.03432	3.60102	-4.20226
H	4.23221	3.51773	-5.27841

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C   2.86450  3.04132 -3.65732
H   2.16835  2.51173 -4.32232
C  -2.92197 -2.75185 -1.78136
C  -3.89036 -3.03468 -2.77247
H  -4.34599 -2.21109 -3.33649
C  -4.28989 -4.35391 -3.05090
H  -5.04538 -4.54388 -3.82441
C  -3.72141 -5.42710 -2.34344
H  -4.03080 -6.45742 -2.55892
C  -2.75238 -5.16957 -1.36008
H  -2.28639 -5.98565 -0.79885
C  -2.36019 -3.84674 -1.08673
H  -1.59298 -3.68649 -0.32078
C  -4.06020  0.44017 -2.08518
C  -3.94284  1.75993 -2.57283
H  -2.95201  2.18309 -2.77640
C  -5.07177  2.57520 -2.76127
H  -4.93731  3.61021 -3.09728
C  -6.35492  2.07227 -2.48842
H  -7.23910  2.70664 -2.62755
C  -6.49765  0.75199 -2.02408
H  -7.49510  0.35377 -1.79865
C  -5.36055 -0.04939 -1.81585
H  -5.48763 -1.05987 -1.40779
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2-BLYP

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SCF Energy = -2805.63392291
Sn -0.00066 -0.07605  3.06750
Sn -1.49114 -2.08821  1.43444
Sn  2.52770 -0.25275  1.45689
Sn -1.07092  2.25199  1.49772
Sn -1.06810 -2.25336 -1.49774
Sn  2.52738  0.25554 -1.45680
Sn -1.49342  2.08654 -1.43457
Sn -0.00065  0.07601 -3.06754
C  -3.68001 -1.89308  1.89997
C  -4.68870 -1.75215  0.91622
H  -4.42458 -1.74298 -0.14409
C  -6.04852 -1.63237  1.26704
H  -6.80135 -1.52220  0.47966
C  -6.43628 -1.65336  2.61820
H  -7.49264 -1.56077  2.89267
C  -5.45321 -1.79394  3.61542
H  -5.74164 -1.81259  4.67245
C  -4.09629 -1.90915  3.25624
H  -3.35156 -2.01540  4.05252
C  -1.19083 -4.12235  2.34520
C  -2.26111 -5.04478  2.45800
H  -3.25687 -4.76674  2.09835
C  -2.07918 -6.31752  3.03371
H  -2.92683 -7.00864  3.10816
C  -0.81327 -6.70205  3.51259
H  -0.66841 -7.69155  3.95995
C   0.26406 -5.80356  3.41023
H   1.25691 -6.08924  3.77352
C   0.07323 -4.53228  2.83505
H   0.93210 -3.85821  2.76739
C   3.56702 -2.22079  1.76927
C   3.20971 -3.37782  1.03310
H   2.42559 -3.32906  0.27184
C   3.84820 -4.61518  1.24678
H   3.54494 -5.48456  0.65569
C   4.86761 -4.72621  2.20954
H   5.36702 -5.68654  2.37804
C   5.24062 -3.59130  2.95251
H   6.03470 -3.66489  3.70484
C   4.59794 -2.35750  2.73241
H   4.91016 -1.48870  3.32033
C   4.03496  1.06892  2.47923
C   3.93678  1.29877  3.87434
H   3.10976  0.85462  4.44007
C   4.87695  2.09209  4.56233
H   4.77395  2.24839  5.64214
C   5.94344  2.68457  3.86265
H   6.67421  3.30620  4.39137
C   6.05906  2.47606  2.47647
H   6.88065  2.93917  1.91920
C   5.11702  1.67814  1.79827
H   5.22712  1.54305  0.71845
C  -2.95321  2.99300  2.48408
C  -3.19097  4.36890  2.72171
H  -2.44760  5.11070  2.41343
C  -4.36569  4.81299  3.35936
H  -4.52055  5.88472  3.53037
C  -5.33922  3.88674  3.77627
H  -6.25428  4.23077  4.27077
C  -5.12390  2.51494  3.55337
H  -5.86834  1.77792  3.87210
C  -3.94453  2.07838  2.91858
H  -3.80421  1.00369  2.76869
C   0.22530  4.06095  1.79713
C   1.26426  4.04469  2.75978
H   1.46224  3.13394  3.33288
C   2.07032  5.17479  2.99783
H   2.87533  5.11962  3.73773
C   1.84988  6.36148  2.27598
H   2.47514  7.24255  2.45682
C   0.82588  6.40363  1.31232
H   0.65055  7.31812  0.73538
C   0.02964  5.26511  1.07433
H  -0.74345  5.32214  0.30306
C  -2.94943 -2.99700 -2.48395
C  -3.94167 -2.08371 -2.91913
H  -3.80246 -1.00878 -2.76995
C  -5.12053 -2.52191 -3.55373
H  -5.86572 -1.78588 -3.87299
C  -5.33440 -3.89408 -3.77574
H  -6.24907 -4.23939 -4.27008
C  -4.35995 -4.81903 -3.35814
H  -4.51368 -5.89103 -3.52845
C  -3.18574 -4.37330 -2.72068
H  -2.44163 -5.11413 -2.41185
C   0.23033 -4.06079 -1.79676
C   0.03620 -5.26494 -1.07352
H  -0.73672 -5.32262 -0.30211
C   0.83374 -6.40261 -1.31126
H   0.65956 -7.31711 -0.73399
C   1.85754 -6.35957 -2.27509
H   2.48380 -7.23996 -2.45573
C   2.07648 -5.17286 -2.99736
H   2.88132 -5.11700 -3.73739
C   1.26914 -4.04362 -2.75956
H   1.46601 -3.13282 -3.33296
C   3.56435  2.22481 -1.76920
C   4.59419  2.36307 -2.73328
H   4.90676  1.49488 -3.32191
C   5.23537  3.59764 -2.95341
H   6.02864  3.67244 -3.70647
C   4.86189  4.73181 -2.20953
H   5.36013  5.69274 -2.37805
C   3.84354  4.61925 -1.24583
H   3.53994  5.48804 -0.65404
C   3.20655  3.38112 -1.03213
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C	4.03609	-1.06429	-2.47935
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H	6.88401	-2.93124	-1.91965
C	5.94638	-2.67756	-3.86302
H	6.67786	-3.29828	-4.39184
C	4.87915	-2.08629	-4.56259
H	4.77627	-2.24262	-5.64240
C	3.93809	-1.29414	-3.87446
H	3.11050	-0.85093	-4.44010
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H	-6.80404	1.52148	-0.48116
C	-4.69117	1.75058	-0.91717
H	-4.42757	1.74385	0.14328
C	-1.19501	4.12115	-2.34490
C	0.06882	4.53268	-2.83398
H	0.92849	3.85967	-2.76593
C	0.25841	5.80426	-3.40894
H	1.25110	6.09119	-3.77163
C	-0.81997	6.70143	-3.51181
H	-0.67608	7.69115	-3.95900
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H	-2.93414	7.00537	-3.10854
C	-2.26637	5.04227	-2.45821
H	-3.26199	4.76297	-2.09913

2-B3LYP

SCF Enrgy = -2807.12244909

Sn	-0.00241	-0.08187	3.04011
Sn	-1.47202	-2.05842	1.41349
Sn	2.48836	-0.25055	1.43990
Sn	-1.05989	2.21335	1.48532
Sn	-1.05811	-2.21421	-1.48524
Sn	2.48803	0.25247	-1.44001
Sn	-1.47380	2.05728	-1.41344
Sn	-0.00269	0.08189	-3.04010
C	-3.63926	-1.85342	1.87767
C	-4.63984	-1.68659	0.90471
H	-4.37882	-1.66740	-0.14913
C	-5.98754	-1.55177	1.25634
H	-6.73384	-1.42059	0.47607
C	-6.37085	-1.58419	2.59795
H	-7.41833	-1.47960	2.87337
C	-5.39572	-1.75222	3.58465
H	-5.68071	-1.77986	4.63480
C	-4.05121	-1.88201	3.22433
H	-3.31104	-2.00804	4.01237
C	-1.17498	-4.08430	2.29164
C	-2.23677	-5.00222	2.39024
H	-3.22793	-4.71816	2.04355
C	-2.05298	-6.27785	2.93325
H	-2.89455	-6.96583	2.99682
C	-0.79329	-6.66972	3.39256
H	-0.64653	-7.66244	3.81372
C	0.27532	-5.77502	3.30567
H	1.26414	-6.06539	3.65407
C	0.08190	-4.50064	2.76416
H	0.93454	-3.82870	2.70866
C	3.51132	-2.20554	1.74482
C	3.16717	-3.34786	0.99951
H	2.39995	-3.29328	0.23112
C	3.79527	-4.57919	1.21228
H	3.50057	-5.43722	0.61360
C	4.79190	-4.69815	2.18307
H	5.28372	-5.65424	2.35113
C	5.15288	-3.57747	2.93452
H	5.92991	-3.65718	3.69328
C	4.51991	-2.35018	2.71526
H	4.82250	-1.49133	3.31008
C	3.98631	1.06241	2.44255
C	3.89718	1.29220	3.82788
H	3.08029	0.84887	4.39544
C	4.83094	2.08539	4.50375
H	4.73428	2.24177	5.57668
C	5.88206	2.67813	3.80122
H	6.60818	3.30036	4.32061
C	5.98911	2.46909	2.42469
H	6.79857	2.93260	1.86440
C	5.05375	1.67089	1.75894
H	5.15679	1.53606	0.68539
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H	-2.42586	5.05292	2.37212
C	-4.33768	4.76308	3.29964
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C	-5.30695	3.84606	3.71257
H	-6.21968	4.19085	4.19466
C	-5.09109	2.48277	3.50242
H	-5.83215	1.75179	3.81815
C	-3.91549	2.04571	2.88382
H	-3.77506	0.97658	2.74372
C	0.24241	3.99522	1.76975
C	1.29678	3.96279	2.69971
H	1.49406	3.05466	3.26372
C	2.12098	5.07135	2.91615
H	2.93905	5.00141	3.62927
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H	2.54170	7.11851	2.36977
C	0.86208	6.31223	1.27551
H	0.68787	7.22297	0.70618
C	0.04911	5.19445	1.05815
H	-0.73605	5.26371	0.31004
C	-2.92659	-2.95316	-2.45211
C	-3.91372	-2.04882	-2.88398
H	-3.77394	-0.97956	-2.74425
C	-5.08901	-2.48682	-3.50248
H	-5.83052	-1.75640	-3.81849
C	-5.30403	-3.85031	-3.71216
H	-6.21653	-4.19583	-4.19417
C	-4.33422	-4.76659	-3.29886
H	-4.48852	-5.83239	-3.45998
C	-3.16387	-4.32063	-2.67712
H	-2.42225	-5.05494	-2.37116
C	0.24562	-3.99502	-1.76971
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H	-0.73184	-5.26428	-0.31000
C	0.86708	-6.31156	-1.27551
H	0.69357	-7.22245	-0.70619
C	1.90707	-6.25197	-2.20605
H	2.54730	-7.11653	-2.36981
C	2.12500	-5.06968	-2.91615
H	2.94301	-4.99910	-3.62927
C	1.29995	-3.96176	-2.69968
H	1.49656	-3.05346	-3.26365
C	3.50968	2.20818	-1.74480
C	4.51787	2.35366	-2.71553

H	4.82080	1.49512	-3.31064
C	5.15004	3.58138	-2.93469
H	5.92678	3.66174	-3.69367
C	4.78860	4.70167	-2.18287
H	5.27980	5.65810	-2.35086
C	3.79234	4.58188	-1.21181
H	3.49731	5.43959	-0.61284
C	3.16505	3.35012	-0.99913
H	2.39810	3.29491	-0.23053
C	3.98686	-1.05938	-2.44278
C	5.05455	-1.66744	-1.75919
H	5.15737	-1.53284	-0.68559
C	5.99046	-2.46493	-2.42503
H	6.80010	-2.92813	-1.86475
C	5.88370	-2.67367	-3.80163
H	6.61024	-3.29535	-4.32108
C	4.83234	-2.08134	-4.50414
H	4.73591	-2.23750	-5.57712
C	3.89803	-1.28886	-3.82818
H	3.08097	-0.84584	-4.39573
C	-3.64087	1.85077	-1.87778
C	-4.05266	1.87847	-3.22451
H	-3.31244	2.00444	-4.01251
C	-5.39706	1.74783	-3.58494
H	-5.68192	1.77480	-4.63514
C	-6.37224	1.57982	-2.59830
H	-7.41962	1.47456	-2.87380
C	-5.98909	1.54827	-1.25662
H	-6.73543	1.41711	-0.47638
C	-4.64150	1.68392	-0.90487
H	-4.38061	1.66536	0.14902
C	-1.17811	4.08338	-2.29155
C	0.07858	4.50069	-2.76371
H	0.93174	3.82943	-2.70795
C	0.27114	5.77520	-3.30524
H	1.25984	6.06633	-3.65334
C	-0.79814	6.66904	-3.39249
H	-0.65206	7.66186	-3.81365
C	-2.05767	6.27620	-2.93354
H	-2.89976	6.96350	-2.99740
C	-2.24060	5.00044	-2.39052
H	-3.23164	4.71561	-2.04412

2-PBE

SCF Energy = -2803.60431828

Sn	0.03757	0.04871	3.09825
Sn	2.00906	1.44624	1.41606
Sn	-2.22837	0.97684	1.44133
Sn	0.29690	-2.40715	1.47674
Sn	1.67344	1.72266	-1.48291
Sn	-2.39184	0.52446	-1.43934
Sn	0.74940	-2.36191	-1.41463
Sn	-0.02128	-0.07779	-3.09803
C	4.03909	0.63029	1.88782
C	5.05620	0.45769	0.92458
H	4.86645	0.70539	-0.12518
C	6.32541	-0.03043	1.28323
H	7.09307	-0.15625	0.51093
C	6.60652	-0.35609	2.61823
H	7.59459	-0.73913	2.89824
C	5.61060	-0.18844	3.59332
H	5.81810	-0.43922	4.64040
C	4.34427	0.29784	3.22729
H	3.57630	0.41392	4.00272
C	2.33586	3.49921	2.24299
C	3.63275	4.04928	2.34185
H	4.49951	3.45328	2.03219
C	3.83794	5.34921	2.83405
H	4.85555	5.75331	2.90092
C	2.74397	6.13103	3.23746
H	2.90152	7.14725	3.61742
C	1.44803	5.60008	3.15057
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C	1.25103	4.29817	2.66227
H	0.22809	3.91032	2.60291
C	-2.61163	3.15845	1.75840
C	-1.98762	4.14972	0.96947
H	-1.31312	3.86702	0.15356
C	-2.21309	5.51745	1.20021
H	-1.71015	6.25609	0.56694
C	-3.07428	5.92454	2.23035
H	-3.25273	6.99065	2.41290
C	-3.70824	4.95505	3.02304
H	-4.38595	5.26225	3.82909
C	-3.47850	3.58968	2.78690
H	-3.98886	2.84828	3.41323
C	-4.07530	0.18608	2.43165
C	-4.07317	-0.04403	3.82522
H	-3.15739	0.14095	4.40270
C	-5.21510	-0.51938	4.49322
H	-5.18504	-0.68763	5.57646
C	-6.38927	-0.78421	3.77188
H	-7.28055	-1.16179	4.28637
C	-6.41099	-0.56730	2.38571
H	-7.31943	-0.78097	1.81071
C	-5.26763	-0.08507	1.72720
H	-5.30633	0.06429	0.64243
C	1.83280	-3.75297	2.39183
C	1.60868	-5.13437	2.57279
H	0.65582	-5.57684	2.25906
C	2.58174	-5.95965	3.16070
H	2.38151	-7.03025	3.29106
C	3.80736	-5.41946	3.58007
H	4.56838	-6.06363	4.03574
C	4.04760	-4.04750	3.41239
H	4.99744	-3.60520	3.73483
C	3.06811	-3.22792	2.82858
H	3.27911	-2.15727	2.72302
C	-1.52339	-3.67843	1.71718
C	-2.54052	-3.29183	2.61601
H	-2.44107	-2.35955	3.18375
C	-3.69979	-4.06560	2.79063
H	-4.48094	-3.72143	3.47760
C	-3.85996	-5.25931	2.07065
H	-4.76394	-5.86560	2.20115
C	-2.86097	-5.66456	1.17169
H	-2.98157	-6.58655	0.59111
C	-1.70999	-4.87757	0.99305
H	-0.96124	-5.20012	0.26131
C	3.69688	1.87093	-2.43281
C	4.39058	0.70461	-2.82552
H	3.94530	-0.28303	-2.66034
C	5.65604	0.77652	-3.43156
H	6.16760	-0.14969	-3.71708
C	6.25450	2.02353	-3.66710
H	7.24134	2.08356	-4.14082
C	5.57672	3.19419	-3.29313
H	6.03336	4.17459	-3.47648
C	4.31423	3.11564	-2.68214
H	3.79997	4.04293	-2.40320
C	0.97252	3.82928	-1.73390
C	1.54946	4.91183	-1.03223
H	2.35839	4.73437	-0.31523
C	1.08677	6.22674	-1.21300

H	1.54830	7.04498	-0.64816
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H	-0.34615	7.50948	-2.22445
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H	-1.41636	5.60479	-3.46360
C	-0.09307	4.11474	-2.61433
H	-0.57746	3.30064	-3.16589
C	-3.98762	-1.01068	-1.75962
C	-4.96484	-0.82850	-2.76321
H	-4.96133	0.08872	-3.36407
C	-5.95021	-1.79931	-3.00700
H	-6.69684	-1.63243	-3.79322
C	-5.98145	-2.97920	-2.24744
H	-6.74989	-3.73789	-2.43625
C	-5.02297	-3.17766	-1.24221
H	-5.03054	-4.08840	-0.63391
C	-4.04008	-2.20218	-1.00342
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H	-4.37552	3.04374	-0.61522
C	-4.89370	4.22613	-2.34473
H	-5.51440	4.91846	-1.76424
C	-4.73860	4.41135	-3.72695
H	-5.24089	5.24400	-4.23294
C	-3.93043	3.52507	-4.45529
H	-3.79976	3.66080	-5.53563
C	-3.28197	2.46504	-3.79802
H	-2.63996	1.79086	-4.38075
C	2.89880	-2.80184	-1.81846
C	3.29326	-3.18548	-3.12075
H	2.53467	-3.31000	-3.90314
C	4.64183	-3.41280	-3.44086
H	4.91921	-3.70892	-4.45969
C	5.63363	-3.25411	-2.45964
H	6.68763	-3.42570	-2.70695
C	5.26413	-2.87338	-1.16113
H	6.02483	-2.73814	-0.38444
C	3.91227	-2.65376	-0.84782
H	3.65522	-2.36331	0.17585
C	-0.13928	-4.22228	-2.27841
C	-1.47671	-4.24111	-2.72933
H	-2.08477	-3.33075	-2.68019
C	-2.06174	-5.41336	-3.23477
H	-3.10691	-5.39611	-3.56439
C	-1.31385	-6.59846	-3.30835
H	-1.76730	-7.51556	-3.70216
C	0.02051	-6.59986	-2.87259
H	0.61460	-7.52035	-2.92709
C	0.59718	-5.42471	-2.36162
H	1.64085	-5.44580	-2.02619

2-M06

SCF Enrgy = -2804.90842006

Sn	0.01542	-0.18799	3.19764
Sn	-1.38252	-1.95239	1.33895
Sn	2.36345	-0.25129	1.42865
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Sn	2.36337	0.25152	-1.42874
Sn	-1.38274	1.95225	-1.33890
Sn	0.01529	0.18799	-3.19766
C	-3.54435	-1.76426	1.78977
C	-4.52631	-1.47786	0.83518
H	-4.25334	-1.34567	-0.21226
C	-5.87015	-1.35680	1.18653
H	-6.60368	-1.14177	0.40892
C	-6.26429	-1.51734	2.51083
H	-7.31367	-1.42119	2.78880
C	-5.30476	-1.80296	3.48082
H	-5.60156	-1.93171	4.52183
C	-3.96519	-1.92648	3.11828
H	-3.22775	-2.15197	3.89308
C	-1.15875	-4.07848	1.92433
C	-2.22394	-4.98120	1.80031
H	-3.21033	-4.61285	1.50811
C	-2.04926	-6.34468	2.03157
H	-2.89222	-7.02754	1.92285
C	-0.79720	-6.83657	2.39504
H	-0.65595	-7.90332	2.56719
C	0.27028	-5.95436	2.54004
H	1.25598	-6.32414	2.82224
C	0.08404	-4.59273	2.31193
H	0.93943	-3.92249	2.42302
C	3.44261	-2.17934	1.57723
C	3.01173	-3.31384	0.87674
H	2.11179	-3.27583	0.25549
C	3.71874	-4.51354	0.92883
H	3.34960	-5.37109	0.36705
C	4.88832	-4.59983	1.67891
H	5.44966	-5.53316	1.71429
C	5.33768	-3.48399	2.38021
H	6.25391	-3.54172	2.96865
C	4.61822	-2.29125	2.33126
H	4.98991	-1.42448	2.88154
C	3.92565	1.06290	2.30931
C	3.92533	1.30131	3.69049
H	3.16141	0.83237	4.31705
C	4.86702	2.13579	4.29079
H	4.83981	2.30192	5.36771
C	5.83652	2.76139	3.51071
H	6.56865	3.42391	3.97172
C	5.86081	2.53520	2.13747
H	6.61005	3.02263	1.51447
C	4.92154	1.68990	1.54952
H	4.96128	1.53894	0.46929
C	-3.02645	2.69043	2.15623
C	-3.54185	3.93856	1.78204
H	-2.89331	4.66989	1.29376
C	-4.87874	4.26448	1.99711
H	-5.25654	5.23924	1.68842
C	-5.73773	3.33930	2.58656
H	-6.78847	3.58575	2.73636
C	-5.24574	2.09670	2.97466
H	-5.90379	1.35217	3.42328
C	-3.90280	1.78512	2.76727
H	-3.54961	0.79386	3.06126
C	0.30196	3.78027	1.80804
C	1.45784	3.64672	2.58802
H	1.66444	2.70326	3.09782
C	2.38258	4.68038	2.71872
H	3.28829	4.51798	3.30416
C	2.15231	5.89566	2.08025
H	2.87276	6.70850	2.17131
C	1.00735	6.05818	1.30333
H	0.82540	6.99596	0.77815
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C	-3.02621	-2.69068	-2.15623
C	-3.90265	-1.78542	-2.76721
H	-3.54956	-0.79411	-3.06114
C	-5.24555	-2.09712	-2.97463
H	-5.90367	-1.35264	-3.42322
C	-5.73742	-3.33980	-2.58663

H	-6.78814	-3.58635	-2.73645
C	-4.87835	-4.26494	-1.99723
H	-5.25605	-5.23975	-1.68861
C	-3.54149	-3.93889	-1.78213
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C	0.30231	-3.78024	-1.80804
C	0.10070	-5.00910	-1.16348
H	-0.76338	-5.15559	-0.51343
C	1.00796	-6.05806	-1.30334
H	0.82613	-6.99586	-0.77814
C	2.15288	-5.89543	-2.08030
H	2.87341	-6.70820	-2.17138
C	2.38299	-4.68014	-2.71881
H	3.28865	-4.51764	-3.30429
C	1.45814	-3.64658	-2.58808
H	1.66460	-2.70311	-3.09791
C	3.44243	2.17963	-1.57729
C	4.61797	2.29163	-2.33141
H	4.98964	1.42491	-2.88177
C	5.33739	3.48440	-2.38034
H	6.25357	3.54219	-2.96886
C	4.88805	4.60017	-1.67894
H	5.44936	5.53352	-1.71430
C	3.71853	4.51380	-0.92876
H	3.34942	5.37131	-0.36689
C	3.01156	3.31407	-0.87670
H	2.11168	3.27600	-0.25538
C	3.92569	-1.06256	-2.30935
C	4.92156	-1.68952	-1.54950
H	4.96123	-1.53858	-0.46927
C	5.86090	-2.53478	-2.13740
H	6.61011	-3.02219	-1.51436
C	5.83671	-2.76095	-3.51065
H	6.56889	-3.42344	-3.97161
C	4.86723	-2.13538	-4.29078
H	4.84010	-2.30150	-5.36771
C	3.92548	-1.30096	-3.69053
H	3.16158	-0.83203	-4.31714
C	-3.54456	1.76399	-1.78973
C	-3.96539	1.92619	-3.11824
H	-3.22796	2.15174	-3.89304
C	-5.30495	1.80260	-3.48080
H	-5.60175	1.93134	-4.52181
C	-6.26447	1.51690	-2.51083
H	-7.31384	1.42068	-2.78881
C	-5.87033	1.35638	-1.18652
H	-6.60386	1.14131	-0.40892
C	-4.52650	1.47753	-0.83516
H	-4.25353	1.34536	0.21228
C	-1.15913	4.07836	-1.92427
C	0.08361	4.59271	-2.31188
H	0.93905	3.92252	-2.42300
C	0.26976	5.95435	-2.53996
H	1.25543	6.32420	-2.82217
C	-0.79776	6.83649	-2.39492
H	-0.65659	7.90325	-2.56705
C	-2.04978	6.34452	-2.03144
H	-2.89279	7.02732	-1.92268
C	-2.22438	4.98102	-1.80021
H	-3.21074	4.61261	-1.50799

2-ωB97xD

SCF Energy = -2806.37878825

Sn	0.03141	0.13956	3.08070
Sn	1.75513	1.58974	1.29049
Sn	-2.21886	0.76553	1.38117
Sn	0.51895	-2.22445	1.50159
Sn	1.36390	1.72495	-1.54344
Sn	-2.38758	0.23576	-1.41344
Sn	0.86581	-2.22718	-1.33088
Sn	-0.10040	-0.20731	-3.12709
C	3.83864	1.03053	1.76394
C	4.84377	0.79805	0.81783
H	4.62098	0.84954	-0.24236
C	6.14808	0.48802	1.20479
H	6.90186	0.31861	0.43993
C	6.47846	0.39928	2.55324
H	7.49352	0.15286	2.85562
C	5.49535	0.63031	3.51381
H	5.73906	0.56461	4.57174
C	4.19686	0.94427	3.11794
H	3.44281	1.11569	3.88507
C	1.90604	3.71834	1.83241
C	3.10874	4.41151	1.63186
H	3.99765	3.86560	1.32027
C	3.18612	5.79281	1.80271
H	4.12809	6.30901	1.63035
C	2.05445	6.51298	2.18315
H	2.10809	7.59244	2.30467
C	0.85676	5.83948	2.40825
H	-0.03823	6.38326	2.69862
C	0.78910	4.45740	2.23903
H	-0.16296	3.96097	2.40766
C	-2.61633	2.91011	1.68282
C	-2.35633	3.88647	0.71311
H	-2.00407	3.60371	-0.27534
C	-2.53265	5.24281	0.98471
H	-2.31041	5.96971	0.21014
C	-2.96839	5.65310	2.24104
H	-3.09935	6.71103	2.45675
C	-3.23095	4.69899	3.22248
H	-3.56923	5.00896	4.20867
C	-3.05774	3.34581	2.94062
H	-3.26845	2.61584	3.72035
C	-4.00763	-0.13368	2.31610
C	-4.02023	-0.38176	3.69573
H	-3.15171	-0.11501	4.29722
C	-5.10785	-0.99136	4.32017
H	-5.08536	-1.17402	5.39205
C	-6.21391	-1.37891	3.56724
H	-7.05905	-1.86779	4.04601
C	-6.22403	-1.14194	2.19515
H	-7.07444	-1.45091	1.59279
C	-5.13661	-0.52114	1.58297
H	-5.16851	-0.36211	0.50861
C	2.38784	-3.23452	2.07383
C	2.73452	-4.49711	1.57399
H	2.00658	-5.07539	1.00858
C	4.01209	-5.02193	1.75396
H	4.25860	-5.99868	1.34411
C	4.98178	-4.28486	2.43101
H	5.98719	-4.68191	2.54831
C	4.65733	-3.03225	2.94374
H	5.40502	-2.43243	3.45602
C	3.37052	-2.52354	2.77294
H	3.14875	-1.53398	3.16453
C	-1.10689	-3.66757	1.85121
C	-2.19387	-3.27694	2.64424
H	-2.19665	-2.29853	3.11712
C	-3.30213	-4.10079	2.83000
H	-4.14089	-3.74208	3.42086
C	-3.33353	-5.35980	2.23626
H	-4.19733	-6.00695	2.37017
C	-2.26128	-5.77545	1.44889

H	-2.28171	-6.74613	0.95963
C	-1.16686	-4.93460	1.25346
H	-0.36640	-5.27473	0.60265
C	3.43638	2.00043	-2.23158
C	4.13244	0.94078	-2.82751
H	3.61625	0.01444	-3.06909
C	5.50030	1.02504	-3.08689
H	6.01249	0.17179	-3.52309
C	6.20160	2.18259	-2.76123
H	7.27058	2.24758	-2.94989
C	5.52474	3.25610	-2.18488
H	6.06454	4.16344	-1.92375
C	4.15980	3.16141	-1.92350
H	3.65764	4.00278	-1.45037
C	0.40183	3.68324	-1.86642
C	0.79604	4.86649	-1.22588
H	1.64003	4.86785	-0.54355
C	0.10234	6.05990	-1.41629
H	0.42726	6.95345	-0.88922
C	-1.01919	6.09586	-2.24220
H	-1.57525	7.02166	-2.37160
C	-1.43529	4.93267	-2.88425
H	-2.32467	4.92933	-3.50909
C	-0.71920	3.75038	-2.70408
H	-1.06468	2.85818	-3.21960
C	-3.78537	-1.46169	-1.53457
C	-4.88823	-1.42581	-2.39879
H	-5.06107	-0.54499	-3.01407
C	-5.78019	-2.49401	-2.48053
H	-6.62922	-2.43939	-3.15867
C	-5.58543	-3.62848	-1.69574
H	-6.27998	-4.46305	-1.75714
C	-4.49770	-3.68431	-0.82869
H	-4.32612	-4.55503	-0.20372
C	-3.61381	-2.60940	-0.75034
H	-2.78251	-2.68423	-0.05349
C	-3.66405	1.79746	-2.31281
C	-4.51371	2.61334	-1.55526
H	-4.56067	2.49236	-0.47584
C	-5.28841	3.60812	-2.14965
H	-5.92228	4.23845	-1.53126
C	-5.24315	3.79976	-3.52804
H	-5.84412	4.57716	-3.99369
C	-4.41755	2.99033	-4.30512
H	-4.37264	3.13069	-5.38262
C	-3.63745	2.00640	-3.69868
H	-2.98072	1.39866	-4.32006
C	3.02066	-2.42275	-1.72151
C	3.44665	-2.83535	-2.99290
H	2.70835	-3.09111	-3.75114
C	4.80006	-2.92341	-3.31473
H	5.10172	-3.24250	-4.30992
C	5.76432	-2.60211	-2.36099
H	6.82153	-2.66905	-2.60714
C	5.36326	-2.19100	-1.09365
H	6.09703	-1.93325	-0.33551
C	4.00794	-2.10114	-0.78356
H	3.73271	-1.77665	0.21482
C	0.21302	-4.25375	-1.88691
C	-1.12520	-4.50955	-2.20808
H	-1.82530	-3.68506	-2.31533
C	-1.60134	-5.80972	-2.36334
H	-2.65365	-5.97112	-2.58337
C	-0.73609	-6.89098	-2.21555
H	-1.10446	-7.90809	-2.32684
C	0.60776	-6.65912	-1.92602
H	1.29318	-7.49674	-1.81633
C	1.07295	-5.35442	-1.76446
H	2.12236	-5.19085	-1.52552

2-BP86(D3)

SCF Energy = -2807.55313321

Sn	-0.06982	-0.01012	3.17468
Sn	1.21348	-2.00385	1.47477
Sn	1.04388	2.04088	1.38753
Sn	-2.41612	-0.12618	1.39829
Sn	1.69201	-1.70706	-1.37237
Sn	0.72093	2.19319	-1.46901
Sn	-2.25084	-0.66470	-1.43819
Sn	0.02883	-0.09434	-3.17365
C	0.08468	-3.91264	1.67948
C	0.45013	-5.10283	1.00615
H	1.32562	-5.12267	0.35078
C	-0.31778	-6.27499	1.12164
H	-0.01164	-7.17081	0.56808
C	-1.48574	-6.28119	1.90300
H	-2.09946	-7.18754	1.97470
C	-1.87487	-5.10865	2.57090
H	-2.80129	-5.08344	3.15652
C	-1.09229	-3.94515	2.46179
H	-1.42967	-3.03867	2.98144
C	3.26070	-2.56400	2.12334
C	3.77562	-3.86881	1.93955
H	3.11235	-4.67822	1.61319
C	5.13827	-4.15026	2.14474
H	5.51613	-5.16791	1.98185
C	6.01847	-3.12713	2.54116
H	7.08495	-3.34118	2.68452
C	5.52113	-1.82969	2.74813
H	6.19003	-1.01284	3.04177
C	4.15768	-1.55567	2.54423
H	3.80663	-0.52731	2.68653
C	3.21826	2.02597	1.85042
C	4.21670	1.58852	0.95215
H	3.95920	1.28835	-0.06877
C	5.56613	1.51789	1.34324
H	6.30829	1.16281	0.62223
C	5.94390	1.87327	2.64773
H	6.99509	1.80846	2.95549
C	4.96486	2.30653	3.55923
H	5.24860	2.58393	4.58256
C	3.62007	2.38373	3.15888
H	2.87106	2.72896	3.88338
C	0.50652	4.04409	2.20556
C	0.29944	4.20478	3.59470
H	0.40958	3.33937	4.26322
C	-0.08379	5.44206	4.14295
H	-0.24184	5.53684	5.22481
C	-0.28019	6.55121	3.30181
H	-0.59314	7.51494	3.72221
C	-0.08561	6.41075	1.91750
H	-0.25270	7.26337	1.24828
C	0.30767	5.17243	1.37976
H	0.43431	5.08763	0.29474
C	-4.18151	-1.34508	1.98948
C	-5.27432	-0.75016	2.66054
H	-5.24753	0.32167	2.89330
C	-6.40737	-1.50187	3.02084
H	-7.24359	-1.01444	3.53902
C	-6.47315	-2.87215	2.71545
H	-7.35718	-3.45949	2.99379
C	-5.39952	-3.47992	2.04240
H	-5.43756	-4.54525	1.78339
C	-4.27147	-2.72223	1.68393

H	-3.45952	-3.22220	1.14829
C	-3.35311	1.88699	1.53581
C	-2.72837	2.90264	2.29135
H	-1.80925	2.68515	2.84513
C	-3.23665	4.21223	2.33950
H	-2.69143	4.98005	2.90016
C	-4.41668	4.52376	1.64504
H	-4.81480	5.54598	1.66468
C	-5.07344	3.52282	0.90687
H	-5.98663	3.75410	0.34509
C	-4.54375	2.22174	0.84908
H	-5.06554	1.46977	0.24958
C	1.81166	-3.85342	-1.92727
C	0.65313	-4.52211	-2.38060
H	-0.25724	-3.95322	-2.60094
C	0.61741	-5.92031	-2.51555
H	-0.31361	-6.40564	-2.83196
C	1.75688	-6.68477	-2.21336
H	1.73135	-7.77775	-2.30427
C	2.93186	-6.03655	-1.79034
H	3.82822	-6.62451	-1.55449
C	2.95601	-4.63727	-1.64836
H	3.87562	-4.15638	-1.29473
C	3.80539	-1.05519	-1.56874
C	4.86818	-1.60487	-0.81482
H	4.68161	-2.40132	-0.08874
C	6.18109	-1.12083	-0.94853
H	6.97709	-1.55991	-0.33511
C	6.45789	-0.05346	-1.82043
H	7.47743	0.34411	-1.90126
C	5.41502	0.51750	-2.56918
H	5.59817	1.37437	-3.22752
C	4.11143	0.00454	-2.45129
H	3.31649	0.46596	-3.04745
C	-0.64867	3.90688	-1.83048
C	-0.28979	4.90757	-2.76339
H	0.67957	4.85078	-3.27455
C	-1.14896	5.98431	-3.04537
H	-0.84611	6.74850	-3.77319
C	-2.39225	6.08143	-2.39721
H	-3.06619	6.91919	-2.61613
C	-2.76316	5.10057	-1.46290
H	-3.72307	5.15499	-0.94032
C	-1.89745	4.02930	-1.18000
H	-2.21806	3.28990	-0.43837
C	2.57902	3.12515	-2.27514
C	3.50947	3.80137	-1.45605
H	3.32930	3.88460	-0.37802
C	4.68914	4.35079	-1.98847
H	5.40478	4.84916	-1.32339
C	4.95531	4.25345	-3.36430
H	5.87692	4.67802	-3.78101
C	4.03432	3.60102	-4.20226
H	4.23221	3.51773	-5.27841
C	2.86450	3.04132	-3.65732
H	2.16835	2.51173	-4.32232
C	-2.92197	-2.75185	-1.78136
C	-3.89036	-3.03468	-2.77247
H	-4.34599	-2.21109	-3.33649
C	-4.28989	-4.35391	-3.05090
H	-5.04538	-4.54388	-3.82441
C	-3.72141	-5.42710	-2.34344
H	-4.03080	-6.45742	-2.55892
C	-2.75238	-5.16957	-1.36008
H	-2.28639	-5.98565	-0.79885
C	-2.36019	-3.84674	-1.08673
H	-1.59298	-3.68649	-0.32078
C	-4.06020	0.44017	-2.08518
C	-3.94284	1.75993	-2.57283
H	-2.95201	2.18309	-2.77640
C	-5.07177	2.57520	-2.76127
H	-4.93731	3.61021	-3.09728
C	-6.35492	2.07227	-2.48842
H	-7.23910	2.70664	-2.62755
C	-6.49765	0.75199	-2.02408
H	-7.49510	0.35377	-1.79865
C	-5.36055	-0.04939	-1.81585
H	-5.48763	-1.05987	-1.40779

2-BLYP(D3)

SCF Energy = -2807.55313321

Sn	0.08286	-0.00829	3.13580
Sn	-1.15445	2.09879	1.48959
Sn	-1.13861	-2.09766	1.40622
Sn	2.48689	0.02852	1.38075
Sn	-1.67245	1.83642	-1.37238
Sn	-0.84536	-2.20806	-1.47765
Sn	2.33855	0.60423	-1.46763
Sn	-0.04143	0.11193	-3.14307
C	-0.00066	3.99541	1.71631
C	-0.35931	5.19285	1.04671
H	-1.23362	5.22007	0.39482
C	0.41333	6.36362	1.16963
H	0.11410	7.26269	0.62129
C	1.57886	6.36292	1.95806
H	2.19294	7.26627	2.03817
C	1.96097	5.18474	2.62442
H	2.88071	5.15591	3.21707
C	1.17445	4.02239	2.50624
H	1.50639	3.11719	3.02465
C	-3.17163	2.67115	2.23447
C	-3.67721	3.99231	2.15622
H	-3.01788	4.81349	1.85942
C	-5.02855	4.27537	2.43567
H	-5.39760	5.30450	2.35720
C	-5.90940	3.23820	2.79958
H	-6.96434	3.45542	2.99925
C	-5.42221	1.92247	2.90253
H	-6.09114	1.09801	3.16824
C	-4.06902	1.65034	2.63025
H	-3.72652	0.61486	2.69711
C	-3.32447	-2.16561	1.84846
C	-4.27390	-1.43744	1.09073
H	-3.96247	-0.85095	0.22388
C	-5.64157	-1.44332	1.42711
H	-6.33954	-0.86360	0.81946
C	-6.09206	-2.18078	2.53654
H	-7.15490	-2.18489	2.80209
C	-5.16698	-2.91673	3.30085
H	-5.50833	-3.49864	4.16485
C	-3.80190	-2.90854	2.95666
H	-3.10225	-3.49616	3.56038
C	-0.55207	-4.09129	2.23128
C	-0.33796	-4.24067	3.62383
H	-0.46988	-3.37908	4.28840
C	0.06992	-5.46842	4.18141
H	0.23083	-5.55177	5.26206
C	0.28329	-6.58235	3.34833
H	0.61241	-7.53601	3.77489
C	0.07935	-6.45614	1.96214
H	0.25541	-7.31084	1.30057
C	-0.33756	-5.22749	1.41528
H	-0.47282	-5.15874	0.33364
C	4.23028	1.22766	2.09079

C	5.28675	0.61587	2.80915
H	5.25816	-0.46150	3.00089
C	6.38781	1.36213	3.27300
H	7.19184	0.86162	3.82504
C	6.45922	2.74607	3.02818
H	7.31468	3.32803	3.38831
C	5.42386	3.37236	2.30985
H	5.46698	4.44651	2.09958
C	4.32848	2.61943	1.84725
H	3.55095	3.13507	1.28283
C	3.40813	-2.00081	1.49567
C	2.79404	-3.02723	2.25109
H	1.88294	-2.82161	2.81564
C	3.31100	-4.33645	2.28536
H	2.78289	-5.10814	2.85232
C	4.48277	-4.64172	1.57058
H	4.88502	-5.66064	1.58056
C	5.12616	-3.63318	0.82789
H	6.03062	-3.85874	0.25342
C	4.59274	-2.33089	0.79084
H	5.10684	-1.57591	0.19382
C	-1.70715	3.98048	-1.97296
C	-0.51070	4.59987	-2.40596
H	0.38480	3.99819	-2.57958
C	-0.42286	5.99293	-2.58259
H	0.53176	6.43691	-2.88251
C	-1.54710	6.80447	-2.34466
H	-1.48272	7.89075	-2.47005
C	-2.75805	6.20719	-1.94319
H	-3.64119	6.83010	-1.76046
C	-2.83399	4.81267	-1.75943
H	-3.78114	4.37529	-1.42986
C	-3.82005	1.26462	-1.53215
C	-4.83986	1.86685	-0.75318
H	-4.59943	2.66203	-0.04621
C	-6.17767	1.43656	-0.84037
H	-6.93515	1.91300	-0.20954
C	-6.52649	0.37642	-1.69793
H	-7.56259	0.02392	-1.74617
C	-5.53113	-0.24198	-2.47605
H	-5.77401	-1.08690	-3.12650
C	-4.20028	0.21044	-2.39735
H	-3.44961	-0.29276	-3.01069
C	0.48838	-3.94864	-1.87479
C	0.10894	-4.95493	-2.79726
H	-0.86105	-4.89208	-3.30131
C	0.95341	-6.04622	-3.07877
H	0.63471	-6.81143	-3.79622
C	2.20319	-6.15516	-2.44080
H	2.86217	-7.00283	-2.65850
C	2.59756	-5.16944	-1.51809
H	3.56040	-5.23353	-1.00675
C	1.74640	-4.08342	-1.23817
H	2.08406	-3.34393	-0.50880
C	-2.74497	-3.02128	-2.33162
C	-3.76078	-3.60609	-1.53882
H	-3.62943	-3.69338	-0.45794
C	-4.96679	-4.05951	-2.10661
H	-5.74166	-4.48769	-1.46205
C	-5.18166	-3.95209	-3.49250
H	-6.12091	-4.30023	-3.93557
C	-4.18124	-3.38565	-4.30421
H	-4.33722	-3.29394	-5.38488
C	-2.98273	-2.92468	-3.72501
H	-2.22768	-2.46541	-4.37317
C	3.04577	2.68912	-1.79275
C	3.99133	2.98658	-2.80555
H	4.41986	2.17629	-3.40407
C	4.40108	4.30893	-3.06395
H	5.13511	4.50764	-3.85341
C	3.86756	5.37362	-2.31406
H	4.18450	6.40306	-2.51339
C	2.92168	5.10449	-1.30879
H	2.48390	5.91307	-0.71931
C	2.51863	3.77844	-1.05750
H	1.76921	3.61301	-0.28016
C	4.08625	-0.55777	-2.20298
C	3.89783	-1.87278	-2.68972
H	2.88698	-2.26020	-2.84231
C	4.98562	-2.72808	-2.94493
H	4.79638	-3.75286	-3.27980
C	6.30101	-2.27362	-2.74040
H	7.15159	-2.93686	-2.93133
C	6.51578	-0.95982	-2.28066
H	7.53655	-0.59770	-2.11387
C	5.41983	-0.11785	-2.00878
H	5.60968	0.88608	-1.61591

2-B3LYP(D3)

SCF Energy = -2807.35880228

Sn	-0.07159	0.02255	3.09254
Sn	1.05372	-2.13010	1.47704
Sn	1.24038	2.02702	1.38346
Sn	-2.46086	0.09410	1.37546
Sn	1.55090	-1.90702	-1.36388
Sn	0.93981	2.15089	-1.47742
Sn	-2.36079	-0.48243	-1.45056
Sn	0.02045	-0.11219	-3.10661
C	-0.17287	-3.95789	1.72266
C	0.10766	-5.15487	1.03578
H	0.94825	-5.21011	0.35171
C	-0.69798	-6.28801	1.18513
H	-0.45753	-7.19045	0.62738
C	-1.81969	-6.24794	2.01724
H	-2.45811	-7.12289	2.12126
C	-2.12554	-5.06853	2.69947
H	-3.00974	-5.01070	3.32995
C	-1.30676	-3.94411	2.55403
H	-1.57777	-3.03603	3.08854
C	3.01806	-2.78961	2.24560
C	3.43470	-4.13254	2.21342
H	2.73398	-4.91070	1.91959
C	4.74533	-4.49488	2.54023
H	5.04450	-5.54098	2.49842
C	5.67396	-3.51663	2.90856
H	6.69785	-3.79589	3.14937
C	5.27550	-2.17901	2.96362
H	5.98396	-1.40013	3.23548
C	3.96244	-1.82675	2.64127
H	3.68951	-0.77590	2.67474
C	3.41130	1.97971	1.81928
C	4.32757	1.25642	1.03588
H	3.99834	0.72620	0.14729
C	5.68392	1.19366	1.37160
H	6.35672	0.61979	0.74219
C	6.15636	1.85664	2.50588
H	7.21087	1.80754	2.77054
C	5.26441	2.58602	3.29708
H	5.62259	3.10973	4.18196
C	3.91111	2.64580	2.95350
H	3.23677	3.22752	3.57898
C	0.76628	4.03327	2.20369
C	0.54719	4.19300	3.58405
H	0.61361	3.32877	4.24371

C	0.21792	5.43519	4.13643
H	0.05117	5.52565	5.20826
C	0.09031	6.55462	3.31017
H	-0.17713	7.52106	3.73276
C	0.30073	6.41904	1.93604
H	0.19113	7.27888	1.27865
C	0.63868	5.17529	1.39450
H	0.78099	5.10075	0.32070
C	-4.22908	-1.01302	2.12304
C	-5.23488	-0.35053	2.84926
H	-5.15086	0.71869	3.03078
C	-6.35444	-1.03336	3.33520
H	-7.11777	-0.49313	3.89306
C	-6.49682	-2.40381	3.10441
H	-7.36798	-2.93695	3.48031
C	-5.51215	-3.08068	2.38074
H	-5.61018	-4.14616	2.18220
C	-4.39667	-2.39093	1.89790
H	-3.65705	-2.94630	1.33226
C	-3.28292	2.14767	1.49291
C	-2.63278	3.13400	2.25282
H	-1.73410	2.88798	2.80854
C	-3.09750	4.45163	2.30585
H	-2.54277	5.19103	2.87759
C	-4.25108	4.80757	1.60513
H	-4.61423	5.83313	1.63253
C	-4.92763	3.84112	0.85480
H	-5.82053	4.10655	0.29267
C	-4.44575	2.53007	0.79770
H	-4.98376	1.80800	0.19227
C	1.48359	-4.02147	-2.00857
C	0.27502	-4.57568	-2.46268
H	-0.59317	-3.93993	-2.61054
C	0.14145	-5.94595	-2.70146
H	-0.81961	-6.34068	-3.02326
C	1.22916	-6.79941	-2.50297
H	1.12873	-7.86866	-2.67860
C	2.44988	-6.26689	-2.07691
H	3.30582	-6.92228	-1.92444
C	2.57220	-4.89521	-1.83374
H	3.52894	-4.50716	-1.49218
C	3.70703	-1.44708	-1.53818
C	4.69093	-2.08468	-0.75911
H	4.41264	-2.84486	-0.03672
C	6.04098	-1.73729	-0.86607
H	6.77204	-2.24116	-0.23758
C	6.43962	-0.72554	-1.74369
H	7.48730	-0.43851	-1.81006
C	5.48073	-0.07100	-2.51992
H	5.76439	0.73984	-3.18584
C	4.13614	-0.44080	-2.42090
H	3.41355	0.08909	-3.03400
C	-0.29940	3.94510	-1.85082
C	0.15169	4.96457	-2.70893
H	1.12630	4.87693	-3.18449
C	-0.62467	6.09977	-2.96132
H	-0.24995	6.87448	-3.62865
C	-1.87747	6.24068	-2.35889
H	-2.48364	7.12346	-2.55313
C	-2.34391	5.24143	-1.50202
H	-3.31086	5.33032	-1.01696
C	-1.55993	4.11159	-1.25074
H	-1.95293	3.36237	-0.56958
C	2.85525	2.87387	-2.33134
C	3.86755	3.45647	-1.54993
H	3.72737	3.57495	-0.47956
C	5.07928	3.86775	-2.11306
H	5.85039	4.29640	-1.47652
C	5.30426	3.71776	-3.48312
H	6.24816	4.03360	-3.92285
C	4.30822	3.15240	-4.28360
H	4.47180	3.02809	-5.35250
C	3.10348	2.73467	-3.70894
H	2.35026	2.27595	-4.34806
C	-3.15307	-2.52074	-1.76902
C	-4.10000	-2.77580	-2.77801
H	-4.48270	-1.95356	-3.37866
C	-4.57003	-4.06828	-3.02934
H	-5.30378	-4.23368	-3.81662
C	-4.09833	-5.14576	-2.27513
H	-4.46288	-6.15272	-2.46832
C	-3.15209	-4.91929	-1.27371
H	-2.76201	-5.73982	-0.67941
C	-2.68823	-3.62257	-1.03022
H	-1.93976	-3.49040	-0.25396
C	-4.04872	0.72824	-2.20198
C	-3.81737	2.00411	-2.74203
H	-2.79987	2.34842	-2.90711
C	-4.86928	2.87389	-3.04232
H	-4.64924	3.86706	-3.42720
C	-6.18993	2.47515	-2.82496
H	-7.01233	3.15066	-3.05185
C	-6.44676	1.20217	-2.30681
H	-7.47223	0.88289	-2.12939
C	-5.38709	0.34491	-1.99487
H	-5.60913	-0.62936	-1.56456

2-PBE(D3)

SCF Energy = -2803.75527400

Sn	0.08146	-0.04532	3.15291
Sn	-0.53523	2.28850	1.49980
Sn	-1.64267	-1.68086	1.40502
Sn	2.36276	-0.63389	1.37876
Sn	-1.07814	2.18816	-1.36333
Sn	-1.37563	-1.87304	-1.47734
Sn	2.37470	-0.04278	-1.46954
Sn	-0.01411	0.11976	-3.15813
C	1.06833	3.81666	1.75889
C	1.06935	5.04308	1.05587
H	0.27285	5.26984	0.34023
C	2.10141	5.98119	1.22718
H	2.07776	6.91600	0.65531
C	3.16730	5.70629	2.09831
H	3.98238	6.42898	2.22017
C	3.19030	4.49091	2.79917
H	4.02773	4.25020	3.46371
C	2.14847	3.56327	2.63121
H	2.19361	2.61462	3.18088
C	-2.30705	3.39327	2.27778
C	-2.39459	4.80232	2.24999
H	-1.52695	5.39713	1.94115
C	-3.58293	5.46408	2.60243
H	-3.62877	6.55939	2.56556
C	-4.71389	4.72663	2.98998
H	-5.64572	5.24176	3.25076
C	-4.64003	3.32611	3.03971
H	-5.51386	2.73079	3.32777
C	-3.44699	2.67267	2.69310
H	-3.42329	1.57805	2.72429
C	-3.78242	-1.19513	1.81223
C	-4.49323	-0.23325	1.06264
H	-4.01340	0.28766	0.22762
C	-5.83028	0.08110	1.35871
H	-6.34443	0.83439	0.75368

C	-6.48670	-0.56459	2.41706
H	-7.52966	-0.32101	2.65118
C	-5.79896	-1.52863	3.17130
H	-6.30449	-2.04290	3.99792
C	-4.46338	-1.83942	2.86857
H	-3.94729	-2.60392	3.46192
C	-1.64523	-3.76121	2.21798
C	-1.46665	-3.97306	3.60271
H	-1.31489	-3.11165	4.26703
C	-1.45403	-5.26696	4.15140
H	-1.31191	-5.40268	5.23023
C	-1.61008	-6.38382	3.31537
H	-1.58837	-7.39572	3.73625
C	-1.78535	-6.19412	1.93598
H	-1.89368	-7.05798	1.27023
C	-1.80850	-4.89716	1.39774
H	-1.93396	-4.77828	0.31644
C	4.35208	0.05622	2.11961
C	5.17983	-0.82120	2.85352
H	4.84756	-1.84932	3.03965
C	6.43095	-0.40800	3.34077
H	7.05455	-1.11085	3.90683
C	6.88497	0.89862	3.10305
H	7.86165	1.22242	3.48136
C	6.07855	1.78376	2.37126
H	6.41984	2.80548	2.16705
C	4.82952	1.36382	1.88664
H	4.22982	2.07491	1.31200
C	2.73343	-2.82876	1.50334
C	1.88814	-3.64761	2.27966
H	1.05662	-3.20172	2.83532
C	2.06718	-5.03922	2.34650
H	1.36741	-5.64462	2.93287
C	3.12027	-5.64019	1.64130
H	3.25979	-6.72697	1.67920
C	3.98579	-4.84276	0.87455
H	4.80513	-5.29963	0.30730
C	3.79133	-3.45331	0.80537
H	4.47007	-2.85885	0.18632
C	-0.53152	4.24757	-2.02052
C	0.76502	4.50850	-2.51152
H	1.46864	3.68345	-2.66540
C	1.19644	5.81671	-2.78279
H	2.22090	5.98285	-3.13498
C	0.32718	6.89949	-2.58013
H	0.66164	7.92374	-2.78199
C	-0.97721	6.65941	-2.11745
H	-1.66706	7.49789	-1.96223
C	-1.39862	5.34795	-1.84096
H	-2.41796	5.18486	-1.47222
C	-3.29710	2.26296	-1.53916
C	-4.10115	3.11809	-0.75241
H	-3.64406	3.77800	-0.00868
C	-5.50083	3.11634	-0.87521
H	-6.09595	3.78238	-0.23987
C	-6.12954	2.24182	-1.77569
H	-7.22282	2.22355	-1.85530
C	-5.35019	1.37632	-2.55850
H	-5.82280	0.66359	-3.24311
C	-3.95071	1.39964	-2.44360
H	-3.36396	0.70964	-3.05990
C	-0.58482	-3.92195	-1.86016
C	-1.27109	-4.80263	-2.72516
H	-2.20515	-4.47875	-3.19968
C	-0.78368	-6.09432	-2.98446
H	-1.33629	-6.76013	-3.65887
C	0.40582	-6.53309	-2.38187
H	0.78708	-7.54132	-2.58195
C	1.10061	-5.67299	-1.51820
H	2.02679	-5.99309	-1.03080
C	0.60644	-4.38387	-1.26031
H	1.16882	-3.74443	-0.57183
C	-3.42177	-2.16205	-2.32392
C	-4.53346	-2.51913	-1.53259
H	-4.41137	-2.66668	-0.45439
C	-5.81268	-2.66269	-2.09442
H	-6.66167	-2.91836	-1.45020
C	-6.00545	-2.46692	-3.47035
H	-7.00386	-2.57523	-3.90975
C	-4.91037	-2.12475	-4.27943
H	-5.04909	-1.96822	-5.35587
C	-3.63652	-1.97038	-3.70644
H	-2.79525	-1.67887	-4.34940
C	3.63194	1.76547	-1.79113
C	4.61092	1.78639	-2.80900
H	4.78196	0.88950	-3.41611
C	5.37958	2.93486	-3.06044
H	6.13340	2.92232	-3.85714
C	5.18336	4.09621	-2.29686
H	5.78324	4.99300	-2.49062
C	4.21068	4.10043	-1.28606
H	4.03024	4.99550	-0.68223
C	3.44523	2.94750	-1.04290
H	2.68094	2.99332	-0.25889
C	3.76051	-1.60863	-2.23058
C	3.25166	-2.78868	-2.81139
H	2.17521	-2.88944	-2.99099
C	4.09156	-3.86611	-3.13605
H	3.65745	-4.78161	-3.55367
C	5.47235	-3.77551	-2.90368
H	6.13123	-4.61583	-3.15132
C	6.00369	-2.60172	-2.34439
H	7.08085	-2.52267	-2.15447
C	5.15390	-1.53539	-2.00575
H	5.58287	-0.63964	-1.54068

3-BP86

SCF Energy = -3038.91146088
Enthalpy 0K = -3037.772035
Enthalpy 298K = -3037.678181
Free Energy 298K = -3037.931452
Lowest Frequency = 5.4547 cm^{-1}
Second Frequency = 13.8220 cm^{-1}

Sn	-0.06793	-0.01395	-3.29291
Sn	-0.61090	-2.48764	-1.76914
Sn	-0.40833	-2.65454	1.14448
Sn	0.03971	0.01006	2.18187
Sn	-2.08234	1.70887	1.18113
Sn	-1.88277	1.71928	-1.73945
Sn	2.38978	0.73374	-1.84098
Sn	2.53202	0.97763	1.07365
C	0.64094	-4.15724	-2.54117
C	1.98071	-3.95080	-2.93884
H	2.43293	-2.95453	-2.86719
C	2.76240	-5.00886	-3.43721
H	3.79862	-4.81712	-3.73814
C	2.21410	-6.29683	-3.54903
H	2.82055	-7.12314	-3.93819
C	0.88191	-6.51972	-3.16192
H	0.44533	-7.52222	-3.24824
C	0.10520	-5.45958	-2.66287
H	-0.93473	-5.65057	-2.37161
C	-2.11127	-3.58099	2.22028
C	-2.01670	-4.92100	2.65937

H	-1.09717	-5.49107	2.48166
C	-3.08352	-5.53763	3.33635
H	-2.98786	-6.57795	3.67003
C	-4.26755	-4.82437	3.58516
H	-5.09927	-5.30412	4.11411
C	-4.37846	-3.49254	3.15366
H	-5.29403	-2.92063	3.34135
C	-3.30951	-2.87838	2.47752
H	-3.42618	-1.83734	2.15430
C	1.25200	-3.94952	1.83275
C	2.10610	-4.63169	0.93741
H	1.97057	-4.52626	-0.14468
C	3.13728	-5.46190	1.41392
H	3.78601	-5.98224	0.70010
C	3.33162	-5.62615	2.79496
H	4.13187	-6.27720	3.16590
C	2.49267	-4.95286	3.69949
H	2.63868	-5.07232	4.77950
C	1.46478	-4.12188	3.22113
H	0.82317	-3.60366	3.94392
C	0.13904	-0.03776	4.39820
C	1.38181	-0.13527	5.06389
H	2.31343	-0.18847	4.48708
C	1.44821	-0.17627	6.46824
H	2.42322	-0.25156	6.96404
C	0.27098	-0.12354	7.23183
H	0.32143	-0.15427	8.32629
C	-0.97215	-0.03437	6.58422
H	-1.89666	0.00247	7.17248
C	-1.03621	0.00719	5.18059
H	-2.01790	0.07112	4.69601
C	-4.05408	0.98226	1.88495
C	-4.45509	1.22687	3.21949
H	-3.79746	1.78867	3.89424
C	-5.69728	0.77696	3.69966
H	-5.98663	0.97858	4.73791
C	-6.56686	0.07320	2.84943
H	-7.53803	-0.27481	3.21990
C	-6.18743	-0.17384	1.52007
H	-6.86167	-0.71343	0.84550
C	-4.94277	0.27682	1.04302
H	-4.67961	0.08391	-0.00303
C	-2.00822	3.69437	2.15792
C	-3.20563	4.41664	2.36500
H	-4.16709	3.98146	2.06722
C	-3.18926	5.68950	2.96136
H	-4.13029	6.23149	3.11415
C	-1.97160	6.26639	3.35805
H	-1.95776	7.25935	3.82226
C	-0.77289	5.56339	3.15675
H	0.18583	5.99794	3.46069
C	-0.79291	4.28906	2.56258
H	0.15854	3.76329	2.42195
C	-3.96750	1.43534	-2.45786
C	-4.86627	2.52465	-2.51531
H	-4.53355	3.52302	-2.20670
C	-6.18404	2.35494	-2.97468
H	-6.86381	3.21492	-3.01174
C	-6.63065	1.08709	-3.38353
H	-7.65867	0.95360	-3.74039
C	-5.75159	-0.00676	-3.33421
H	-6.08303	-1.00205	-3.65135
C	-4.43267	0.16909	-2.87736
H	-3.76678	-0.70205	-2.85531
C	3.16540	2.66193	-2.63488
C	2.29879	3.73689	-2.93485
H	1.21900	3.64274	-2.76890
C	2.79519	4.94788	-3.45051
H	2.09823	5.76408	-3.67163
C	4.17193	5.10383	-3.67957
H	4.56101	6.04601	-4.08325
C	5.04781	4.04383	-3.39118
H	6.12421	4.15655	-3.56938
C	4.54771	2.83626	-2.87327
H	5.24512	2.01733	-2.65974
C	4.06371	-0.59941	-2.44595
C	4.99489	-1.15709	-1.54169
H	4.91078	-0.95484	-0.46797
C	6.04473	-1.97789	-1.99278
H	6.75235	-2.39896	-1.26912
C	6.18536	-2.25760	-3.36143
H	7.00402	-2.89598	-3.71357
C	5.26931	-1.71312	-4.27737
H	5.37011	-1.92452	-5.34859
C	4.22060	-0.89532	-3.82099
H	3.51516	-0.48320	-4.55392
C	4.22437	-0.04725	2.08013
C	5.34798	0.70387	2.49504
H	5.36857	1.78864	2.33718
C	6.44319	0.08264	3.12031
H	7.30413	0.68490	3.43464
C	6.43471	-1.30418	3.34303
H	7.28771	-1.78914	3.83180
C	5.32612	-2.06516	2.93792
H	5.30006	-3.14695	3.10870
C	4.23217	-1.44166	2.31133
H	3.38001	-2.06188	2.00967
C	2.86690	3.05461	1.77091
C	2.88179	3.33007	3.15891
H	2.69418	2.52673	3.88194
C	3.13141	4.62816	3.63857
H	3.14030	4.81759	4.71843
C	3.36853	5.67822	2.73506
H	3.56528	6.69063	3.10660
C	3.35231	5.42265	1.35461
H	3.53393	6.23497	0.64164
C	3.10445	4.12279	0.87724
H	3.10119	3.94875	-0.20446
C	-2.61758	-3.28407	-2.30684
C	-5.13519	-4.31585	-3.13659
H	-6.10504	-4.71507	-3.45562
C	-4.21377	-3.85068	-4.09016
H	-4.46127	-3.88594	-5.15784
C	-2.97083	-3.34015	-3.67616
H	-2.26727	-2.98117	-4.43823
C	-4.80401	-4.26674	-1.77311
H	-5.51520	-4.62669	-1.02048
C	-3.55834	-3.75603	-1.36444
H	-3.32620	-3.73302	-0.29364
C	-1.13274	4.84233	-1.40377
H	-0.93301	4.59104	-0.35600
C	-0.93793	6.17041	-1.82501
H	-0.58937	6.92089	-1.10623
C	-1.58723	3.85033	-2.30119
C	-1.19302	6.53356	-3.15732
H	-1.04406	7.56876	-3.48591
C	-1.64421	5.56121	-4.06580
H	-1.84638	5.83428	-5.10844
C	-1.83692	4.23575	-3.63968
H	-2.19366	3.49413	-4.36526

3-BP86(C/H-optimised)

SCF Energy = -3038.89478311

Enthalpy 0K = -3037.754908

Enthalpy 298K = -3037.661547
Free Energy 298K = -3037.911993
Lowest Frequency = 7.4063 cm^{-1}
Second Frequency = 11.8393 cm^{-1}

Sn	0.02153	-0.07617	-3.14505
Sn	2.00884	-1.50884	-1.68471
Sn	1.51390	-1.99954	1.03826
Sn	-0.06327	0.02765	2.12203
Sn	-2.61692	-0.28601	1.07372
Sn	-2.23517	-0.98414	-1.63830
Sn	0.33267	2.35398	-1.71246
Sn	0.94652	2.39334	1.04879
C	4.09063	-0.78496	-1.94345
C	4.41475	0.58850	-1.92407
H	3.63659	1.34250	-1.76128
C	5.73368	1.02670	-2.13660
H	5.95209	2.10002	-2.12252
C	6.75616	0.09432	-2.37305
H	7.78485	0.43422	-2.54062
C	6.45157	-1.27685	-2.40168
H	7.24230	-2.01227	-2.59403
C	5.13065	-1.71060	-2.19116
H	4.90766	-2.78364	-2.23194
C	0.71726	-3.99160	1.59133
C	1.62695	-5.02487	1.91358
H	2.70635	-4.83360	1.88004
C	1.17060	-6.29707	2.30023
H	1.89420	-7.08319	2.54743
C	-0.20750	-6.55694	2.38000
H	-0.56529	-7.54647	2.68712
C	-1.12339	-5.53919	2.07073
H	-2.20145	-5.72142	2.13924
C	-0.66199	-4.27128	1.67680
H	-1.40210	-3.49570	1.45124
C	3.38966	-2.07054	2.23124
C	4.66598	-2.07839	1.62473
H	4.75987	-1.99516	0.53571
C	5.83742	-2.18272	2.39837
H	6.81560	-2.19063	1.90303
C	5.75281	-2.27969	3.79644
H	6.66408	-2.35965	4.40055
C	4.49237	-2.27217	4.41640
H	4.41567	-2.34299	5.50777
C	3.32478	-2.16961	3.64062
H	2.35310	-2.16491	4.14799
C	0.10664	-0.01194	4.33020
C	1.14915	0.69219	4.97510
H	1.87488	1.26509	4.38492
C	1.28388	0.66323	6.37467
H	2.09972	1.21748	6.85315
C	0.38043	-0.07660	7.15462
H	0.48398	-0.09993	8.24547
C	-0.65386	-0.79004	6.52743
H	-1.36032	-1.37547	7.12761
C	-0.78841	-0.75858	5.12800
H	-1.60161	-1.32653	4.66142
C	-3.77197	-1.80533	2.21670
C	-4.18955	-1.52491	3.53890
H	-3.93455	-0.56369	4.00160
C	-4.94706	-2.45212	4.27654
H	-5.25658	-2.21154	5.30060
C	-5.30953	-3.68112	3.70133
H	-5.90107	-4.40484	4.27373
C	-4.91416	-3.97236	2.38614
H	-5.20323	-4.92230	1.92135
C	-4.15281	-3.04331	1.65249
H	-3.86284	-3.29411	0.62550
C	-3.89411	1.47995	1.46398
C	-5.26617	1.29014	1.74917
H	-5.68301	0.27671	1.78902
C	-6.11144	2.38502	2.00133
H	-7.17192	2.21401	2.22254
C	-5.59788	3.69199	1.97601
H	-6.25465	4.54643	2.17630
C	-4.23779	3.89695	1.69568
H	-3.81813	4.90832	1.67851
C	-3.39735	2.79980	1.43961
H	-2.33978	2.99583	1.23383
C	-2.62505	-3.15922	-1.87655
C	-3.94403	-3.62162	-2.09292
H	-4.77614	-2.90751	-2.10995
C	-4.20861	-4.98652	-2.30356
H	-5.23920	-5.32207	-2.47200
C	-3.15528	-5.91632	-2.30615
H	-3.35945	-6.98023	-2.47417
C	-1.83925	-5.47358	-2.10002
H	-1.00545	-6.18396	-2.10898
C	-1.58020	-4.10814	-1.88703
H	-0.54002	-3.79311	-1.74557
C	-1.29998	3.81141	-2.09538
C	-2.65487	3.42000	-2.14289
H	-2.94012	2.37735	-1.96302
C	-3.66929	4.34574	-2.44444
H	-4.71125	4.00929	-2.47935
C	-3.34448	5.68625	-2.70529
H	-4.13379	6.40928	-2.94203
C	-2.00041	6.09349	-2.66992
H	-1.73573	7.13645	-2.88291
C	-0.98943	5.16306	-2.37079
H	0.05651	5.49372	-2.36767
C	2.00014	3.47093	-2.68216
C	2.95590	4.23057	-1.97016
H	2.92965	4.26389	-0.87432
C	3.96781	4.94464	-2.63929
H	4.69722	5.52431	-2.06107
C	4.04263	4.91443	-4.04089
H	4.83047	5.46877	-4.56407
C	3.10332	4.16447	-4.76776
H	3.15615	4.13036	-5.86251
C	2.09745	3.45154	-4.09332
H	1.37817	2.86688	-4.68128
C	3.06073	2.70225	1.62967
C	3.47991	3.99350	2.02528
H	2.75957	4.82017	2.04570
C	4.81046	4.23520	2.40959
H	5.11424	5.24406	2.71407
C	5.74511	3.18662	2.41189
H	6.78153	3.37266	2.71651
C	5.34267	1.89788	2.02708
H	6.05532	1.06620	2.03354
C	4.01327	1.66112	1.63656
H	3.73060	0.64185	1.35173
C	0.02702	4.11993	2.10461
C	-0.08732	4.12518	3.51433
H	0.23343	3.25315	4.09671
C	-0.61746	5.23369	4.19658
H	-0.70038	5.21110	5.28956
C	-1.04508	6.36411	3.48086
H	-1.45981	7.22873	4.01190
C	-0.94274	6.37663	2.08068
H	-1.27689	7.25180	1.51106
C	-0.41240	5.26406	1.40089
H	-0.36095	5.29146	0.30638
C	2.20949	-3.50541	-2.64972

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C   2.51025 -5.98918 -4.00600
H   2.62432 -6.94618 -4.52832
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H   2.43730 -4.81351 -5.83129
C   2.25521 -3.56892 -4.06215
H   2.16743 -2.64813 -4.65293
C   2.46193 -5.95008 -2.60347
H   2.53933 -6.87754 -2.02365
C   2.31440 -4.72005 -1.93515
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C  -5.14706  0.37169 -2.05159
H  -5.15330  0.48768 -0.96147
C  -6.26332  0.82313 -2.78075
H  -7.11427  1.26758 -2.25096
C  -4.03194 -0.20454 -2.70036
C  -6.28700  0.70456 -4.17932
H  -7.15500  1.05626 -4.74905
C  -5.18765  0.13628 -4.84388
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C  -4.07479 -0.30925 -4.11050
H  -3.22409 -0.74274 -4.65158
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3-BLYP

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SCF Energy = -3037.17330226
Sn  0.02953 -0.00940 -3.29850
Sn -0.04566  2.57519 -1.80316
Sn -0.42434  2.69458  1.12514
Sn -0.01247  0.00921  2.20004
Sn  2.53660 -0.97784  1.16607
Sn  2.26411 -1.25190 -1.75967
Sn -2.18463 -1.33502 -1.80100
Sn -2.11473 -1.71244  1.12973
C  -1.59924  3.92264 -2.66933
C  -2.82441  3.41203 -3.16191
H  -3.03366  2.33908 -3.11789
C  -3.79998  4.26324 -3.71757
H  -4.73864  3.83854 -4.08608
C  -3.56616  5.64743 -3.79543
H  -4.32169  6.31109 -4.22778
C  -2.35317  6.17384 -3.31517
H  -2.16166  7.25054 -3.37346
C  -1.38302  5.31938 -2.75804
H  -0.44419  5.75036 -2.39658
C   0.82627  4.14842  2.25231
C   0.30080  5.41559  2.60344
H  -0.72899  5.67355  2.33930
C   1.07870  6.35727  3.30374
H   0.64914  7.32977  3.56593
C   2.40315  6.05179  3.66474
H   3.00864  6.78357  4.20858
C   2.94365  4.80003  3.32138
H   3.97273  4.54708  3.59306
C   2.16149  3.86008  2.62291
H   2.61121  2.89677  2.36758
C  -2.46301  3.36423  1.70669
C  -3.47741  3.63114  0.75575
H  -3.27920  3.51216 -0.31234
C  -4.75514  4.06758  1.15781
H  -5.51926  4.27004  0.40109
C  -5.04555  4.24732  2.52162
H  -6.03670  4.59070  2.83397
C  -4.05139  3.98629  3.48267
H  -4.26614  4.12450  4.54722
C  -2.77587  3.54826  3.07731
H  -2.01956  3.35376  3.84426
C  -0.04542  0.04779  4.42774
C  -1.22118 -0.26898  5.15006
H  -2.13896 -0.53831  4.61865
C  -1.24072 -0.23573  6.55800
H  -2.16216 -0.48559  7.09376
C  -0.08298  0.11814  7.27284
H  -0.09636  0.14307  8.36683
C   1.09209  0.44220  6.57155
H   1.99785  0.72246  7.11880
C   1.10873  0.40760  5.16442
H   2.03542  0.66876  4.64400
C   4.15933  0.43699  1.71589
C   4.73442  0.39260  3.01078
H   4.39580 -0.35525  3.73466
C   5.75498  1.28636  3.38809
H   6.18409  1.22958  4.39377
C   6.22416  2.24752  2.47401
H   7.01950  2.94119  2.76377
C   5.66796  2.30608  1.18390
H   6.02567  3.04629  0.46208
C   4.64704  1.41029  0.81106
H   4.24493  1.47442 -0.20315
C   3.17496 -2.81031  2.24609
C   4.55217 -3.12390  2.35199
H   5.30272 -2.44778  1.93118
C   4.98444 -4.29494  3.00286
H   6.05485 -4.51439  3.07334
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H   4.37967 -6.09334  4.06341
C   2.67340 -4.88923  3.46012
H   1.92983 -5.57015  3.88447
C   2.24531 -3.71512  2.81121
H   1.17185 -3.51639  2.75241
C   4.22932 -0.60854 -2.59277
C   5.33185 -1.49612 -2.63669
H   5.22361 -2.52026 -2.26637
C   6.57395 -1.09174 -3.16193
H   7.41083 -1.79775 -3.18591
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C  -2.58419 -3.35380 -2.66211
C  -1.53110 -4.16643 -3.14724
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C  -1.78326 -5.43927 -3.69593
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C  -3.10037 -5.92479 -3.77511
H  -3.29948 -6.91279 -4.20218
C  -4.16127 -5.13113 -3.30241
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C  -3.90342 -3.86163 -2.75107
H  -4.74529 -3.25956 -2.39568
C  -4.12472 -0.33322 -2.25548
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H  -4.62423  0.31960 -0.23416
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H  -6.71914  1.45868 -0.86464
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H  -7.48552  1.47954 -3.25328
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H  -6.10124  0.33720 -5.00441
C  -4.57669 -0.30861 -3.59931
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H	-3.79387	0.80455	2.43358
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C	-1.69140	-4.15982	3.10745
H	-1.88746	-3.39819	3.86877
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H	-1.45989	-5.72816	4.59098
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C	-1.42596	-4.83237	0.79167
H	-1.41937	-4.60967	-0.27790
C	1.78239	3.77316	-2.25897
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H	4.98385	5.85436	-3.26031
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H	1.54374	3.50442	-4.41194
C	3.74905	5.11500	-1.63073
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H	2.35867	4.27455	-0.21523
C	2.09736	-4.43977	-1.21335
H	1.87696	-4.16444	-0.17886
C	2.13029	-5.80792	-1.54651
H	1.92933	-6.55657	-0.77399
C	2.35480	-3.43993	-2.18169
C	2.42192	-6.20917	-2.86201
H	2.44979	-7.27201	-3.12184
C	2.68086	-5.23295	-3.84138
H	2.91131	-5.53324	-4.86885
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3-B3LYP

SCF Enrgy = -3038.77052438

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Sn	0.01515	-0.01572	2.17850
Sn	-1.90172	1.88619	1.15499
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Sn	2.50117	0.33973	-1.78866
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C	-0.12460	-4.17972	-2.65241
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C	1.74038	-5.37407	-3.68633
H	2.76554	-5.36530	-4.04777
C	0.97191	-6.53657	-3.76659
H	1.39303	-7.44344	-4.19415
C	-0.34293	-6.52655	-3.29549
H	-0.94994	-7.42733	-3.35584
C	-0.88164	-5.36091	-2.74392
H	-1.90922	-5.37454	-2.38783
C	-2.40601	-3.41638	2.22193
C	-2.45361	-4.78597	2.53478
H	-1.63446	-5.43874	2.24313
C	-3.53630	-5.33198	3.22976
H	-3.54909	-6.39473	3.46120
C	-4.59877	-4.51699	3.62530
H	-5.44176	-4.94077	4.16570
C	-4.57041	-3.15457	3.32289
H	-5.38927	-2.50600	3.62285
C	-3.48398	-2.61234	2.62976
H	-3.49279	-1.54823	2.40875
C	0.89587	-4.02365	1.67228
C	1.70594	-4.67314	0.72511
H	1.56184	-4.49407	-0.33622
C	2.70271	-5.57116	1.12048
H	3.31196	-6.06185	0.36554
C	2.90945	-5.84016	2.47439
H	3.68164	-6.54112	2.78202
C	2.11441	-5.20537	3.43199
H	2.26584	-5.40896	4.48951
C	1.12092	-4.30661	3.03268
H	0.51539	-3.82487	3.79710
C	0.04240	-0.07950	4.38413
C	1.24610	-0.22630	5.09492
H	2.19011	-0.31150	4.56176
C	1.25871	-0.27679	6.49222
H	2.20340	-0.39066	7.01883
C	0.06431	-0.18353	7.20833
H	0.07252	-0.22153	8.29482
C	-1.14173	-0.04380	6.51888
H	-2.07820	0.02555	7.06738
C	-1.15039	0.00660	5.12247
H	-2.10399	0.11093	4.61024
C	-3.93493	1.23513	1.69615
C	-4.41910	1.44631	3.00061
H	-3.79925	1.95730	3.73406
C	-5.69740	1.02474	3.37779
H	-6.04834	1.20188	4.39189
C	-6.52310	0.38102	2.45287
H	-7.51899	0.05474	2.74249
C	-6.06285	0.16611	1.15269
H	-6.69620	-0.32896	0.42117
C	-4.78331	0.58967	0.78054
H	-4.46132	0.41866	-0.24240
C	-1.75330	3.80056	2.22861
C	-2.88827	4.62015	2.35876
H	-3.84444	4.29403	1.95615
C	-2.81779	5.85504	3.00921
H	-3.71010	6.47058	3.09852
C	-1.60509	6.29906	3.54027
H	-1.54831	7.26054	4.04483
C	-0.46688	5.50054	3.41830
H	0.48530	5.83263	3.82350
C	-0.54321	4.26424	2.77034
H	0.36028	3.66549	2.69352
C	-3.58453	2.23293	-2.56070
C	-4.23995	3.47646	-2.58513
H	-3.73658	4.36213	-2.20411
C	-5.53226	3.60475	-3.10189
H	-6.01733	4.57849	-3.11050
C	-6.20118	2.48618	-3.60400
H	-7.20766	2.58439	-4.00385
C	-5.56804	1.24237	-3.58959
H	-6.07513	0.36153	-3.97544
C	-4.27311	1.12143	-3.07582
H	-3.80474	0.14003	-3.08246
C	3.66813	2.01432	-2.63765
C	3.03375	3.16534	-3.13612
H	1.95003	3.24833	-3.11419
C	3.77076	4.22882	-3.66715
H	3.24987	5.10768	-4.03851

C	5.16393	4.15872	-3.71670
H	5.73979	4.98325	-4.13032
C	5.81360	3.02121	-3.23225
H	6.89900	2.95707	-3.26822
C	5.07210	1.96402	-2.69761
H	5.59879	1.08612	-2.33067
C	3.85154	-1.35470	-2.22426
C	4.22571	-2.31747	-1.27171
H	3.89349	-2.22933	-0.24151
C	5.03923	-3.40217	-1.61300
H	5.31259	-4.12787	-0.85103
C	5.49874	-3.54993	-2.92273
H	6.13303	-4.39171	-3.18988
C	5.13965	-2.60529	-3.88711
H	5.49333	-2.70892	-4.91048
C	4.32536	-1.52385	-3.53887
H	4.06354	-0.80015	-4.30810
C	4.18984	-0.38000	2.17226
C	5.41488	0.25769	2.43528
H	5.56333	1.29307	2.13828
C	6.45464	-0.41298	3.08505
H	7.39286	0.10259	3.27758
C	6.29072	-1.74043	3.48621
H	7.09929	-2.26317	3.99136
C	5.08160	-2.39077	3.23476
H	4.93637	-3.42345	3.54042
C	4.04373	-1.71562	2.58488
H	3.11375	-2.24969	2.40697
C	3.03582	2.78276	1.70007
C	3.17936	3.10369	3.06297
H	3.06457	2.33165	3.82069
C	3.46991	4.40757	3.47488
H	3.57874	4.62832	4.53423
C	3.62102	5.42296	2.52730
H	3.84784	6.43785	2.84458
C	3.48123	5.12467	1.17118
H	3.60005	5.90517	0.42384
C	3.19251	3.81824	0.76340
H	3.10033	3.61561	-0.29946
C	-3.13251	-2.66560	-2.22880
C	-5.85038	-3.03757	-2.93609
H	-6.89354	-3.18163	-3.20679
C	-4.87334	-2.93392	-3.92904
H	-5.15255	-2.99826	-4.97829
C	-3.53354	-2.74897	-3.57577
H	-2.79266	-2.67213	-4.36921
C	-5.47532	-2.95850	-1.59414
H	-6.22468	-3.04417	-0.81078
C	-4.13252	-2.77484	-1.24765
H	-3.87494	-2.72837	-0.19370
C	-0.07965	4.82801	-1.16926
H	0.01718	4.47259	-0.14744
C	0.45672	6.07958	-1.48664
H	0.95729	6.65915	-0.71501
C	-0.73784	4.04771	-2.13487
C	0.34739	6.58149	-2.78447
H	0.76211	7.55551	-3.03268
C	-0.30236	5.82348	-3.76143
H	-0.39566	6.20521	-4.77570
C	-0.83571	4.57267	-3.43721
H	-1.34078	4.00415	-4.21544

3-PBE

SCF Energy = -3034.94570776

Sn	-0.04905	0.02249	-3.30736
Sn	-1.42887	-2.07249	-1.77950
Sn	-1.16630	-2.39282	1.10482
Sn	0.03567	-0.00781	2.18595
Sn	-1.48682	2.21403	1.16088
Sn	-1.11627	2.25846	-1.72994
Sn	2.47001	-0.16754	-1.81042
Sn	2.68377	0.19519	1.07411
C	-0.93208	-4.05034	-2.66069
C	0.36890	-4.32901	-3.13129
H	1.15552	-3.56820	-3.06932
C	0.68658	-5.58080	-3.68452
H	1.70698	-5.77088	-4.03430
C	-0.29795	-6.57476	-3.78491
H	-0.05370	-7.55113	-4.21739
C	-1.59909	-6.31078	-3.33038
H	-2.37426	-7.08157	-3.40847
C	-1.91066	-5.06082	-2.77148
H	-2.93289	-4.87007	-2.42485
C	-3.00008	-2.85491	2.25631
C	-3.29106	-4.19116	2.60278
H	-2.60208	-4.99348	2.31539
C	-4.45157	-4.51236	3.32522
H	-4.65874	-5.55634	3.58580
C	-5.34391	-3.50116	3.71133
H	-6.24973	-3.75181	4.27378
C	-5.06838	-2.16782	3.37444
H	-5.75366	-1.36593	3.66861
C	-3.90510	-1.84877	2.65502
H	-3.71470	-0.79861	2.40685
C	0.12713	-4.10441	1.64811
C	0.78838	-4.88953	0.68013
H	0.65740	-4.68030	-0.38662
C	1.61562	-5.95918	1.06194
H	2.11608	-6.55513	0.29107
C	1.79388	-6.26464	2.41920
H	2.43646	-7.10039	2.71650
C	1.14074	-5.49535	3.39510
H	1.27263	-5.72722	4.45773
C	0.31722	-4.42412	3.01131
H	-0.18024	-3.83239	3.78857
C	0.07399	-0.09787	4.39993
C	1.25490	-0.43939	5.09214
H	2.17287	-0.66757	4.53780
C	1.27336	-0.50553	6.49512
H	2.20069	-0.77275	7.01369
C	0.10966	-0.23336	7.22893
H	0.12354	-0.28367	8.32284
C	-1.07352	0.10067	6.55330
H	-1.98825	0.30999	7.11867
C	-1.09048	0.16670	5.15115
H	-2.02720	0.42383	4.64323
C	-3.61360	1.95792	1.71449
C	-4.02824	2.19627	3.04396
H	-3.30358	2.54478	3.78949
C	-5.36491	2.00593	3.43122
H	-5.66500	2.19776	4.46739
C	-6.31394	1.57303	2.49184
H	-7.35701	1.42505	2.79141
C	-5.91962	1.33798	1.16649
H	-6.65079	1.00579	0.42187
C	-4.58225	1.53002	0.78217
H	-4.30712	1.35139	-0.26234
C	-0.95772	4.06379	2.24942
C	-1.94195	5.04604	2.48862
H	-2.97443	4.87934	2.16082
C	-1.62153	6.24034	3.15417
H	-2.40053	6.99017	3.33199
C	-0.30807	6.47470	3.58746
H	-0.05742	7.40729	4.10429

C	0.68135	5.50802	3.35552
H	1.71169	5.67516	3.68674
C	0.35734	4.31264	2.69420
H	1.14956	3.57311	2.53189
C	-3.09577	2.83022	-2.55633
C	-3.50803	4.17887	-2.60130
H	-2.83941	4.96655	-2.23513
C	-4.76425	4.53387	-3.11905
H	-5.06461	5.58750	-3.14644
C	-5.63540	3.54278	-3.59657
H	-6.61714	3.81932	-3.99619
C	-5.24116	2.19728	-3.56031
H	-5.90966	1.41123	-3.92779
C	-3.98052	1.84750	-3.04868
H	-3.69442	0.78918	-3.03763
C	3.92255	1.26584	-2.68568
C	3.49420	2.52067	-3.16915
H	2.43470	2.79880	-3.12552
C	4.40937	3.43986	-3.70900
H	4.04922	4.41011	-4.06744
C	5.77161	3.11384	-3.78305
H	6.48729	3.82802	-4.20465
C	6.21319	1.86668	-3.31515
H	7.27575	1.60439	-3.37187
C	5.29640	0.95395	-2.76893
H	5.65822	-0.01652	-2.40984
C	3.48393	-2.09859	-2.22093
C	3.63104	-3.11335	-1.25206
H	3.29678	-2.94943	-0.22229
C	4.21459	-4.34897	-1.57589
H	4.31608	-5.11670	-0.80119
C	4.66462	-4.59528	-2.88134
H	5.12091	-5.55805	-3.13556
C	4.52982	-3.59758	-3.85924
H	4.88102	-3.77893	-4.88124
C	3.94418	-2.36413	-3.53006
H	3.85062	-1.59785	-4.30880
C	4.03340	-1.17722	2.17045
C	5.34630	-0.76628	2.48413
H	5.68768	0.23658	2.20341
C	6.22693	-1.62294	3.16423
H	7.24226	-1.28442	3.39918
C	5.80945	-2.90792	3.54204
H	6.49678	-3.57635	4.07157
C	4.50666	-3.33027	3.23955
H	4.16278	-4.32875	3.52926
C	3.62707	-2.47108	2.56088
H	2.61255	-2.82572	2.34551
C	3.53013	2.16278	1.63215
C	3.72027	2.47618	2.99676
H	3.44630	1.74976	3.77102
C	4.25428	3.71513	3.38770
H	4.39459	3.93648	4.45151
C	4.60477	4.66668	2.41707
H	5.02047	5.63378	2.71963
C	4.42179	4.37063	1.05857
H	4.69505	5.10354	0.29179
C	3.89080	3.12919	0.66959
H	3.76844	2.92078	-0.39837
C	-3.61065	-1.98720	-2.18688
C	-6.36611	-1.79185	-2.84761
H	-7.42888	-1.71681	-3.10175
C	-5.40840	-1.96282	-3.85936
H	-5.72109	-2.02299	-4.90781
C	-4.04645	-2.05746	-3.52930
H	-3.31487	-2.18954	-4.33565
C	-5.95253	-1.72255	-1.50928
H	-6.69046	-1.59683	-0.70925
C	-4.58903	-1.81988	-1.18440
H	-4.29870	-1.77322	-0.12951
C	0.88180	4.71068	-1.15584
H	0.92020	4.31887	-0.13403
C	1.66238	5.83503	-1.46992
H	2.29221	6.28690	-0.69602
C	0.05706	4.10067	-2.12415
C	1.63308	6.37400	-2.76452
H	2.24037	7.25164	-3.01098
C	0.81688	5.78320	-3.74164
H	0.78429	6.19882	-4.75505
C	0.03941	4.65777	-3.42240
H	-0.59291	4.21284	-4.19998

3-M06

SCF Enrgy = -3036.36238947

Sn	-0.08721	0.01857	-3.50091
Sn	-0.81027	-2.25785	-1.82864
Sn	-0.53970	-2.48015	1.03208
Sn	0.04807	-0.00140	2.27330
Sn	-1.88989	1.73453	1.14407
Sn	-1.59607	1.78613	-1.73518
Sn	2.29103	0.46217	-1.86891
Sn	2.44982	0.79512	0.99552
C	0.11119	-4.15910	-2.42902
C	1.40055	-4.19302	-2.97238
H	1.91574	-3.26325	-3.22671
C	2.06983	-5.40106	-3.16508
H	3.08158	-5.39537	-3.56846
C	1.45135	-6.60044	-2.82545
H	1.97353	-7.54508	-2.96867
C	0.16089	-6.58825	-2.30040
H	-0.32759	-7.52444	-2.03369
C	-0.49812	-5.37791	-2.10202
H	-1.50287	-5.38180	-1.67284
C	-2.40847	-3.26060	1.85167
C	-2.73739	-4.60666	1.65350
H	-2.00678	-5.28430	1.20610
C	-3.99037	-5.09937	2.00867
H	-4.22921	-6.14867	1.84161
C	-4.94213	-4.24823	2.56381
H	-5.92650	-4.62986	2.82953
C	-4.63125	-2.90844	2.77547
H	-5.36655	-2.22727	3.20261
C	-3.37223	-2.42469	2.42632
H	-3.16242	-1.36379	2.58474
C	0.97386	-3.93354	1.64875
C	1.78245	-4.62066	0.73622
H	1.66395	-4.45969	-0.33569
C	2.75107	-5.52280	1.17307
H	3.35460	-6.05464	0.43748
C	2.93501	-5.74557	2.53427
H	3.69202	-6.44904	2.87740
C	2.14488	-5.06395	3.45782
H	2.28501	-5.23063	4.52474
C	1.17186	-4.17002	3.01618
H	0.56366	-3.64119	3.75369
C	0.16988	-0.15821	4.44965
C	1.39773	-0.39808	5.07865
H	2.30951	-0.49087	4.48401
C	1.47812	-0.53092	6.46286
H	2.44221	-0.71671	6.93348
C	0.32941	-0.42746	7.24145
H	0.39118	-0.52978	8.32338
C	-0.89951	-0.19554	6.63076
H	-1.80258	-0.11793	7.23402

C	-0.97664	-0.06399	5.24669
H	-1.95004	0.11139	4.78391
C	-3.91975	1.19692	1.75756
C	-4.29870	1.32617	3.10050
H	-3.59089	1.72995	3.82838
C	-5.57257	0.95881	3.52883
H	-5.84516	1.06491	4.57778
C	-6.49967	0.46665	2.61258
H	-7.49823	0.18582	2.94338
C	-6.14471	0.34416	1.27276
H	-6.86468	-0.01985	0.54002
C	-4.86524	0.70173	0.85205
H	-4.61744	0.60111	-0.20565
C	-1.61257	3.75130	1.93152
C	-2.62468	4.70489	1.77202
H	-3.59300	4.40748	1.36368
C	-2.41603	6.03691	2.12092
H	-3.21420	6.76537	1.98562
C	-1.18464	6.43938	2.63065
H	-1.01739	7.48276	2.89262
C	-0.16885	5.50366	2.80254
H	0.80232	5.80133	3.19630
C	-0.38691	4.17173	2.45937
H	0.43282	3.46172	2.59255
C	-3.71588	1.94741	-2.28498
C	-4.46133	3.07879	-1.92812
H	-3.95498	3.94545	-1.49638
C	-5.84212	3.11540	-2.10225
H	-6.40438	4.00211	-1.81279
C	-6.50617	2.01150	-2.63259
H	-7.58766	2.03308	-2.75697
C	-5.78247	0.88154	-3.00116
H	-6.29029	0.00920	-3.41046
C	-4.39856	0.85516	-2.83272
H	-3.85441	-0.05104	-3.11120
C	3.45801	2.21943	-2.47854
C	2.82041	3.35114	-3.00044
H	1.75057	3.32842	-3.22508
C	3.51855	4.54045	-3.20609
H	2.99115	5.41199	-3.59180
C	4.87445	4.61257	-2.90138
H	5.42122	5.54142	-3.05561
C	5.52977	3.49221	-2.39496
H	6.59048	3.54437	-2.15336
C	4.82473	2.31055	-2.18257
H	5.34666	1.44575	-1.76585
C	3.68719	-1.21624	-2.11482
C	3.74537	-2.25546	-1.17859
H	3.13445	-2.22345	-0.27314
C	4.58282	-3.35225	-1.35984
H	4.61261	-4.13208	-0.59907
C	5.37106	-3.44178	-2.50311
H	6.02718	-4.29813	-2.65113
C	5.31504	-2.42987	-3.45836
H	5.92573	-2.49526	-4.35799
C	4.48388	-1.32849	-3.26153
H	4.46139	-0.54034	-4.01684
C	4.10487	-0.41414	1.75518
C	5.41911	0.02968	1.56685
H	5.60317	1.02047	1.14543
C	6.50396	-0.77690	1.90109
H	7.51889	-0.41518	1.74250
C	6.29226	-2.04794	2.42828
H	7.14022	-2.68223	2.68085
C	4.99304	-2.50492	2.62709
H	4.80749	-3.49986	3.03053
C	3.91205	-1.69155	2.29406
H	2.90318	-2.08583	2.44256
C	2.98074	2.82896	1.60409
C	3.19612	3.10932	2.96033
H	3.09959	2.31409	3.70299
C	3.52486	4.39399	3.38713
H	3.68469	4.59028	4.44623
C	3.65255	5.42465	2.45820
H	3.91517	6.42828	2.78877
C	3.44360	5.16377	1.10769
H	3.54957	5.95665	0.36738
C	3.10680	3.87836	0.68681
H	2.94520	3.70269	-0.37718
C	-2.96208	-2.63417	-2.07025
C	-5.72638	-2.97199	-2.49987
H	-6.79427	-3.10684	-2.66492
C	-4.81218	-3.37196	-3.47151
H	-5.16445	-3.81902	-4.40022
C	-3.44580	-3.20508	-3.25477
H	-2.74412	-3.53059	-4.02575
C	-5.26672	-2.39757	-1.31855
H	-5.96611	-2.07826	-0.54604
C	-3.90012	-2.22700	-1.11412
H	-3.57425	-1.76973	-0.17757
C	0.02778	4.42498	-1.07587
H	0.30038	3.90267	-0.15619
C	0.55908	5.69420	-1.28692
H	1.21786	6.12738	-0.53448
C	-0.83866	3.83176	-2.00139
C	0.24366	6.39467	-2.44725
H	0.65649	7.38783	-2.61769
C	-0.60225	5.81716	-3.39122
H	-0.85024	6.35757	-4.30390
C	-1.13782	4.55042	-3.16642
H	-1.80565	4.11735	-3.91412

3-ωB97xD

SCF Energy = -3037.95545049

Sn	0.14198	0.38523	-3.38729
Sn	-2.25892	-0.33517	-1.98612
Sn	-2.42175	-0.98627	0.76596
Sn	-0.09489	-0.22892	2.12436
Sn	0.32958	2.41846	1.31870
Sn	0.70072	2.47895	-1.50235
Sn	1.70975	-1.50003	-1.89010
Sn	1.99117	-1.66517	0.93362
C	-3.30681	-2.02750	-2.88393
C	-2.58962	-3.06791	-3.48717
H	-1.51320	-2.98798	-3.62197
C	-3.22664	-4.23887	-3.89593
H	-2.63961	-5.03904	-4.33742
C	-4.59973	-4.38325	-3.71789
H	-5.09793	-5.29742	-4.02921
C	-5.33334	-3.35033	-3.13710
H	-6.40568	-3.45689	-2.99612
C	-4.68984	-2.18676	-2.72196
H	-5.27306	-1.39620	-2.25344
C	-4.07908	-0.03831	1.82126
C	-5.29167	-0.71846	1.98043
H	-5.40380	-1.72638	1.58675
C	-6.36329	-0.12832	2.64846
H	-7.29653	-0.67391	2.76058
C	-6.23991	1.15644	3.17093
H	-7.07604	1.61715	3.68986
C	-5.03913	1.84623	3.02644
H	-4.92158	2.84916	3.42665
C	-3.97224	1.24934	2.35921
H	-3.04764	1.81314	2.26417

C	-2.80233	-3.09150	1.17978
C	-3.04411	-4.04193	0.18086
H	-3.03984	-3.75404	-0.86652
C	-3.28958	-5.37559	0.50739
H	-3.48098	-6.09260	-0.28648
C	-3.29294	-5.78289	1.83815
H	-3.48040	-6.82284	2.09105
C	-3.05685	-4.84915	2.84544
H	-3.05555	-5.15726	3.88733
C	-2.81756	-3.51666	2.51689
H	-2.62763	-2.80439	3.31776
C	-0.39803	-0.67012	4.23392
C	0.27016	-1.73521	4.85023
H	0.98573	-2.33123	4.28710
C	0.01400	-2.06762	6.17941
H	0.54113	-2.89955	6.63821
C	-0.91974	-1.34122	6.91325
H	-1.12151	-1.60052	7.94875
C	-1.60139	-0.28665	6.31071
H	-2.34097	0.27671	6.87284
C	-1.34400	0.04319	4.98202
H	-1.90304	0.85660	4.52407
C	-1.24919	3.73394	2.04200
C	-1.51657	3.80205	3.41671
H	-0.92195	3.21740	4.11609
C	-2.54303	4.60260	3.91271
H	-2.73617	4.63550	4.98145
C	-3.32039	5.35866	3.03729
H	-4.12139	5.98463	3.42056
C	-3.06303	5.30880	1.67060
H	-3.65468	5.90202	0.97869
C	-2.03887	4.50125	1.17701
H	-1.86609	4.47771	0.10497
C	2.19890	3.15744	2.14508
C	2.61936	4.45861	1.84261
H	1.94508	5.14335	1.33185
C	3.90380	4.88996	2.16046
H	4.21519	5.89875	1.90406
C	4.79672	4.02015	2.78212
H	5.80678	4.34850	3.01097
C	4.39297	2.72735	3.10134
H	5.08139	2.03293	3.57348
C	3.10204	2.30628	2.78891
H	2.81809	1.28573	3.03189
C	-0.25910	4.37952	-2.00054
C	0.28488	5.59223	-1.55459
H	1.26058	5.60004	-1.07163
C	-0.40405	6.79261	-1.70988
H	0.03353	7.71991	-1.34964
C	-1.66020	6.80134	-2.31325
H	-2.20584	7.73456	-2.42338
C	-2.21183	5.60908	-2.77347
H	-3.19346	5.59840	-3.23829
C	-1.51325	4.41172	-2.62207
H	-1.97573	3.49261	-2.97477
C	3.81167	-1.48944	-2.48326
C	4.42894	-0.29591	-2.87627
H	3.83766	0.60534	-3.02145
C	5.81058	-0.22179	-3.04878
H	6.26517	0.72550	-3.32435
C	6.59847	-1.35141	-2.84530
H	7.67633	-1.29563	-2.97148
C	5.99912	-2.55478	-2.47722
H	6.60919	-3.43991	-2.31772
C	4.61975	-2.61891	-2.29454
H	4.16834	-3.55966	-1.98454
C	1.01442	-3.52005	-2.34500
C	0.10998	-4.18006	-1.50457
H	-0.21950	-3.71922	-0.57633
C	-0.39496	-5.43676	-1.82508
H	-1.08824	-5.92134	-1.14466
C	-0.01225	-6.05703	-3.01089
H	-0.40618	-7.03686	-3.26693
C	0.87889	-5.41476	-3.86764
H	1.18124	-5.89196	-4.79621
C	1.38831	-4.16081	-3.53334
H	2.08975	-3.67823	-4.21103
C	1.88485	-3.71887	1.65373
C	3.04824	-4.49142	1.75080
H	4.01283	-4.05360	1.50249
C	2.99325	-5.81977	2.16837
H	3.90741	-6.40372	2.23530
C	1.77002	-6.39950	2.49624
H	1.72689	-7.43668	2.81721
C	0.60413	-5.64351	2.41173
H	-0.35981	-6.07706	2.66219
C	0.66649	-4.31554	1.99711
H	-0.25988	-3.74948	1.94339
C	3.94729	-1.06032	1.68448
C	4.19657	-1.12835	3.06262
H	3.40404	-1.43102	3.74473
C	5.44717	-0.81028	3.58704
H	5.61531	-0.86772	4.65901
C	6.47969	-0.42017	2.73605
H	7.45707	-0.17327	3.14127
C	6.25094	-0.35085	1.36559
H	7.04846	-0.05653	0.68877
C	4.99630	-0.66785	0.84540
H	4.84931	-0.60471	-0.22836
C	-3.66559	1.33275	-2.11077
C	-5.34889	3.58244	-2.32463
H	-5.99983	4.44859	-2.40704
C	-5.23035	2.69139	-3.38897
H	-5.78836	2.86187	-4.30598
C	-4.39927	1.57729	-3.27884
H	-4.32548	0.88924	-4.11864
C	-4.62788	3.35677	-1.15563
H	-4.70636	4.03985	-0.31525
C	-3.79304	2.24750	-1.05856
H	-3.23571	2.10738	-0.13595
C	3.73182	2.30164	-0.68952
H	3.37766	1.55347	0.01593
C	5.09252	2.59065	-0.70283
H	5.75304	2.07306	-0.01415
C	2.83424	2.96115	-1.53795
C	5.59006	3.54288	-1.58828
H	6.65180	3.77394	-1.60248
C	4.71874	4.20093	-2.45269
H	5.09995	4.94406	-3.14846
C	3.35451	3.91353	-2.42287
H	2.68721	4.44817	-3.09598

3-BP86(D3)

SCF (BP86) Energy = -3038.87849082
Enthalpy 0K = -3037.735343
Enthalpy 298K = -3037.643983
Free Energy 298K = -3037.877938
Lowest Frequency = 16.3516 cm^{-1}
Second Frequency = 18.3460 cm^{-1}

Sn	0.70249	0.13645	-3.41944
Sn	-1.62624	1.43215	-2.24577
Sn	-2.44410	1.09614	0.47197
Sn	-0.40451	-0.04054	2.08997
Sn	1.86087	1.53336	1.47612

Sn	2.43576	1.18086	-1.33190
Sn	0.29512	-2.30888	-1.88580
Sn	0.13605	-2.58819	0.97702
C	-3.50915	0.88640	-3.24824
C	-3.64816	-0.40873	-3.79473
H	-2.78105	-1.07619	-3.86448
C	-4.90260	-0.89194	-4.20743
H	-4.98531	-1.91579	-4.58813
C	-6.04009	-0.07567	-4.09469
H	-7.02152	-0.45207	-4.40548
C	-5.91678	1.22478	-3.57388
H	-6.80258	1.86403	-3.47931
C	-4.66336	1.69708	-3.14844
H	-4.58994	2.70062	-2.71071
C	-2.98943	2.87715	1.64908
C	-4.25377	2.95375	2.27275
H	-5.00242	2.17407	2.09131
C	-4.56516	4.00805	3.14911
H	-5.54996	4.04225	3.63050
C	-3.61695	5.01037	3.41176
H	-3.85702	5.83103	4.09785
C	-2.35847	4.95450	2.78999
H	-1.60286	5.72210	2.98557
C	-2.04913	3.89542	1.91972
H	-1.04991	3.86840	1.47442
C	-4.21735	-0.17372	0.77392
C	-4.97983	-0.70023	-0.29234
H	-4.71132	-0.48198	-1.33037
C	-6.09732	-1.51738	-0.04222
H	-6.68074	-1.90187	-0.88697
C	-6.46808	-1.82795	1.27655
H	-7.33595	-2.46933	1.46899
C	-5.71988	-1.31053	2.34795
H	-5.99029	-1.55234	3.38202
C	-4.60680	-0.48940	2.09868
H	-4.03608	-0.10455	2.95126
C	-1.48946	-0.06709	4.00217
C	-1.97449	-1.28998	4.51692
H	-1.64295	-2.24235	4.08573
C	-2.93218	-1.30450	5.54640
H	-3.30947	-2.26263	5.92216
C	-3.42186	-0.09664	6.07158
H	-4.18125	-0.10805	6.86183
C	-2.94310	1.12658	5.57089
H	-3.33310	2.07463	5.95794
C	-1.98354	1.14191	4.54453
H	-1.66096	2.10766	4.13757
C	1.62219	3.63180	2.08691
C	1.16377	3.93559	3.38856
H	0.92048	3.12678	4.08882
C	0.99718	5.26764	3.80357
H	0.63454	5.48187	4.81541
C	1.27665	6.32178	2.91656
H	1.14179	7.36098	3.23743
C	1.72617	6.03488	1.61757
H	1.95581	6.84576	0.91660
C	1.89735	4.70085	1.20536
H	2.24675	4.50802	0.18704
C	3.66361	0.73031	2.43301
C	4.90954	1.35323	2.19949
H	4.95043	2.33059	1.70218
C	6.10931	0.72376	2.56835
H	7.06821	1.21434	2.36479
C	6.08163	-0.54601	3.16962
H	7.01911	-1.04867	3.43341
C	4.85084	-1.17393	3.41860
H	4.81142	-2.17239	3.86660
C	3.65302	-0.53552	3.05529
H	2.70722	-1.06050	3.23143
C	3.24002	3.18507	-1.78333
C	4.46020	3.61404	-1.21093
H	5.09997	2.88971	-0.69056
C	4.85851	4.95993	-1.28040
H	5.80250	5.27574	-0.82050
C	4.03597	5.90565	-1.91849
H	4.33514	6.95955	-1.95375
C	2.83012	5.49317	-2.50955
H	2.17270	6.22050	-2.99907
C	2.44425	4.14213	-2.44954
H	1.48727	3.84829	-2.89589
C	1.88832	-3.77776	-2.28238
C	3.21060	-3.33750	-2.51096
H	3.42320	-2.27111	-2.64830
C	4.28676	-4.24288	-2.51098
H	5.30613	-3.86568	-2.64745
C	4.05167	-5.61153	-2.29991
H	4.88890	-6.31901	-2.28791
C	2.73778	-6.07127	-2.09919
H	2.54944	-7.13864	-1.93323
C	1.66773	-5.16037	-2.08503
H	0.65137	-5.52877	-1.89663
C	-1.55947	-3.34378	-2.46024
C	-2.77230	-3.04325	-1.80227
H	-2.79651	-2.31252	-0.98504
C	-3.97671	-3.65790	-2.17740
H	-4.89607	-3.40575	-1.63963
C	-3.99164	-4.58328	-3.23403
H	-4.93037	-5.06497	-3.53121
C	-2.79635	-4.89148	-3.90612
H	-2.80136	-5.61331	-4.73178
C	-1.59104	-4.27861	-3.51874
H	-0.66455	-4.53823	-4.04643
C	-1.45345	-3.93100	1.68753
C	-1.13087	-5.22083	2.16351
H	-0.08543	-5.55201	2.18099
C	-2.13492	-6.08711	2.63129
H	-1.86608	-7.08495	2.99846
C	-3.47820	-5.67541	2.63024
H	-4.26091	-6.35096	2.99467
C	-3.81248	-4.39311	2.16433
H	-4.85180	-4.04810	2.16263
C	-2.80730	-3.53030	1.69778
H	-3.09819	-2.53042	1.35964
C	1.89801	-3.52801	1.90546
C	1.91868	-3.69410	3.30968
H	1.08414	-3.32108	3.91744
C	2.99366	-4.33540	3.94932
H	2.99152	-4.44952	5.03960
C	4.06905	-4.82891	3.18953
H	4.90800	-5.33079	3.68498
C	4.06025	-4.67497	1.79420
H	4.88610	-5.06285	1.18693
C	2.98511	-4.02888	1.15770
H	3.00918	-3.92166	0.06963
C	-1.49412	3.62896	-2.32540
C	-1.24882	6.45737	-2.36026
H	-1.15881	7.54966	-2.37251
C	-2.03701	5.80300	-3.32245
H	-2.56041	6.38548	-4.09029
C	-2.15876	4.40167	-3.30294
H	-2.78254	3.90810	-4.05881
C	-0.57927	5.70460	-1.38142
H	0.04000	6.19348	-0.62217
C	-0.70164	4.30647	-1.37207

H -0.14868 3.74376 -0.60853
C 4.34694 -1.10648 -0.24487
H 3.49041 -1.36810 0.38612
C 5.51743 -1.86860 -0.11572
H 5.54312 -2.68782 0.60906
C 4.27416 -0.01992 -1.14311
C 6.63942 -1.56957 -0.90563
H 7.55630 -2.16241 -0.80732
C 6.58279 -0.50333 -1.81898
H 7.45431 -0.26523 -2.44087
C 5.41085 0.26680 -1.93113
H 5.38943 1.10776 -2.63580

3-BLYP(D3)

SCF Energy = -3037.46524203

Sn 0.15403 0.15277 -3.43784
Sn 2.30568 1.16054 -1.70220
Sn 1.96683 1.53393 1.13859
Sn -0.19128 -0.04198 2.13015
Sn 0.24552 -2.61177 0.95555
Sn 0.05368 -2.37128 -1.92193
Sn -2.00732 1.44471 -1.88877
Sn -2.56217 0.97450 0.91582
C 3.01142 3.17486 -2.27684
C 2.08720 4.17847 -2.64635
H 1.03435 3.92864 -2.79693
C 2.48430 5.52023 -2.79318
H 1.73668 6.27777 -3.04690
C 3.82834 5.88131 -2.59015
H 4.14142 6.92474 -2.69600
C 4.77133 4.89087 -2.25338
H 5.82098 5.16366 -2.10191
C 4.36443 3.55179 -2.09623
H 5.10700 2.79744 -1.81632
C 3.79270 1.15805 2.31061
C 4.63580 2.22676 2.69351
H 4.37181 3.25556 2.42817
C 5.81489 1.98934 3.42591
H 6.45472 2.82990 3.71398
C 6.17073 0.67742 3.78883
H 7.08775 0.49415 4.35744
C 5.34061 -0.39600 3.41856
H 5.59801 -1.42278 3.69179
C 4.16350 -0.15500 2.68613
H 3.53863 -1.00877 2.41452
C 1.53488 3.66817 1.48848
C 2.32742 4.67049 0.87536
H 3.15598 4.39842 0.21832
C 2.05469 6.03671 1.07737
H 2.67468 6.78715 0.57800
C 0.97712 6.42868 1.89256
H 0.75706 7.49024 2.04224
C 0.17400 5.44804 2.50202
H -0.67859 5.73616 3.12248
C 0.45317 4.08301 2.30161
H -0.19639 3.34466 2.78104
C -0.19212 -0.00250 4.33321
C -1.32289 0.42843 5.06612
H -2.22002 0.77635 4.54476
C -1.30846 0.44282 6.47428
H -2.19263 0.78237 7.02313
C -0.16036 0.02908 7.17298
H -0.14849 0.03987 8.26710
C 0.97668 -0.38979 6.45742
H 1.87856 -0.70119 6.99387
C 0.96158 -0.40337 5.05038
H 1.86342 -0.71627 4.51545
C 2.21625 -3.27393 1.69827
C 2.41610 -3.38038 3.09826
H 1.59910 -3.14728 3.78849
C 3.65932 -3.77076 3.63093
H 3.79182 -3.83612 4.71532
C 4.73040 -4.06893 2.76816
H 5.69869 -4.37208 3.17788
C 4.54780 -3.97455 1.37733
H 5.36834 -4.21508 0.69561
C 3.30476 -3.57796 0.84691
H 3.20104 -3.50722 -0.23660
C -1.09101 -4.17759 1.73585
C -0.56915 -5.30502 2.41384
H 0.50646 -5.38596 2.59680
C -1.41758 -6.33469 2.86380
H -0.99435 -7.19806 3.38779
C -2.80436 -6.25655 2.63996
H -3.46370 -7.05807 2.98767
C -3.33718 -5.14296 1.96668
H -4.41287 -5.06118 1.78871
C -2.48706 -4.11566 1.51963
H -2.93138 -3.26421 1.00413
C 1.67709 -3.77574 -2.44880
C 1.60620 -5.13602 -2.05669
H 0.68452 -5.53092 -1.61699
C 2.71387 -5.99229 -2.19703
H 2.63928 -7.03687 -1.87811
C 3.92187 -5.50088 -2.72661
H 4.78961 -6.16135 -2.81976
C 4.00987 -4.15631 -3.12854
H 4.94565 -3.75424 -3.52494
C 2.89532 -3.30578 -2.99353
H 3.00313 -2.25934 -3.28989
C -4.00393 0.94454 -2.69930
C -4.21416 -0.30463 -3.32860
H -3.36616 -0.95829 -3.55049
C -5.51008 -0.75834 -3.63971
H -5.64159 -1.74602 -4.09114
C -6.62590 0.04523 -3.34427
H -7.63560 -0.30646 -3.57752
C -6.43731 1.30423 -2.74271
H -7.30129 1.93445 -2.50870
C -5.13991 1.74386 -2.41842
H -5.01724 2.71160 -1.92146
C -1.92353 3.65050 -2.01089
C -1.00827 4.38054 -1.21507
H -0.35219 3.86792 -0.50694
C -0.90453 5.78145 -1.31266
H -0.18310 6.30723 -0.68396
C -1.71977 6.48217 -2.21960
H -1.64349 7.57095 -2.30049
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3-PBE(D3)

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1-IGLOII

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2-IGLOII

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3-IGLOII

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Sn -0.08910 -0.07906  2.16040
Sn  1.39877 -2.19298  1.06929
Sn  0.96504 -2.19103 -1.75554
Sn  1.68273  1.94692 -1.58072
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H   6.28634  3.70757  1.87662
C   5.42252  3.19535  3.81421
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H	2.55497	-7.08141	2.82396
C	2.01442	-5.07153	2.17740
H	3.05571	-4.78054	1.99508
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H	-1.07136	-2.25745	4.29517
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H	-1.93651	-0.15951	7.99962
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H	-6.29948	-3.29440	-4.83156
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H	2.47711	-5.08695	-2.03831
C	4.59819	-4.79364	-2.40914
H	4.83021	-5.86305	-2.33790

In order to understand the origin of the broad absorbances in **1**–**3**, TD-DFT calculations at the BPBE-GD3/IGLOII//BPBE-GD3/SDD40-42 level of theory were carried out. Calculation of the 50 lowest energy transitions for **1**–**3** predict electronic spectra with excitations from 582-413 nm for **1**, 600-393 nm for **2** and 508-355 nm for **3**. The calculated transitions are closely spaced in energy but show very low oscillator strength resulting in broad absorption bands rather than isolated absorption maxima. The transitions essentially represent symmetry forbidden excitations from the Sn σ-skeleton into π*-orbitals located at the phenyl substituents and reproduce the bathochromic shift observed for bicyclo[2.2.2]-dianion **2** with respect to the monoanion **3** and bicyclo[2.2.1]-dianion **1**.

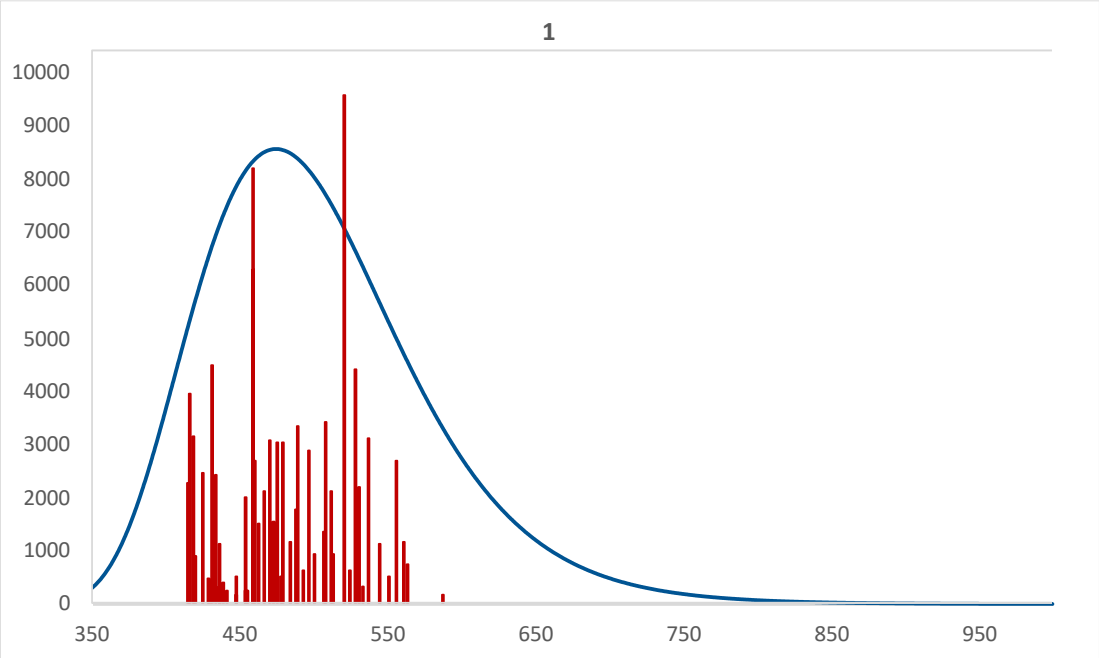

Figure S5.3 Calculated UV/Vis spectrum for **1**. (BPBE-GD3/IGLOII//BPBE-GD3/SDD level of theory, first 50 excitations)

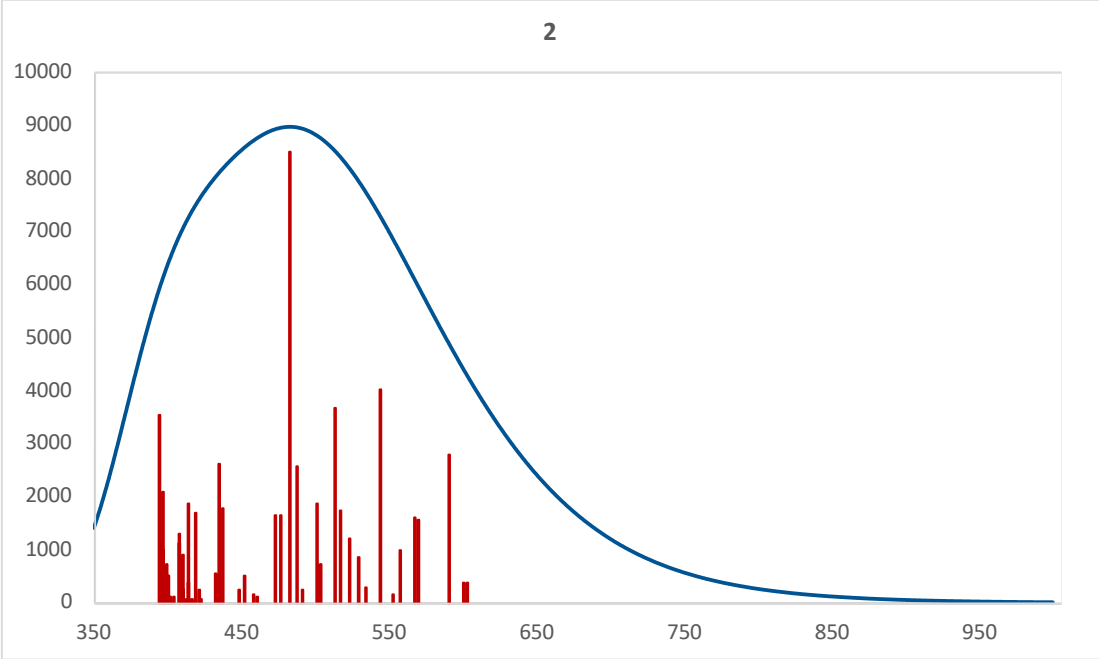

Figure S5.4 Calculated UV/Vis spectrum for **2**. (BPBE-GD3/IGLOII//BPBE-GD3/SDD level of theory, first 50 excitations)

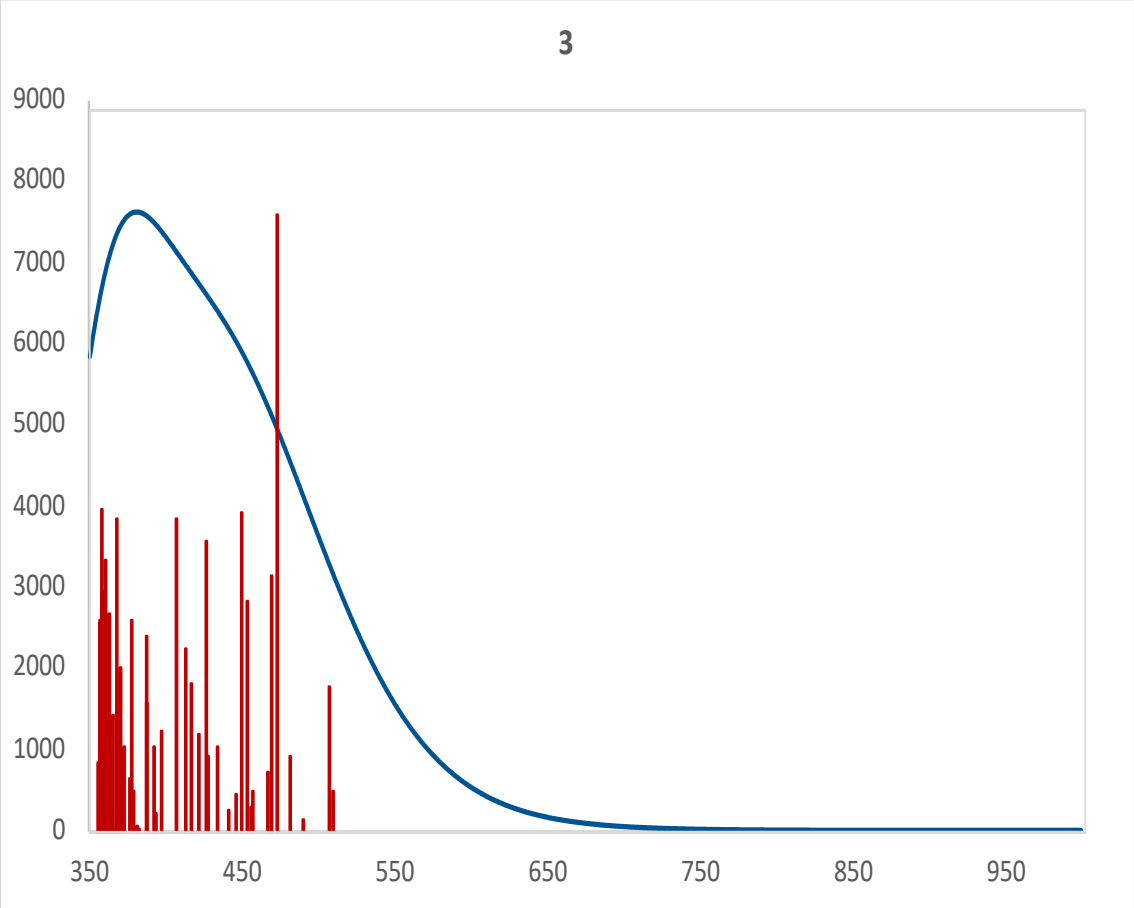

Figure S5.5 Calculated UV/Vis spectrum for **3**. (BPBE-GD3/IGLOII//BPBE-GD3/SDD level of theory, first 50 excitations)

6. References

1.) (a) R. H. Blessing, *Acta Crystallogr. Sect. A* 1995, **A51**, 33–38. (b) G. M. Sheldrick, SADABS Version 2.10 Siemens Area Detector Correction., Universitaet Goettingen, Goettingen, Germany, 2003.

2.) (a) G. M. Sheldrick, SHELXTL Version 6.1. Bruker AXS, Inc., Madison, WI, 2002. (b) G. M. Sheldrick SHELXS97 and SHELXL97, Universitaet Goettingen, Goettingen, Germany, 2002.

3.) (a) A. L. Spek *J. Appl. Crystallogr*. 2003, **36**, 7–13. (b) A. L. Spek *Acta Crystallogr. Sect. D* Biol. Crystallogr. 2009, **65**, 148–155.

4.) O. V. Dolomanov, R. J. Bourhis, J. A. K. Gildea, H. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339–341.

5.) (a) Gaussian 09, Revision D.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, T. Keith, 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013. (b) J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett*. **77**, 3865-3868. (c) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys*., 2010, **132**, 154104; (d) W. Kutzelnigg, U. Fleischer and M. Schindler, The IGLO-Method: Ab-initio Calculation and Interpretation of NMR Chemical Shifts and Magnetic Susceptibilities, In: Deuterium and Shift Calculation. NMR Basic Principles and Progress, vol 23. Springer, Berlin, Heidelberg, 2011, 165–262

6.) D. Andrae, U. Häußermann, M. Dolg, H. Stoll, and H. Preuß, *Theor. Chim. Acta*., 1990, **77**, 123−141.

7.) (a) P. C. Hariharan, and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213−222. (b) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261.

8.) A. Höllwarth, M. Böhme, S. Dapprich, A. Ehlers, A. Gobbi, V. Jonas, K. Köhler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett*., 1993, **208**, 237-240.

9.) (a) A. D. Becke, *Phys. Rev. A: At., Mol., Opt. Phys.* 1988, **38**, 3098-3100; (b) J. P. Perdew, *Phys. Rev. B: Condens. Matter Mater. Phys.* **33**, 1986, 8822−8824.

10.) C. Lee, W. Yang, and R. G. Parr, R. G., *Phys. Rev. B*, 1988, **37**, 785-789.

11.) A. D. Becke, *J. Chem. Phys*., 1993, **98**, 5648-5652.

12.) J.-D. Chai, and M. Head-Gordon, *PCCP*, 2008, **10**, 6615-6620.

13.) Y. Zhao, and D. G. Truhlar, *Acc. Chem. Res*., 2008, **41**, 157-167.

14.) A. Grimme, J. Antony, S. Ehrlich, and H. Krieg, H., *J. Chem. Phys*., 2010, **132**, 154104.

15.) W. Kutzelnigg, U. Fleischer and M. Schindler, The IGLO-Method: Ab-initio Calculation and Interpretation of NMR Chemical Shifts and Magnetic Susceptibilities, in: In: Deuterium and Shift Calculation. NMR Basic Principles and Progress, vol 23. Springer, Berlin, Heidelberg, 2011, pp. 165–262