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Supporting Information for the Paper Entitled:

Synthesis, Isolation and Characterization of a Stable Lithium Stannenolate. A Keto or an Enol Tautomer?

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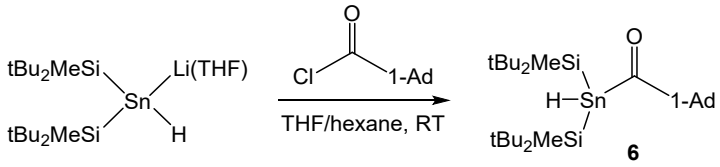
1. Experimental – general

Standard Schlenk techniques were used for all syntheses and all sample manipulations. Solvents were dried and kept over anhydrous $CaCl_2$, filtered, degassed, kept on n-BuLi (except THF which was kept over Ph_3CLi) in vacuum and were distilled prior to use. 1-adamantanecarbonyl chloride was sublimed and stored in vacuum prior to use. 12-crown-4 ether was dried in hexane solution over Li metal, filtered, and stored in vacuum prior to use. All other commercially available reagents were degassed from air and used without additional purification. LDA,[1] $tBu_2MeSiLi$[2] and $(tBu_2MeSi)_2SnHLi(THF)$[3] were synthesized according to literature procedures. NMR spectra were recorded on a Bruker Avance 600 instrument. All NMR samples were measured at room temperature in benzene or THF solutions in Young vacuum NMR tubes equipped with DMSO-d_6 capillary in order to provide an external lock frequency signal. ^{1}H and ^{13}C NMR spectra were referenced to benzene solvent resonance ($\delta(^{1}H)$ = 7.16 ppm, $\delta(^{13}C)$ = 128.0 ppm). ^{119}Sn NMR chemical shifts were referenced to $SnMe_4$ as an external standard. ^{29}Si chemical shifts were referenced to tetramethylsilane (TMS) as an external standard. The INEPT pulse sequence was used to enhance ^{29}Si NMR signals.[4] If not stated otherwise, the NMR experiments were carried out ^{1}H decoupled. UV-Vis absorption spectra were measured with Evolution 201 spectrometer (Thermo Scientific) in a quartz glass vacuum cuvette. Infrared spectroscopy was carried out on a Bruker Alpha IR spectrometer. High-resolution mass spectrometry (HRMS) measurements were performed on a Bruker Maxis Impact mass spectrometer using APCI (Atmospheric Pressure Chemical Ionization) technique in a positive ion mode. 1-Ad = 1-adamantyl.

2. Synthesis of acylstannane 6



Scheme 1. Synthesis of acylstannane **6**.

An hexane solution (3 ml) of 1-adamantanecarbonyl chloride (0.22 gr, 1.10 mmol) was added to a THF solution (20 ml) of hydrido stannyl lithium (0.58 gr, 1.13 mmol) at RT. The reaction mixture was stirred for 15 minutes at RT. All the volatiles were evaporated under vacuum (0.2 Torr) at RT to dryness. 20 ml of hexane were added to the residue and the organic phase was separated from

the salt by centrifugation. Evaporation of the solvent under vacuum (0.2 Torr) at RT yields yellow oil of acylstannane **6** (Scheme 1) in 90% yield (0.59 gr, 0.99 mmol), which was characterized by NMR, UV-Vis and IR spectroscopy. Acylstannane **6** was used in the next step without additional purification.

NMR of **6** (in benzene with DMSO-d_6 capillary, 25 °C), δ in ppm: ^{1}H NMR: δ = 0.37 (s, 6H, tBu_2MeSi); 1.15 (s, 18H, tBu_2MeSi); 1.16 (s, 18H, tBu_2MeSi); 1.59, 1.96, 2.00 (15H, 1-Ad); 4.96 (s, 1H, Sn-H), $J(^{119/117}Sn\text{-}^{1}H)$ = 1074/1024 Hz. ^{13}C NMR: δ = -3.5 (tBu_2MeSi); 29.1, 28.8 (tBu_2MeSi); 28.2, 36.6, 37.7, 54.7 (1-Ad); 252.9 (C=O). ^{29}Si NMR: δ = 28.0 (tBu_2MeSi), $J(^{117/119}Sn\text{-}^{29}Si$ = 398/380 Hz). ^{119}Sn{^{1}H} NMR: δ = -512.5. ^{119}Sn NMR: δ = -512.5 (d, $J(^{119}Sn\text{-}^{1}H)$ = 1074 Hz). (see Figures 1-5).

UV-Vis (hexane): λ [nm] (ε [$L\cdot mol^{-1}\cdot cm^{-1}$]) = 388 (ε = 595).

IR (neat): ν(C=O) = 1633 cm^{-1}.

HRMS (APCI positive ion; benzene): m/z calc. for [$C_{29}H_{58}OSi_2Sn$ - H]: 597.2969. Found: 597.3000 $[M - H]^+$.

3. Synthesis of stannenolates 7a and 7b

Method A: Reaction of acylstannane **6** with LDA

A THF solution (5 ml) of LDA[1] (59 mg, 0.55 mmol) was added to a THF solution (10 ml) of acylstannane **6** (300 mg, 0.51 mmol) at RT. The solution color turned violet after several minutes. The reaction mixture was stirred for 15 minutes at RT. All the volatiles were evaporated under vacuum (0.2 Torr) at RT and the residue was dissolved in hexane (20 ml). Upon concentration of the hexane solution, violet crystals of stannenolate **7a** were obtained in 82% yield (370 mg, 0.42 mmol), which disappointingly were not suitable for X-ray diffraction analysis. **7a** was characterized by NMR spectroscopy and UV-Vis spectroscopy (see below). Addition of one equivalent of 12-crown-4 (77 mg, 0.44 mmol) to **7a** in hexane (3 ml) followed by recrystallization from THF at RT yields violet crystals of stannenolate **7b**. The molecular structure of **7b** was determined by X-ray crystallography.

Method B: Reaction of acylstannane **6** with tBu_2MeSiLi

A THF solution (2 ml) of tBu_2MeSiLi[2] (26 mg, 0.16 mmol) was added to a THF solution (5 ml) of acylstannane **5** (88 mg, 0.14 mmol) at RT. The solution color immediately changed to violet. All

the volatiles were evaporated under vacuum (0.2 Torr) at RT and the residue was dissolved in hexane (10 ml). Upon concentration of the hexane solution, violet crystals of stannenolate **7a** were obtained. The formation of **7a** was confirmed by NMR spectroscopy.

NMR of **7a**, δ in ppm: ^{1}H NMR (in benzene with DMSO-d_6 capillary, 25 °C): δ = 0.65 (s, 6H, tBu_2MeSi); 1.46 (s, 36H, tBu_2MeSi); 1.73, 1.77, 2.10 (15H, 1-Ad). ^{13}C NMR (in THF with DMSO-d_6 capillary, 25 °C): δ = -1.8 (tBu_2MeSi); 30.4 (tBu_2MeSi); 28.9, 37.2, 38.4, 55.3 (1-Ad); 290.7 (C=O). ^{29}Si NMR (in THF with DMSO-d_6 capillary, 25 °C): δ = 21.6 (tBu_2MeSi), J($^{117/119}$Sn-^{29}Si = 590/564 Hz). ^{119}Sn{^{1}H} NMR (in THF with DMSO-d_6 capillary, 25 °C): δ = -432.8. (see Figures 6-9).

UV-Vis of **7a** (hexane): λ [nm] (ε [L·mol^{-1}·cm^{-1}]) = 273 (ε = 6930), 504 (ε = 850).

4. Synthesis of deuterated acylstannane 14

Degassed D_2O (ca. 0.1 ml) was added to a THF solution (0.5 ml) of **7a** (49 mg, 0.056 mmol) at RT. The solution color changed immediately from violet to yellow. All the volatiles were evaporated under vacuum (0.2 Torr) at RT. The residue was extracted with hexane (3 ml) from the resulting salt. Evaporation of hexane under vacuum (0.2 Torr) at RT, yields yellow oil of deuterated acylstannane **14**, in 94% yield (30 mg, 0.05 mmol). The formation of **14** was confirmed by ^{119}Sn NMR spectroscopy. The ^{119}Sn NMR spectrum of **14** shows, as expected, a triplet signal at -514 ppm with a J(^{119}Sn-D) coupling constant of 166 Hz (Figure 10).

HRMS (APCI positive ion; hexane): m/z calc. for [$C_{29}H_{57}DOSi_2Sn$ - D]: 597.2969. Found: 597.2785 [M - D]$^{+}$.

5. Synthesis of methylated acylstannane 15

An excess of MeCl gas was added via a rubber balloon to a THF solution (0.5 ml) of **7a** (62 mg, 0.069 mmol) at -196 °C. The reaction mixture was allowed to warm to RT, during which time the solution color turned from violet to yellow. All the volatiles were evaporated under vacuum (0.2 Torr) at RT. The residue was extracted with hexane (3 ml) from the resulting salt. Evaporation of hexane under vacuum (0.2 Torr) at RT yields yellow oil of methylated acylstannane **15** in 92% yield (39 mg, 0.064 mmol). Acylstannane **15** was characterized by NMR spectroscopy.

NMR of **15** (in benzene with DMSO-d_6 capillary, 25 °C), δ in ppm: ^{1}H NMR: δ = 0.37 (s, 6H, tBu_2MeSi); δ = 0.84 (s, 3H, MeSn); 1.11 (s, 18H, tBu_2MeSi); 1.13 (s, 18H, tBu_2MeSi); 1.61, 1.93, 1.96 (15H, 1-Ad). ^{13}C NMR: δ = -3.9 (tBu_2MeSi); -2.7 (MeSn); 29.5, 29.6 (tBu_2MeSi); 28.1, 36.5, 37.5, 55.5 (1-Ad); 254.4 (C=O). ^{29}Si NMR: δ = 25.3 (tBu_2MeSi), J($^{119/117}$Sn-^{29}Si = 392/374 Hz). ^{119}Sn{^{1}H} NMR: δ = -322.4. (see Figures 11-14).

HRMS (APCI positive ion; benzene): m/z calc. for [$C_{30}H_{60}OSi_2Sn$ + H]: 613.3282. Found: 613.3234 $[M + H]^+$.

6. Synthesis of silylated acylstannane 16

Method A: Reaction of stannenolate **7a** with Me_3SiCl

Me_3SiCl (0.2 ml, 1.57 mmol) was added to THF solution (0.5 ml) of stannenolate **7a** (56 mg, 0.063 mmol) at RT. The solution color changed immediately from violet to yellow. All the volatiles were evaporated under vacuum (0.2 Torr) at RT. The residue was extracted with hexane (3 ml) from the resulting salt. Evaporation of hexane under vacuum (0.2 Torr) at RT yields yellow oil of silylated acylstannane **16**, in 87% yield (36 mg, 0.055 mmol). Acylstannane **16** was characterized by NMR spectroscopy.

NMR of **16** (in benzene with DMSO-d_6 capillary, 25 °C), δ in ppm: ^{1}H NMR: δ = 0.49 (s, 6H, tBu_2MeSi); δ = 0.60 (s, 9H, Me_3Si); 1.13 (s, 18H, tBu_2MeSi); 1.14 (s, 18H, tBu_2MeSi); 1.62, 1.89, 1.97 (15H, 1-Ad). ^{13}C NMR: δ = -1.8 (tBu_2MeSi); 5.1 (Me_3Si) 30.2, 30.3 (tBu_2MeSi); 28.2, 36.6, 38.4, 53.4 (1-Ad); 254.7 (C=O). ^{29}Si NMR: δ = -8.4 (Me_3Si), J($^{119/117}$Sn -^{29}Si) = 248/238 Hz; 31.1 (tBu_2MeSi), J($^{119/117}$Sn-^{29}Si = 300/287 Hz). ^{119}Sn{^{1}H} NMR: δ = -450.2. (see Figures 15-18).

HRMS (APCI positive ion; benzene): m/z calc. for [$C_{32}H_{66}OSi_3Sn$ + H]: 671.3521. Found: 671.3501 $[M + H]^+$.

Method B: Reaction of stannenolate **7a** with Me_3SiOTf

Hexane solution (0.5 ml) of Me_3SiOTf (36 mg, 0.16 mmol) was added to a THF solution (0.5 ml) of stannenolate **7a** (26 mg, 0.029 mmol) at RT. The solution color changed immediately from violet to yellow. According to NMR spectroscopy acylstannae **16** was obtained quantitatively.

7. NMR spectra

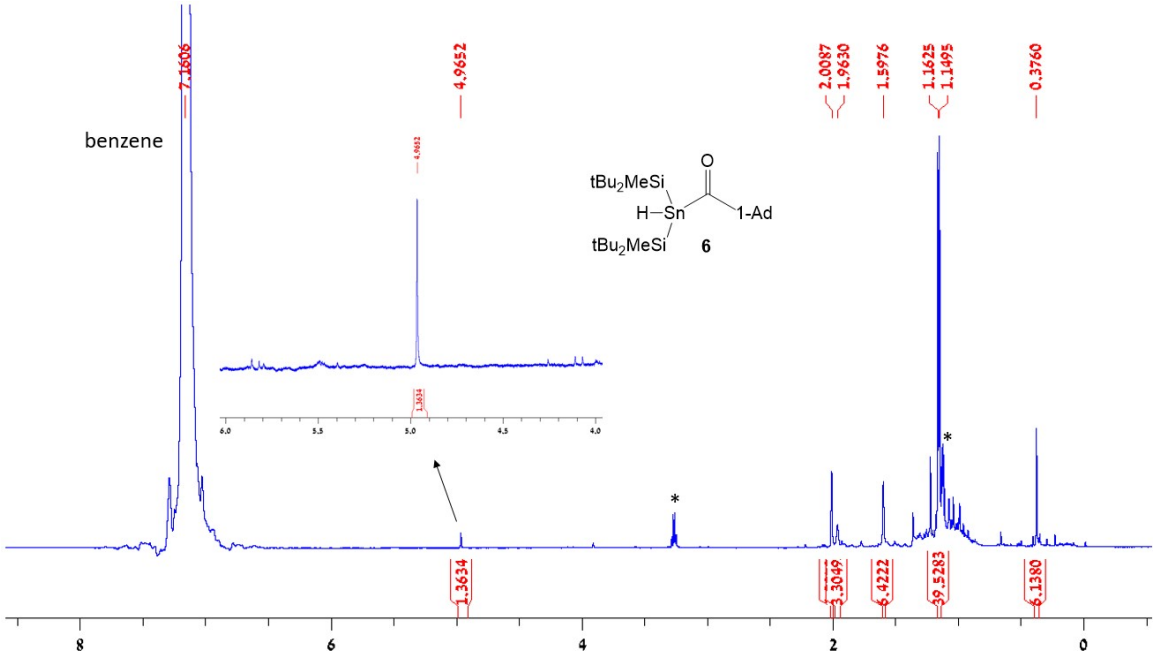


Figure 1. ^{1}H NMR spectrum of **6** in benzene (* impurity of Et_2O).

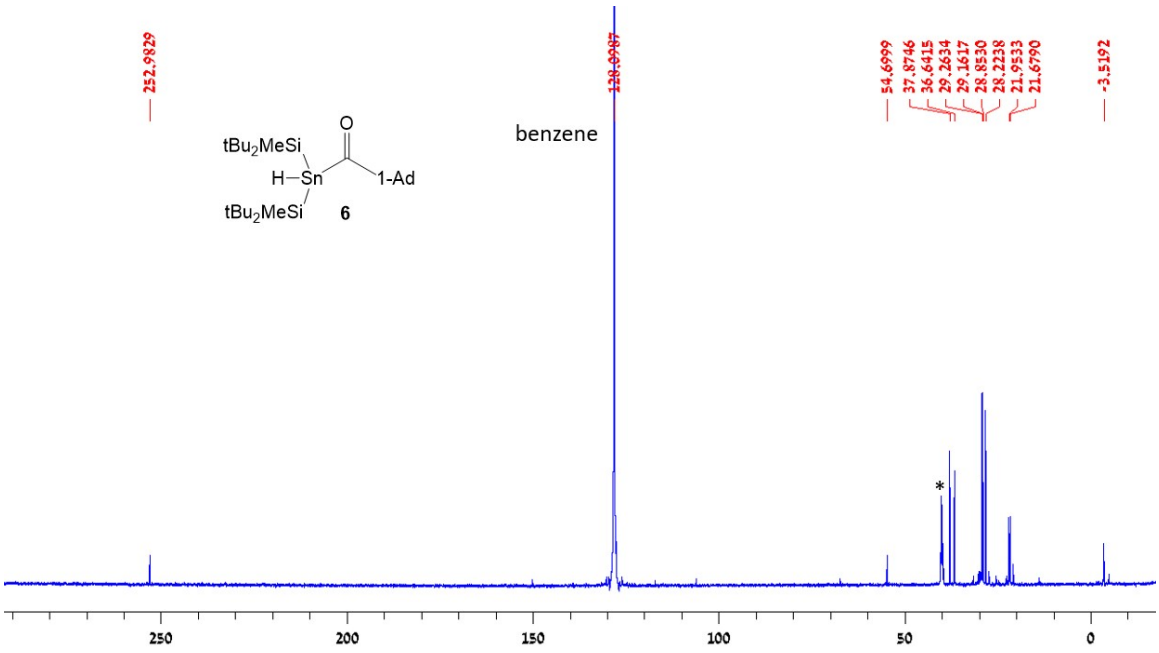


Figure 2. ^{13}C NMR spectrum of **6** in benzene (* DMSO-d_6 capillary).

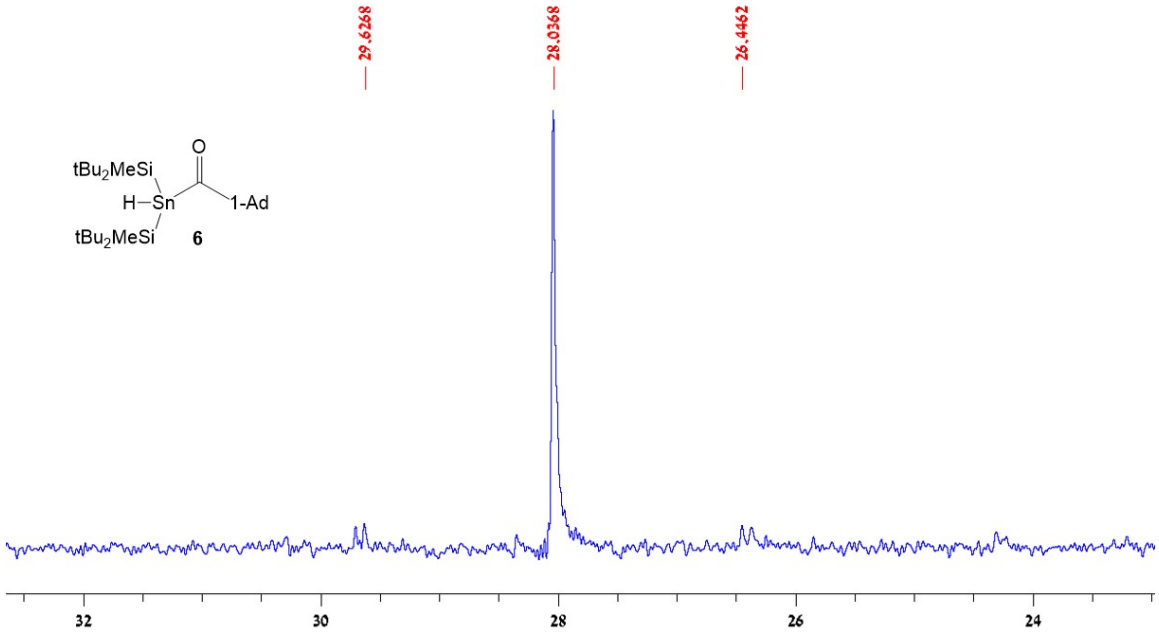


Figure 3. ^{29}Si NMR spectrum of **6** in benzene.

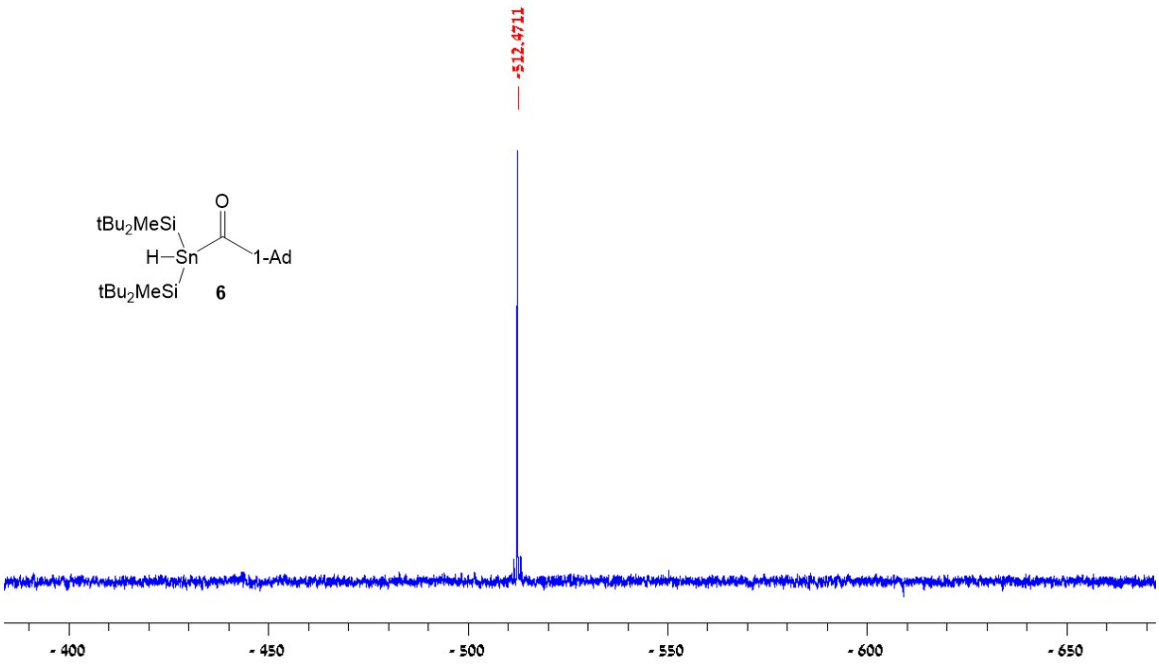


Figure 4. $^{119}Sn\{^{1}H\}$ NMR spectrum of **6** in benzene.

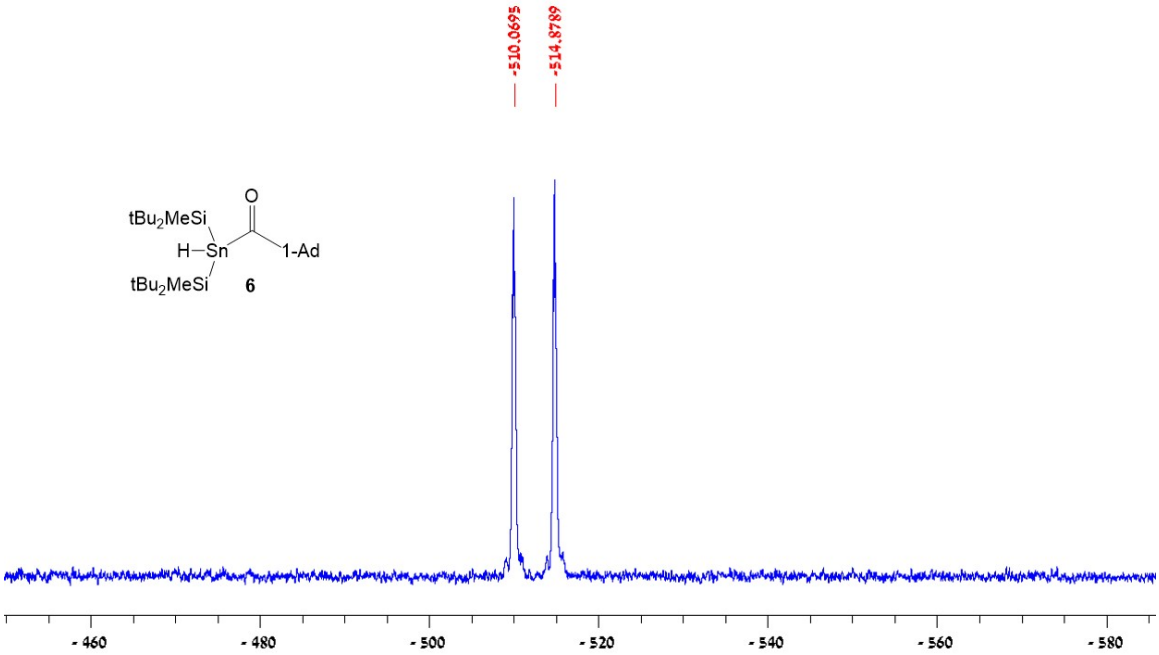


Figure 5. ^{119}Sn NMR spectrum of **6** in benzene.

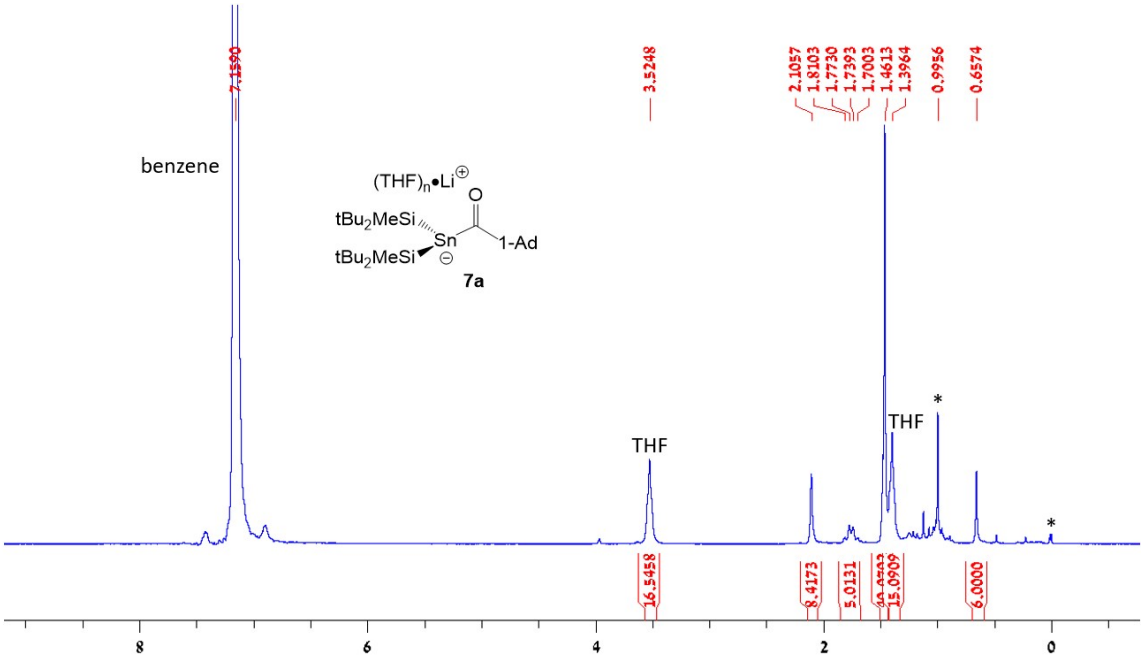


Figure 6. ^{1}H NMR spectrum of **7a** in benzene (* tBu_2MeSiH).

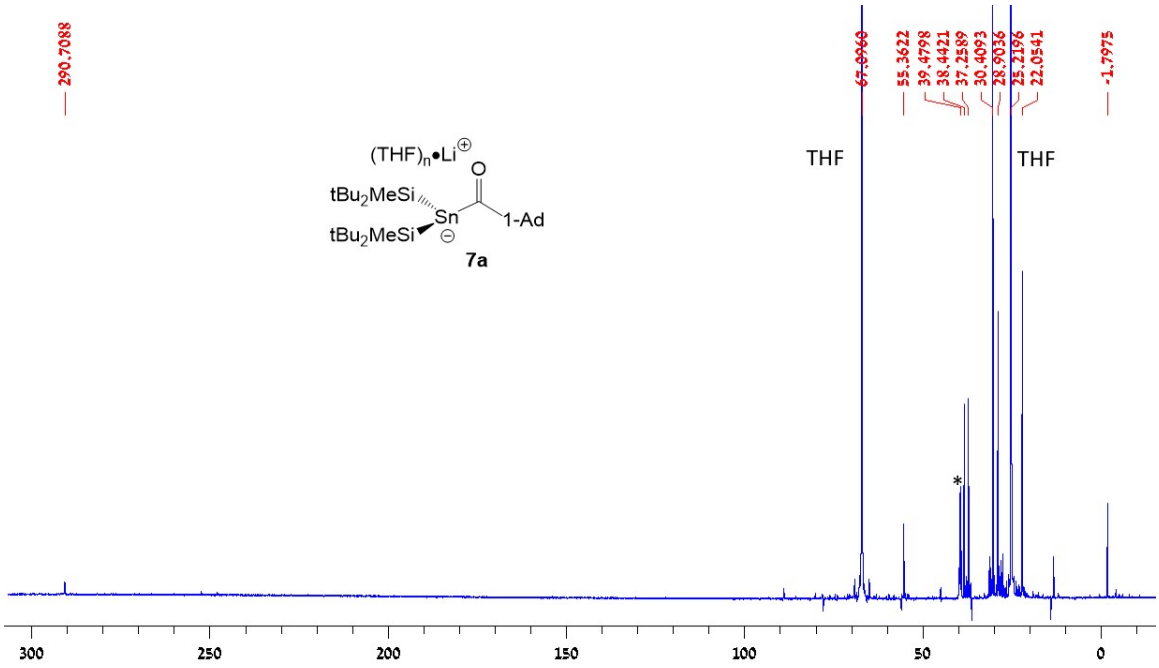


Figure 7. ^{13}C NMR spectrum of **7a** in THF (* DMSO-d_6 capillary).

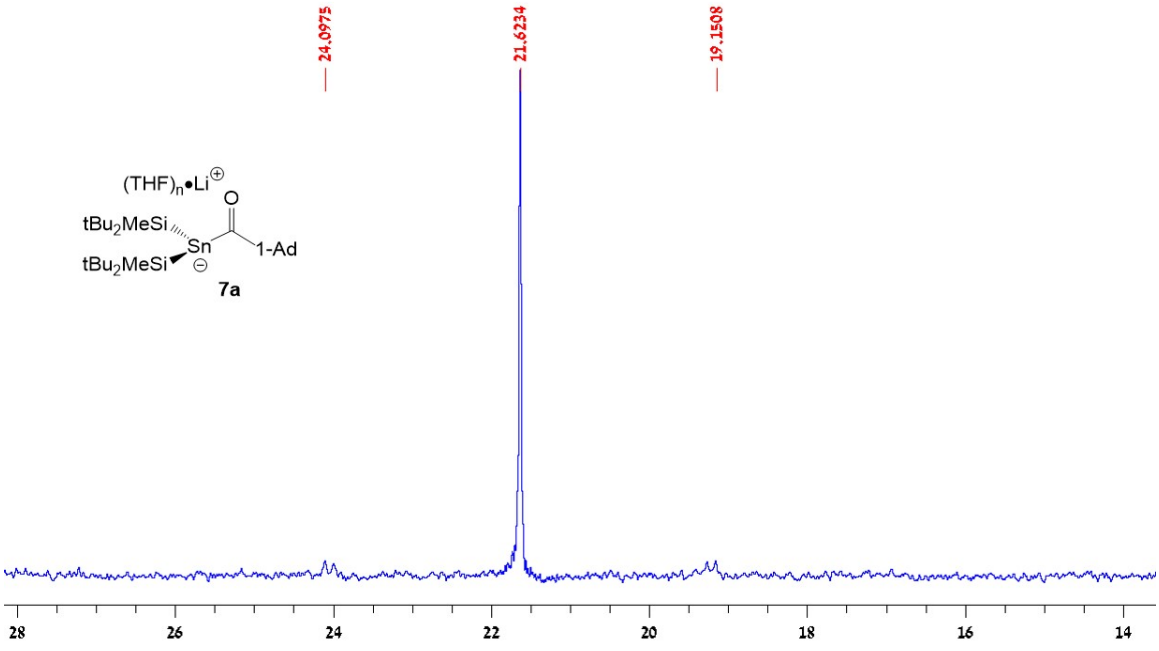


Figure 8. ^{29}Si NMR spectrum of **7a** in THF.

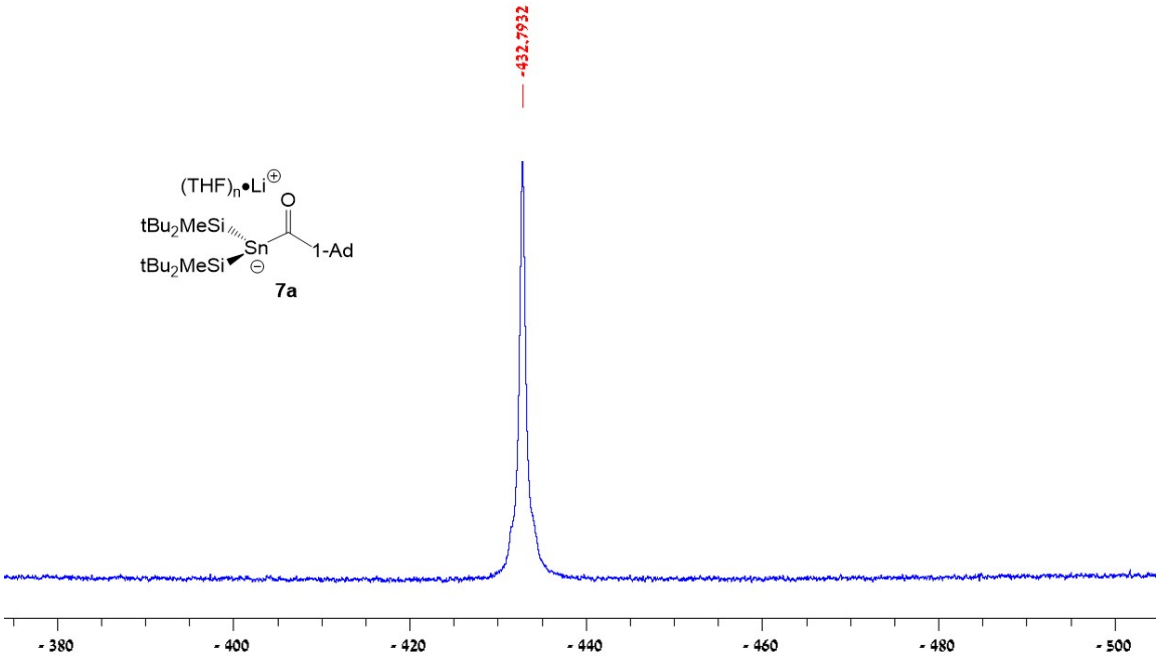


Figure 9. $^{119}Sn\{^{1}H\}$ NMR spectrum of **7a** in THF.

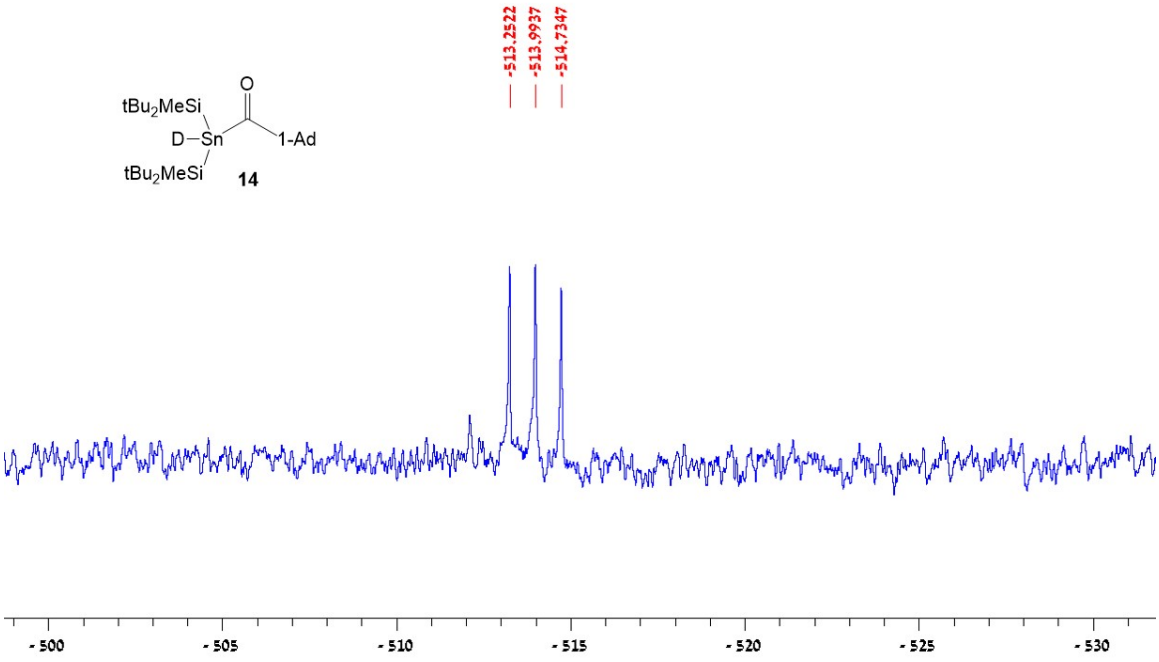


Figure 10. $^{119}Sn\{^{1}H\}$ NMR spectrum of **14** in benzene.

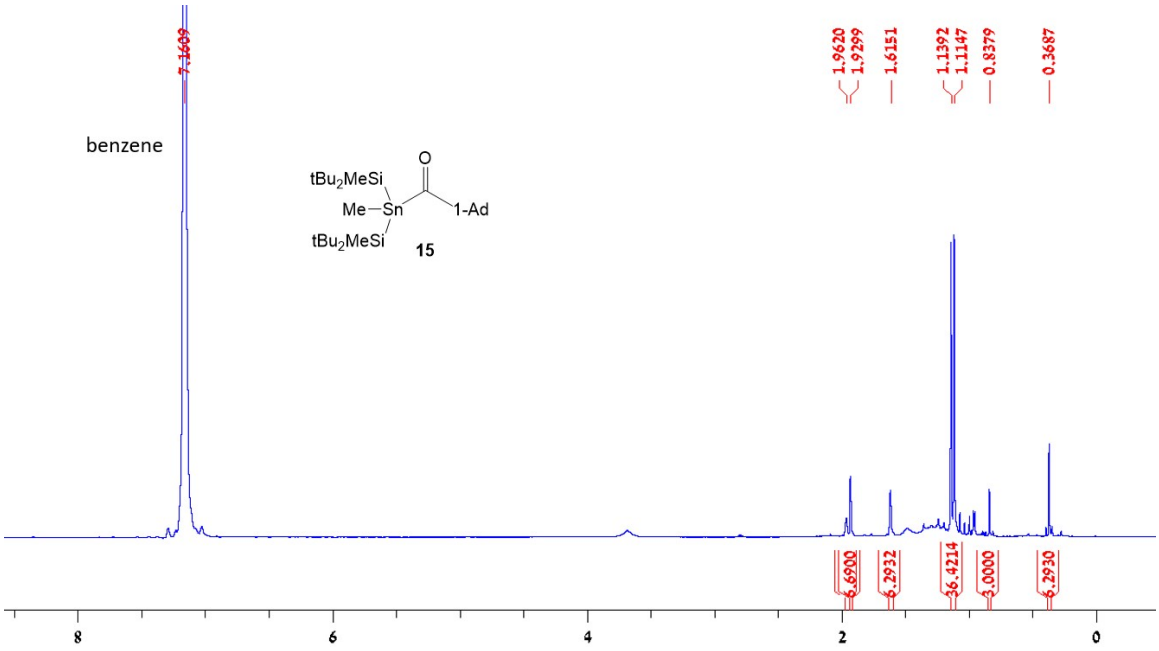


Figure 11. ^{1}H NMR spectrum of **15** in benzene.

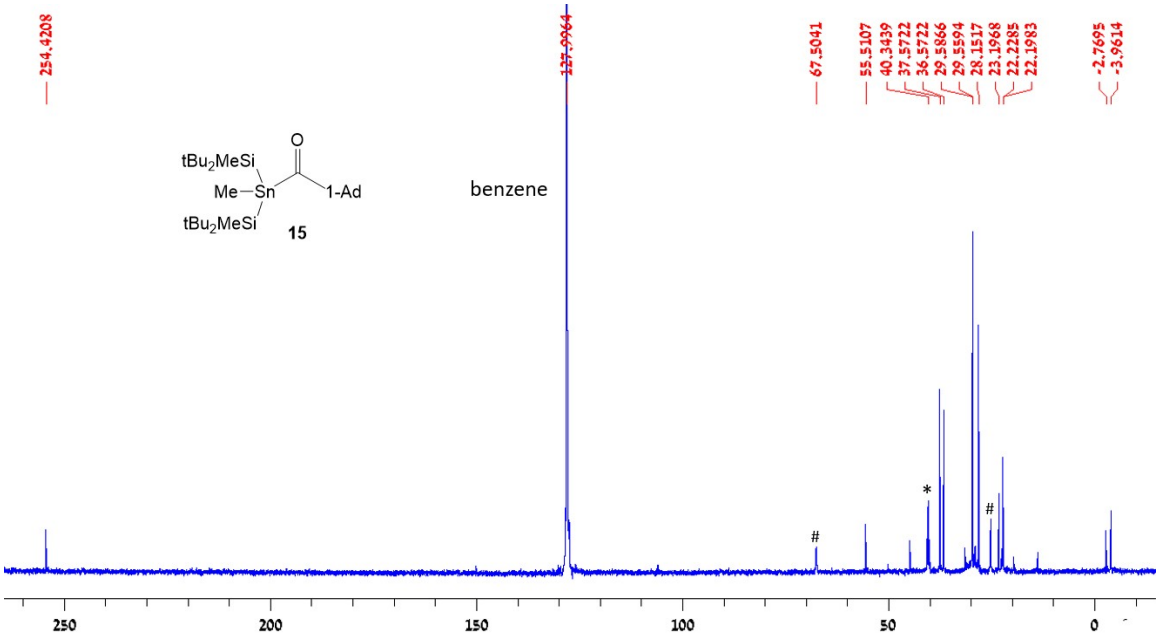


Figure 12. ^{13}C NMR spectrum of **15** in benzene (* DMSO-d_6 capillary; # THF).

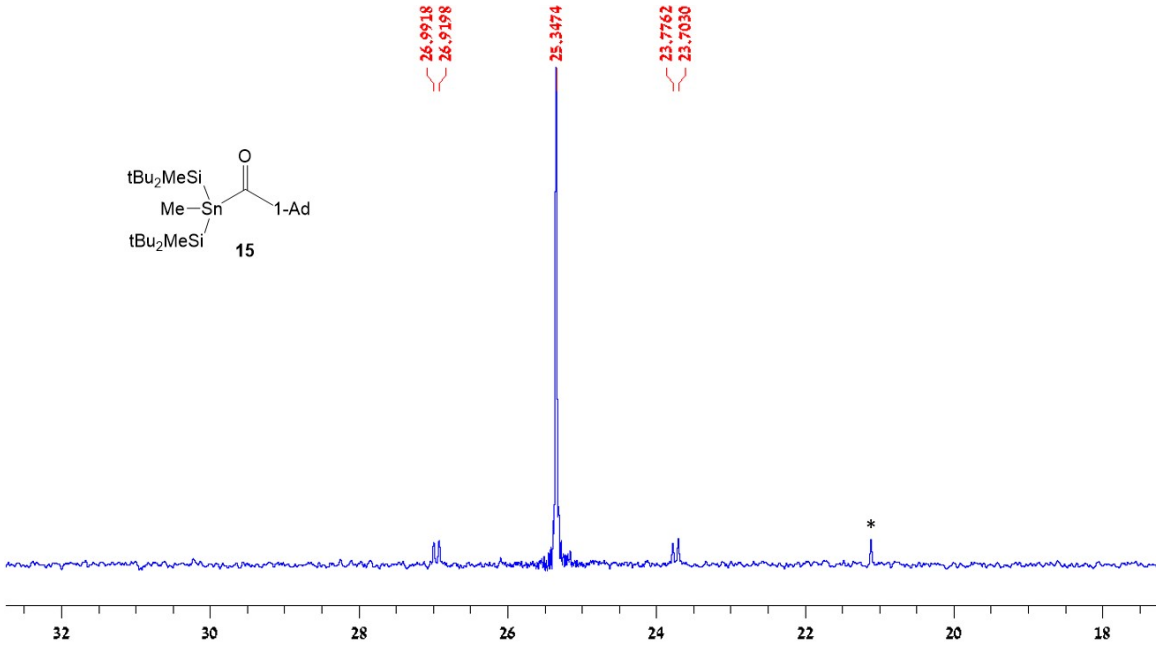


Figure 13. ^{29}Si NMR spectrum of **15** in benzene (* unknown impurity).

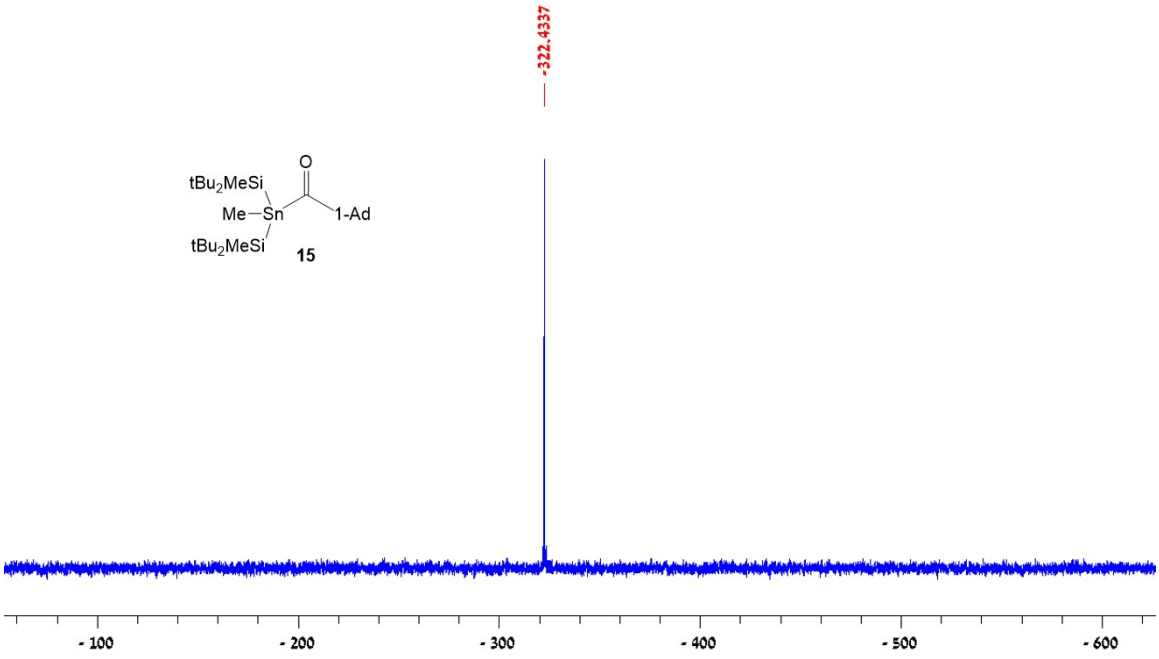


Figure 14. $^{119}Sn\{^{1}H\}$ NMR spectrum of **15** in benzene.

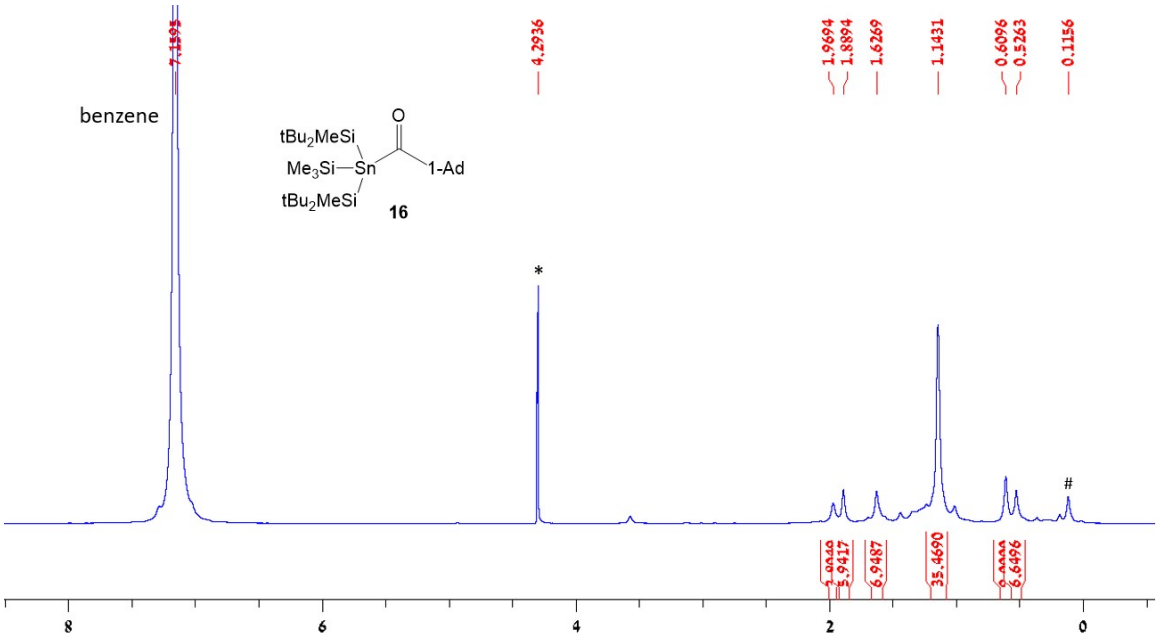


Figure 15. ^{1}H NMR spectrum of **16** in benzene (* traces of H_2O in DMSO-d_6 capillary; # unknown impurity).

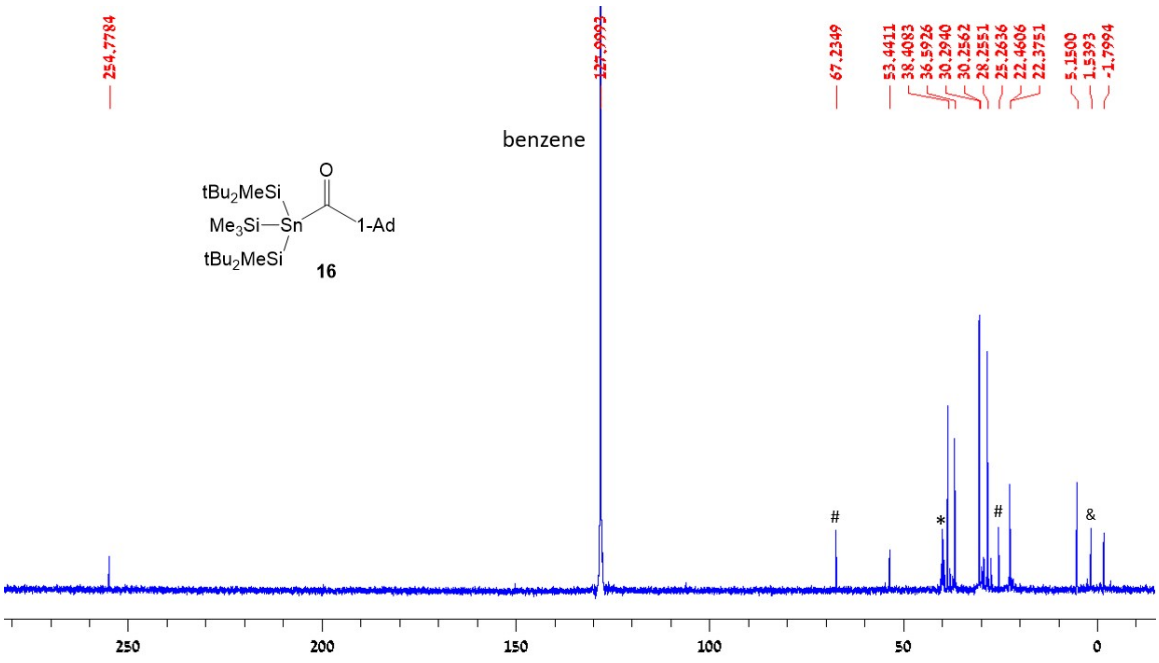


Figure 16. ^{13}C NMR spectrum of **16** in benzene (* DMSO-d_6 capillary; # THF; & unknown impurity).

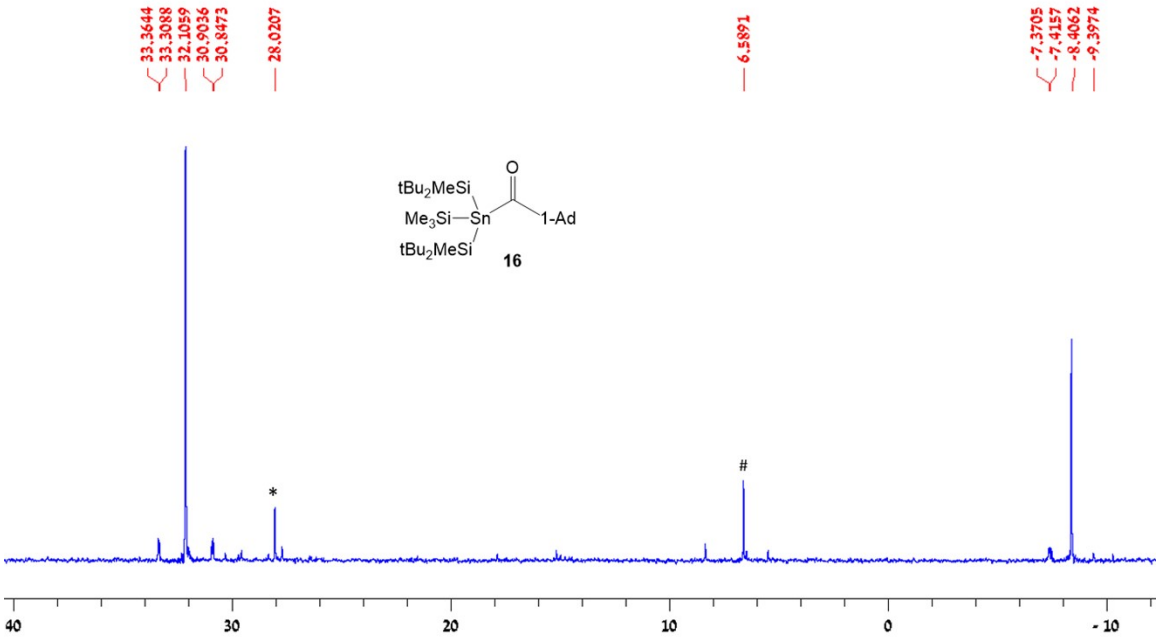


Figure 17. ^{29}Si NMR spectrum of **16** in benzene (* traces of acylstannane **6**; # unknown impurity).

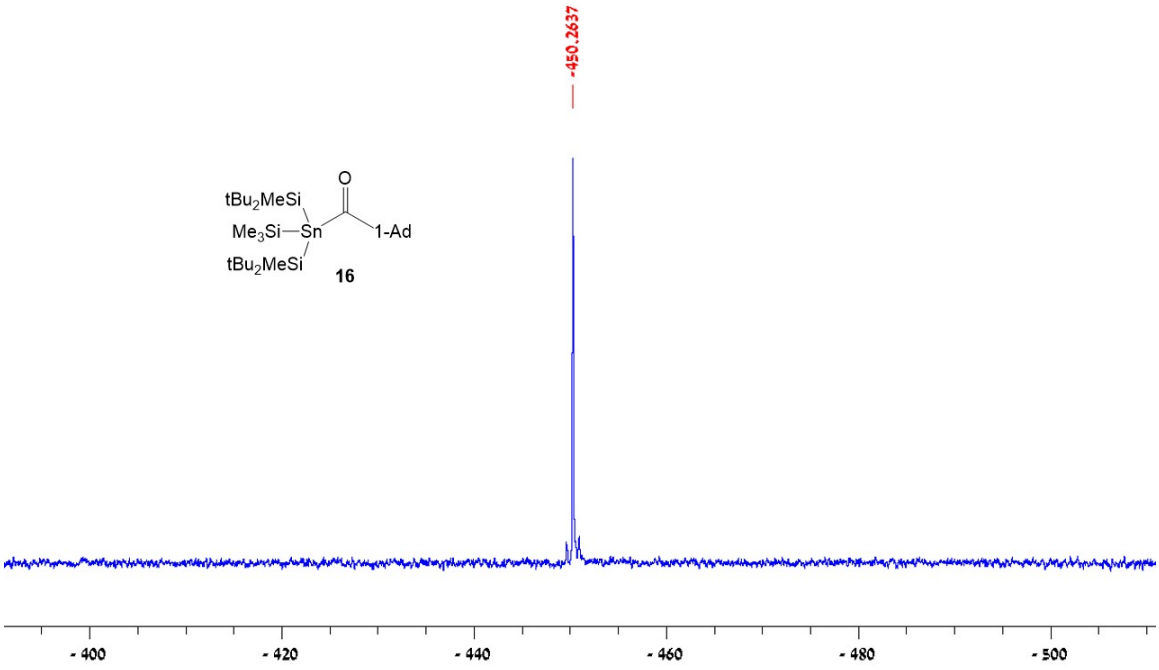


Figure 18. ^{119}Sn{^{1}H} NMR spectrum of **16** in benzene.

8. X-ray crystallographic analysis

Single-crystals of **7b** immersed in Paratone-N oil were mounted on a Bruker ApexII diffractometer at 200K. Data collection was performed using monochromated Mo Kα radiation, λ = 0.71073 Å, using ϕ and ω scans to cover the Ewald sphere. Accurate cell parameters were obtained with the amount of indicated reflections. Using Olex2,[5] the structure was solved with the olex2.solve[6] structure solution program using Charge Flipping and refined with the ShelXL[7] refinement package using Least Squares minimization. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. The Software used for molecular graphics is Olex2. The crystallographic details for **7b** (CCDC 2096073) have also been deposited to the Cambridge Structural Database.

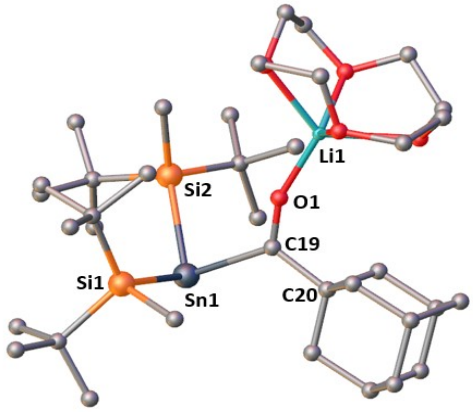


Figure 19. Olex2 drawing of the X-ray crystallographic molecular structure of **7b**. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å], angles [°], and dihedral angles [°]: Sn1-C19 2.312(5), Sn1-Si2 2.673 (17), Sn1-Si1 2.684(18), O1-C19 1.235(5), O1-Li1 1.895(9), C19-C20 1.553(7); C19-Sn1-Si2 96.3 (12), C19-Sn1-Si1 90.0 (13), Si2-Sn1-Si1 113.3(5), O1-C19-Sn1 122.8(4), O1-C19-C20 116.1(4), C20-C19-Sn1 121.0(3); Si1-Sn1-C19-O1 78.5(0), Si2-Sn1-C19-O 34.9(0), Si1-Sn1-Si2-C19 92.8(0), C20-C19-O1-Sn1 176.1(0).

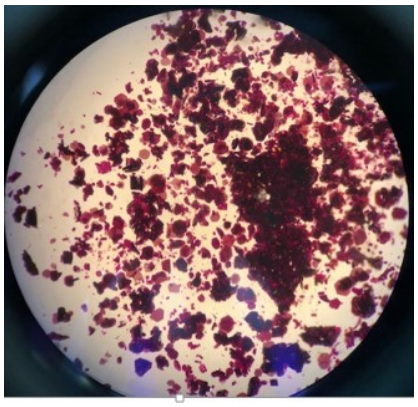


Figure 20. Photograph of the violet crystals of **7b**.

9. Experimental UV-Vis spectrum of stannenolate 7a

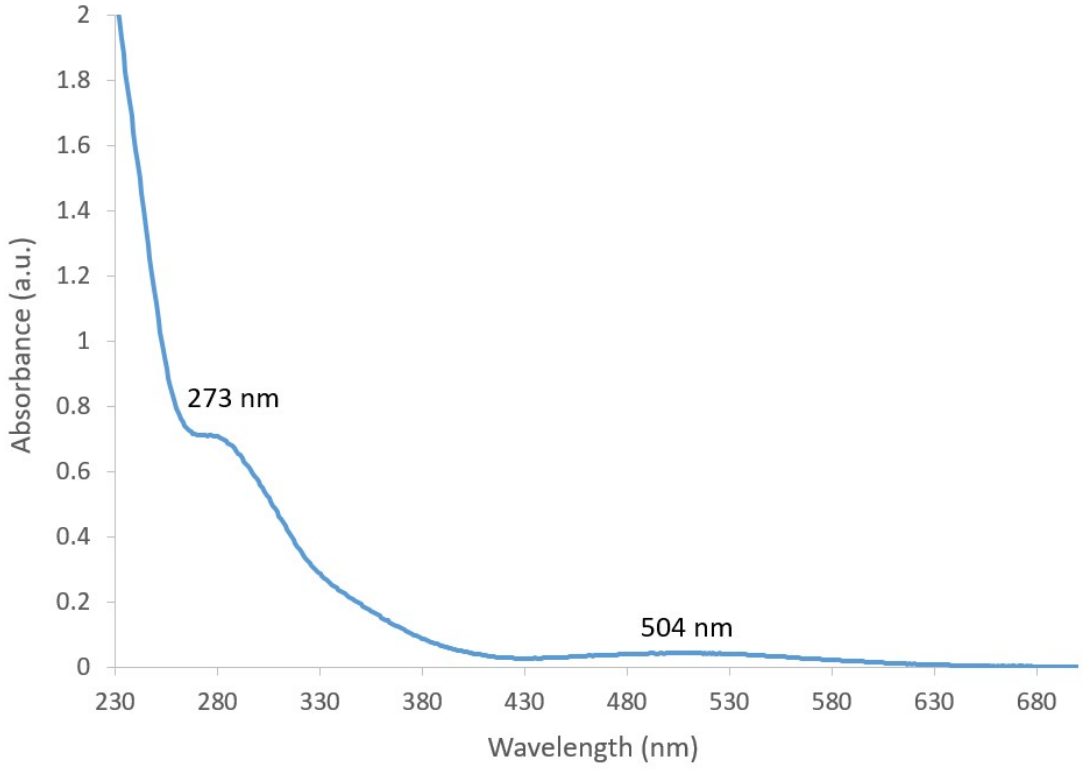


Figure 21. UV-Vis spectrum of **7a** in hexane (0.1 mM).

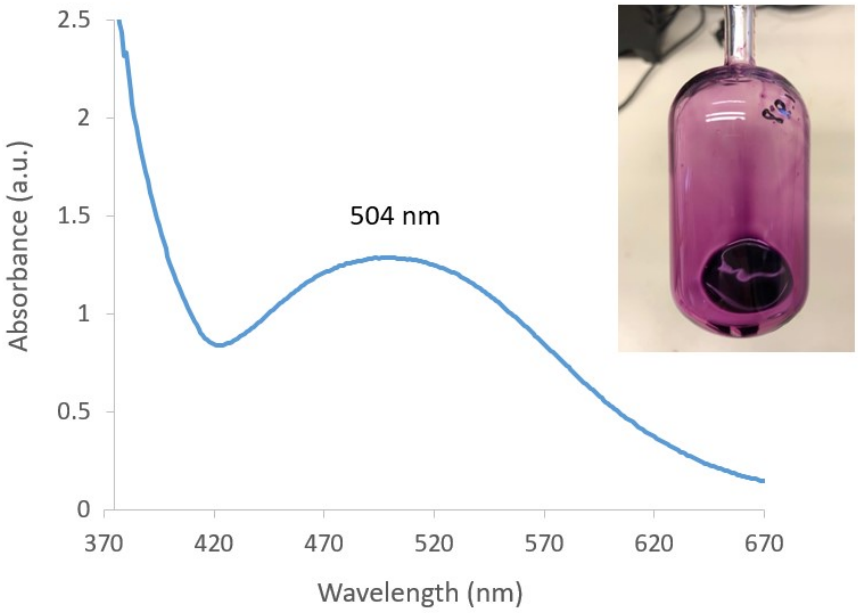


Figure 22. UV-Vis spectrum of **7a** in hexane (1.6 mM).

10. DFT calculations

All calculations were performed with the Gaussian 09 series of programs: Gaussian 09, Revision C.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, 2010.

All calculations were performed using Density Functional Theory (DFT).[8] All geometries were optimized at the B3PW91[9]-D3[10]/6-31+G(d,p)[11] [H, Li, C, O, Si], SDD[12] [Sn, Pb] level of theory. Frequency calculations at the same level were performed to validate each structure as either a minimum (no imaginary frequencies) or a transition state (one imaginary frequency). All transition state structures were confirmed to connect the corresponding reactants and products by Intrinsic Reaction Coordinate (IRC)[13] calculations. UV-Vis spectrum of **7c** was calculated using TD-DFT[14] method at the B3PW91-D3/6-31+G(d,p) [H, C, O, Si], SDD [Sn] level of theory (using PCM[15] in hexane). The NMR chemical shifts of **7c** were calculated at the HCTH407[16]/6-311+G(d,p) [H, C, O, Si], NMR-DKH (TZ2P)[17] [Sn] level of theory (using PCM in THF). NBO[18] and NRT[19] calculations were performed at the B3PW91-D3/6-31+G(d,p) [H, C, O, Si], SDD [Sn, Pb] level of theory.

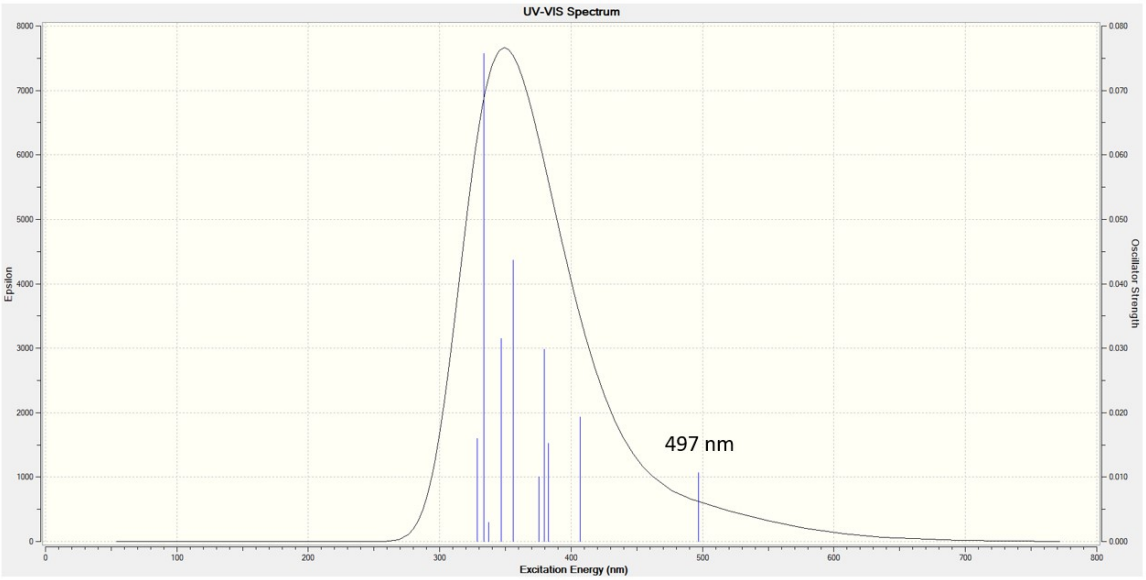
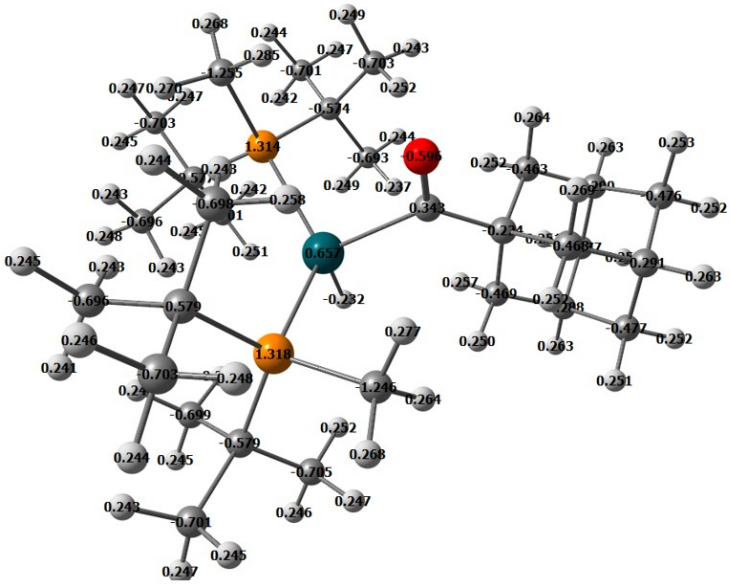
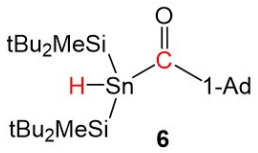


Figure 23. Calculated UV-Vis spectrum of **7c**.





6

$q((tBu_2MeSi)_2Sn)$ = +0.56 el.

q(Sn) = +0.65 el.

q(Sn-H) = -0.23 el.

q(Sn-C) = +0.34 el.

q(O) = -0.59 el.

Figure 24. Calculated NPA charges of acylstannane **6**.

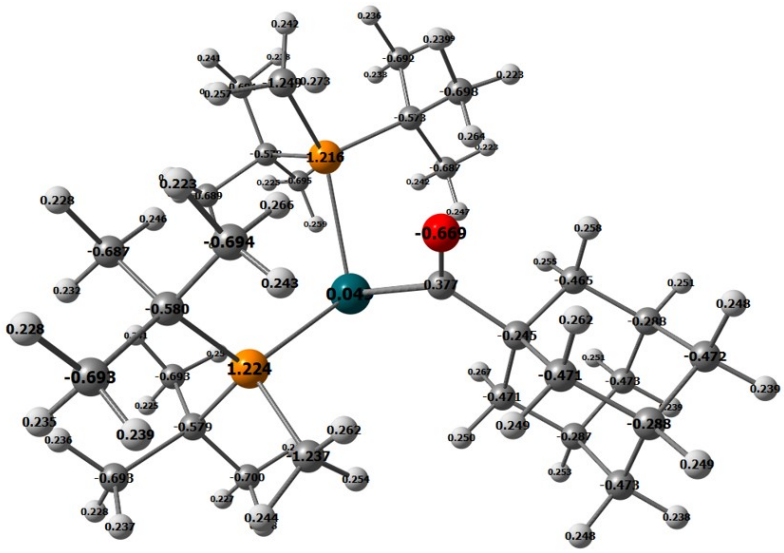


Figure 25. Calculated NPA charges of stannenolate anion **7c**.

NRT analysis

Table 1. Main calculated NRT resonance structures for enolate **9**.

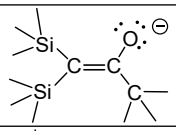
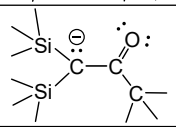
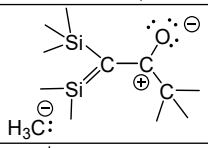
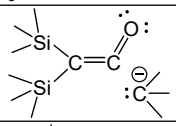
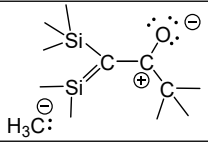
	resonance structure	NRT resonance weight (%)
1		33.16
2		23.57
3		2.84
4		2.23
5		1.32

Table 2. Main calculated NRT resonance structures for silenolate **10**.

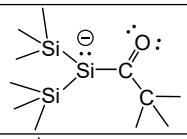
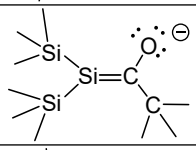
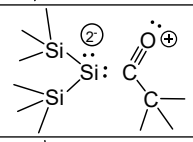
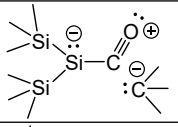
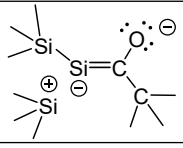
	resonance structure	NRT resonance weight (%)
1		46.55
2		8.05
3		3.23
4		3.21
5		3.12

Table 3. Main calculated NRT resonance structures for germenolate **11**.

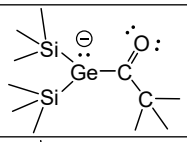
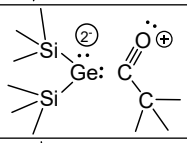
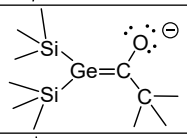
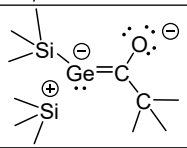
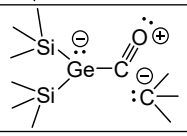
	resonance structure	NRT resonance weight (%)
1		48.85
2		3.91
3		3.85
4		3.75
5		3.35

Table 4. Main calculated NRT resonance structures for stannenolate **12**.

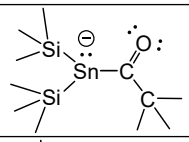
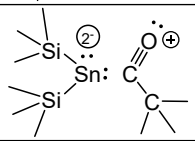
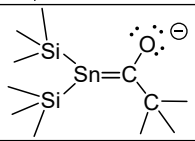
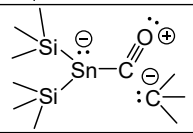
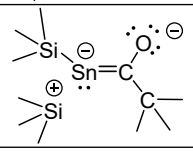
	resonance structure	NRT resonance weight (%)
1		53.31
2		4.37
3		3.43
4		3.29
5		1.29

Table 5. Main calculated NRT resonance structures for plumbenolate **13**.

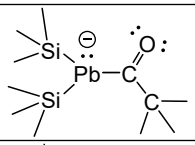
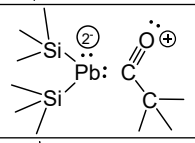
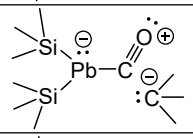
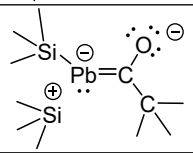
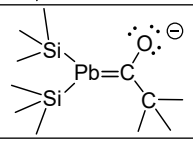
	resonance structure	NRT resonance weight (%)
1		55.49
2		4.71
3		3.23
4		2.60
11		0.67

Table 6. Calculated energies for 1,3 silyl shift in equations 1-3.[a,b]

Equation	ΔH	TΔS	ΔG	ΔH‡	TΔS‡	ΔG‡
1	-20.48	2.17	-22.65	-	-	-
2	-12.11	2.61	-14.72	-	-	-
3	-22.90	-0.44	-22.46	6.25	-2.08	8.33

a) Calculated at B3PW91-D3/6-31+G(d,p) [H, C, O, Si], SDD [Sn].
b) at 298.15 K, kcal/mol.

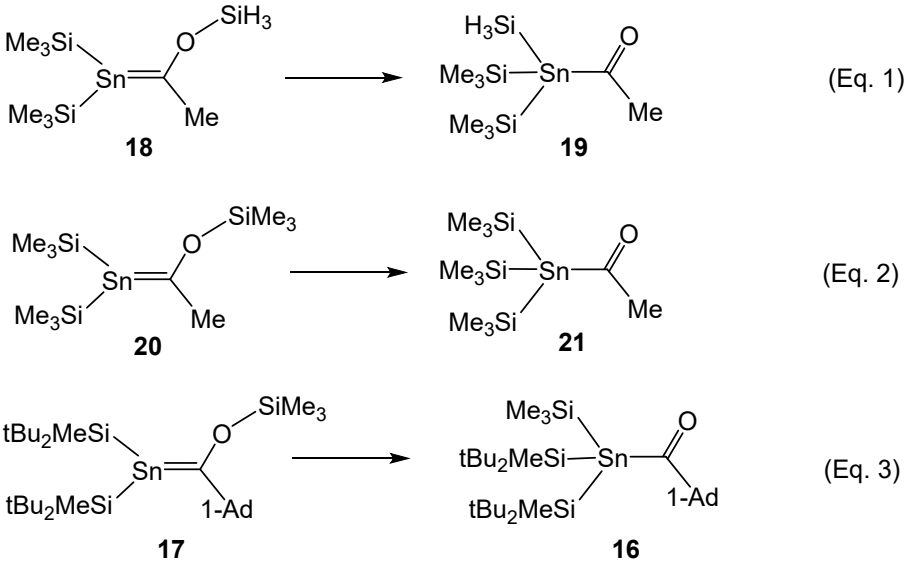


Table 7. Calculated rotation barrier about Sn-C bond in $[(Me_3Si)_2SnC(O)tBu]^-$ (**12**).[a,b]

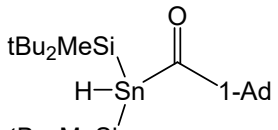
ΔH‡	TΔS‡	ΔG‡
1.81	-1.59	3.40

a) Calculated at B3PW91-D3/6-31+G(d,p) [H, C, O, Si], SDD [Sn].
b) at 298.15 K, kcal/mol.

Table 8. Calculated NMR chemical shifts of **7c**.

atom	σ_{iso} (ppm)	chemical shift (ppm)
$\underline{Sn}(CH_3)_4$	2238.1	0
$Si(\underline{C}H_3)_4$	185.8	0
Sn1	2731.8	-493.7
C65	-111.2	297.0

Optimized Cartesian coordinates for 6



6

Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.818759 (Hartree/Particle)
Thermal correction to Energy= 0.861286
Thermal correction to Enthalpy= 0.862230
Thermal correction to Gibbs Free Energy= 0.747380
Sum of electronic and zero-point Energies= -1796.589636
Sum of electronic and thermal Energies= -1796.547109
Sum of electronic and thermal Enthalpies= -1796.546165
Sum of electronic and thermal Free Energies= -1796.661015
Number of imaginary frequencies: 0

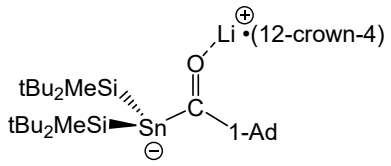
Charge = 0 Multiplicity = 1

Sn	0.435053000	-0.045739000	-0.344958000
Si	1.261519000	2.391769000	0.124232000
Si	1.565111000	-2.312146000	0.337285000
O	-1.279148000	0.027854000	2.110083000
C	1.983525000	3.146741000	-1.506793000
C	3.028770000	2.224190000	-2.152492000
H	3.871477000	2.015189000	-1.486682000
H	3.435902000	2.692983000	-3.060171000
H	2.590953000	1.265917000	-2.455515000
C	2.621487000	4.518980000	-1.231503000
H	1.923588000	5.209449000	-0.743677000
H	2.931288000	4.984873000	-2.178449000
H	3.514089000	4.439733000	-0.603193000
C	0.823616000	3.338776000	-2.502076000
H	0.304290000	2.397563000	-2.718124000
H	1.212168000	3.723485000	-3.456134000
H	0.084266000	4.059871000	-2.137067000
C	2.411621000	2.471441000	1.677152000
C	3.848600000	2.049114000	1.345932000
H	3.881545000	1.056314000	0.886550000
H	4.451757000	2.006596000	2.264473000
H	4.342882000	2.751450000	0.666523000
C	1.846462000	1.510584000	2.737465000
H	0.801636000	1.721719000	2.988239000
H	2.432995000	1.587860000	3.664410000
H	1.894030000	0.468792000	2.407378000
C	2.416894000	3.893125000	2.267608000
H	2.794151000	4.642260000	1.564888000

H	3.065620000	3.922413000	3.155169000
H	1.417167000	4.204404000	2.588622000
C	-0.325561000	3.339222000	0.559911000
H	-1.100267000	3.195171000	-0.199209000
H	-0.131606000	4.414895000	0.646188000
H	-0.727798000	2.986086000	1.514964000
C	3.151487000	-2.598588000	-0.738697000
C	2.787953000	-2.857875000	-2.208426000
H	3.700494000	-2.928543000	-2.817907000
H	2.174299000	-2.050943000	-2.626812000
H	2.240946000	-3.797282000	-2.338236000
C	3.977431000	-3.778083000	-0.192350000
H	4.902483000	-3.884498000	-0.777579000
H	3.446546000	-4.731099000	-0.252087000
H	4.270923000	-3.620956000	0.851676000
C	4.035756000	-1.342602000	-0.666808000
H	4.334512000	-1.109665000	0.361289000
H	3.541055000	-0.460161000	-1.084656000
H	4.958406000	-1.498942000	-1.244122000
C	0.193820000	-3.675476000	0.142118000
C	0.800392000	-5.088436000	0.122574000
H	1.387033000	-5.275469000	-0.782357000
H	-0.005127000	-5.837011000	0.145231000
H	1.441972000	-5.277809000	0.991111000
C	-0.629216000	-3.475522000	-1.140392000
H	-1.147489000	-2.510597000	-1.150141000
H	-1.397846000	-4.257799000	-1.221413000
H	-0.013011000	-3.522363000	-2.043698000
C	-0.745094000	-3.578989000	1.359851000
H	-0.237997000	-3.866598000	2.287148000
H	-1.597299000	-4.260950000	1.226877000
H	-1.149387000	-2.573900000	1.506756000
C	2.085593000	-2.277871000	2.157471000
H	2.981266000	-1.667255000	2.310435000
H	2.307982000	-3.293605000	2.506048000
H	1.286912000	-1.869944000	2.784403000
C	-1.460691000	0.054535000	0.904567000
C	-2.882720000	0.180914000	0.347446000
C	-2.917282000	0.530322000	-1.147201000
H	-2.371619000	-0.226837000	-1.724228000
H	-2.410182000	1.489608000	-1.321148000
C	-4.371722000	0.604260000	-1.638022000
H	-4.379128000	0.860181000	-2.705317000
C	-5.043964000	-0.762199000	-1.429789000
H	-6.078544000	-0.732088000	-1.796772000
H	-4.517331000	-1.532388000	-2.009494000
C	-5.025920000	-1.121825000	0.064266000
H	-5.500417000	-2.100322000	0.215633000

C	-3.572869000	-1.189625000	0.556617000
H	-3.027903000	-1.970224000	0.011277000
H	-3.534855000	-1.449764000	1.621372000
C	-5.130517000	1.677546000	-0.841901000
H	-6.165986000	1.749524000	-1.201035000
H	-4.666505000	2.660937000	-0.998752000
C	-5.111601000	1.318093000	0.651909000
H	-5.650403000	2.085028000	1.223632000
C	-5.784457000	-0.048002000	0.859697000
H	-5.790941000	-0.305036000	1.927348000
H	-6.831365000	-0.006355000	0.530405000
C	-3.658284000	1.252501000	1.142871000
H	-3.614697000	1.008570000	2.209831000
H	-3.169939000	2.227277000	1.013517000
H	0.079638000	-0.151856000	-2.037439000

Optimized Cartesian coordinates for 7b



7b

Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 1.062497 (Hartree/Particle)
Thermal correction to Energy= 1.118894
Thermal correction to Enthalpy= 1.119839
Thermal correction to Gibbs Free Energy= 0.976152
Sum of electronic and zero-point Energies= -2418.502947
Sum of electronic and thermal Energies= -2418.446549
Sum of electronic and thermal Enthalpies= -2418.445605
Sum of electronic and thermal Free Energies= -2418.589292
Number of imaginary frequencies: 0

Charge = 0 Multiplicity = 1

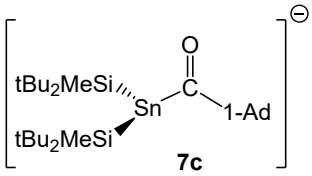
Sn	1.904072000	0.700251000	-0.966529000
Si	2.227530000	1.574657000	1.567723000
Si	1.931736000	-2.001623000	-1.109215000
O	-0.996271000	-0.029433000	0.123748000
O	-2.257386000	-1.776494000	2.923764000
O	-2.460861000	-3.024898000	0.555026000
O	-4.109560000	-1.005092000	-0.224009000
O	-3.917838000	0.257750000	2.181276000
C	3.943193000	2.510507000	1.630902000

C	5.071788000	1.641844000	1.056867000
H	5.195179000	0.700804000	1.603090000
H	6.031136000	2.179946000	1.104013000
H	4.886723000	1.399129000	0.004258000
C	4.327999000	2.945750000	3.052739000
H	3.540731000	3.539215000	3.532978000
H	5.235177000	3.569327000	3.024404000
H	4.547784000	2.088581000	3.697857000
C	3.820896000	3.772823000	0.756765000
H	3.500203000	3.531990000	-0.263989000
H	4.796919000	4.277449000	0.687354000
H	3.110278000	4.494828000	1.175300000
C	1.967597000	0.351138000	3.070237000
C	3.116794000	-0.657862000	3.157127000
H	3.263138000	-1.169445000	2.201193000
H	2.904993000	-1.425045000	3.918929000
H	4.064462000	-0.181131000	3.429650000
C	0.667768000	-0.412248000	2.788656000
H	-0.192643000	0.266216000	2.753190000
H	0.474137000	-1.158132000	3.575953000
H	0.701508000	-0.925339000	1.826315000
C	1.805232000	1.064886000	4.421799000
H	2.706216000	1.599033000	4.732387000
H	1.578053000	0.326829000	5.208574000
H	0.979514000	1.785962000	4.405241000
C	0.913230000	2.935391000	1.864764000
H	0.804907000	3.587892000	0.993262000
H	1.175192000	3.567060000	2.723350000
H	-0.063903000	2.482310000	2.063920000
C	3.785534000	-2.592501000	-1.321137000
C	4.364529000	-2.114187000	-2.661453000
H	5.440740000	-2.340190000	-2.715174000
H	4.245846000	-1.031709000	-2.790504000
H	3.889757000	-2.607343000	-3.516210000
C	3.946215000	-4.118890000	-1.209502000
H	5.012242000	-4.388718000	-1.272144000
H	3.430156000	-4.661325000	-2.005501000
H	3.573878000	-4.498010000	-0.250498000
C	4.616544000	-1.965802000	-0.190215000
H	4.278129000	-2.300835000	0.796371000
H	4.578332000	-0.872729000	-0.203668000
H	5.673795000	-2.258342000	-0.285219000
C	0.845114000	-2.503300000	-2.677205000
C	1.157465000	-3.918128000	-3.185915000
H	2.164044000	-3.989801000	-3.607894000
H	0.451965000	-4.197231000	-3.985464000
H	1.068706000	-4.673135000	-2.395294000
C	1.024513000	-1.512925000	-3.838388000

H	0.741684000	-0.494688000	-3.549518000
H	0.393463000	-1.808589000	-4.691984000
H	2.058488000	-1.466162000	-4.192465000
C	-0.634175000	-2.476760000	-2.258734000
H	-0.865426000	-3.239551000	-1.507675000
H	-1.274704000	-2.664660000	-3.137108000
H	-0.916443000	-1.509408000	-1.837223000
C	1.201771000	-3.064485000	0.302067000
H	1.830250000	-3.028409000	1.197957000
H	1.078719000	-4.114668000	0.005046000
H	0.220946000	-2.656250000	0.559999000
C	-0.392695000	0.815907000	-0.560982000
C	-1.294009000	1.876287000	-1.225946000
C	-0.533977000	3.042695000	-1.874292000
H	0.203439000	2.656781000	-2.588607000
H	0.032000000	3.590556000	-1.110676000
C	-1.519688000	3.989061000	-2.581336000
H	-0.960115000	4.819853000	-3.029876000
C	-2.266245000	3.219008000	-3.681512000
H	-2.957604000	3.888864000	-4.211337000
H	-1.552177000	2.837077000	-4.422942000
C	-3.040755000	2.053155000	-3.049712000
H	-3.572678000	1.493723000	-3.831722000
C	-2.063302000	1.112565000	-2.333799000
H	-1.349827000	0.681584000	-3.048511000
H	-2.612148000	0.283728000	-1.872944000
C	-2.533762000	4.541391000	-1.567319000
H	-3.230427000	5.229956000	-2.065570000
H	-2.012937000	5.114597000	-0.788777000
C	-3.305666000	3.375039000	-0.929614000
H	-4.027166000	3.766676000	-0.197699000
C	-4.050316000	2.597037000	-2.026738000
H	-4.611084000	1.759866000	-1.586169000
H	-4.779238000	3.251355000	-2.524202000
C	-2.311608000	2.445220000	-0.219499000
H	-2.832396000	1.616687000	0.267766000
H	-1.778359000	2.994530000	0.565990000
C	-2.740484000	-3.111102000	2.938494000
H	-3.841013000	-3.131394000	2.893848000
H	-2.423978000	-3.626798000	3.857040000
C	-2.141659000	-3.782258000	1.717864000
H	-1.050842000	-3.782911000	1.790121000
H	-2.488358000	-4.819855000	1.627586000
C	-3.665967000	-3.384204000	-0.101921000
H	-4.458232000	-3.601327000	0.630592000
H	-3.515998000	-4.282626000	-0.717989000
C	-4.047944000	-2.208461000	-0.983554000
H	-3.269580000	-2.043450000	-1.732861000

H	-4.998896000	-2.401637000	-1.498857000
C	-5.305094000	-0.796951000	0.510565000
H	-5.539679000	-1.670421000	1.139052000
H	-6.153227000	-0.630009000	-0.170364000
C	-5.073292000	0.432228000	1.370720000
H	-4.871174000	1.295629000	0.731770000
H	-5.961306000	0.651007000	1.979272000
C	-4.147111000	-0.361934000	3.437698000
H	-4.885388000	-1.172569000	3.343577000
H	-4.536564000	0.367189000	4.163560000
C	-2.809932000	-0.907886000	3.904112000
H	-2.089009000	-0.093539000	4.016773000
H	-2.913075000	-1.417099000	4.872133000
Li	-2.322070000	-0.921234000	0.973412000

Optimized Cartesian coordinates for anion 7c



7c

Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.808551 (Hartree/Particle)
Thermal correction to Energy= 0.850836
Thermal correction to Enthalpy= 0.851780
Thermal correction to Gibbs Free Energy= 0.737504
Sum of electronic and zero-point Energies= -1796.051535
Sum of electronic and thermal Energies= -1796.009251
Sum of electronic and thermal Enthalpies= -1796.008306
Sum of electronic and thermal Free Energies= -1796.122582
Number of imaginary frequencies: 0

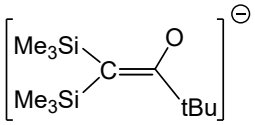
Charge = -1 Multiplicity = 1

Sn	0.351722000	-0.058373000	-0.857782000
Si	0.932826000	2.369638000	0.155579000
Si	1.833749000	-1.980961000	0.341284000
O	-1.203312000	-0.412820000	1.904367000
C	1.789708000	3.420999000	-1.265954000
C	2.963227000	2.658808000	-1.898333000
H	3.733735000	2.398177000	-1.164850000
H	3.441659000	3.271364000	-2.680331000
H	2.623990000	1.730769000	-2.372337000
C	2.297796000	4.787183000	-0.784201000

H	1.519653000	5.360360000	-0.265884000
H	2.634888000	5.391987000	-1.642684000
H	3.153010000	4.689358000	-0.106335000
C	0.733266000	3.660380000	-2.359905000
H	0.292998000	2.717921000	-2.708159000
H	1.193443000	4.157376000	-3.229663000
H	-0.080075000	4.304887000	-2.006859000
C	1.868970000	2.511295000	1.866684000
C	3.320060000	2.041246000	1.714108000
H	3.360330000	1.047351000	1.257747000
H	3.815385000	1.979510000	2.696616000
H	3.912583000	2.721639000	1.090723000
C	1.149492000	1.571211000	2.847981000
H	0.128989000	1.906362000	3.063816000
H	1.695219000	1.535240000	3.805155000
H	1.064737000	0.553594000	2.463863000
C	1.852485000	3.920612000	2.482657000
H	2.412061000	4.651670000	1.892828000
H	2.311265000	3.892779000	3.485029000
H	0.831054000	4.299108000	2.607006000
C	-0.724396000	3.276406000	0.474810000
H	-1.428522000	3.128880000	-0.349652000
H	-0.577499000	4.357195000	0.602230000
H	-1.193019000	2.886312000	1.384083000
C	3.486151000	-2.197734000	-0.705645000
C	3.186118000	-2.739214000	-2.111258000
H	4.101814000	-2.738707000	-2.725694000
H	2.437594000	-2.126218000	-2.627233000
H	2.815599000	-3.769776000	-2.086080000
C	4.522447000	-3.105556000	-0.022126000
H	5.447559000	-3.139374000	-0.621824000
H	4.174916000	-4.135592000	0.093656000
H	4.793774000	-2.731737000	0.971949000
C	4.128026000	-0.810858000	-0.860245000
H	4.403054000	-0.378047000	0.107932000
H	3.458107000	-0.106835000	-1.361678000
H	5.050162000	-0.877109000	-1.460956000
C	0.775094000	-3.646013000	0.309703000
C	1.639812000	-4.908870000	0.445296000
H	2.282027000	-5.070853000	-0.426592000
H	0.994083000	-5.798040000	0.540587000
H	2.278894000	-4.876781000	1.336042000
C	-0.059150000	-3.763831000	-0.974691000
H	-0.741235000	-2.915391000	-1.091801000
H	-0.667052000	-4.683585000	-0.951747000
H	0.562071000	-3.797300000	-1.875288000
C	-0.189756000	-3.620795000	1.509061000
H	0.348006000	-3.676541000	2.462520000

H	-0.866817000	-4.489840000	1.463387000
H	-0.802085000	-2.717363000	1.534495000
C	2.416767000	-1.847180000	2.156894000
H	3.170729000	-1.062131000	2.278273000
H	2.849596000	-2.793323000	2.509679000
H	1.570131000	-1.594083000	2.801833000
C	-1.395906000	-0.190159000	0.714978000
C	-2.883567000	-0.094877000	0.269695000
C	-3.079639000	0.503361000	-1.129712000
H	-2.490657000	-0.062785000	-1.861785000
H	-2.694969000	1.530877000	-1.151248000
C	-4.568085000	0.490758000	-1.514150000
H	-4.688983000	0.925291000	-2.516230000
C	-5.079436000	-0.959037000	-1.517052000
H	-6.139575000	-0.987098000	-1.809634000
H	-4.521341000	-1.550318000	-2.255736000
C	-4.901998000	-1.567764000	-0.117480000
H	-5.263399000	-2.606187000	-0.117970000
C	-3.415393000	-1.546719000	0.265737000
H	-2.831935000	-2.150924000	-0.441866000
H	-3.266803000	-1.982362000	1.261666000
C	-5.372452000	1.312625000	-0.494335000
H	-6.437627000	1.322599000	-0.769804000
H	-5.025655000	2.355251000	-0.498010000
C	-5.192005000	0.707153000	0.906951000
H	-5.763228000	1.295822000	1.639384000
C	-5.702785000	-0.743062000	0.903263000
H	-5.594409000	-1.181074000	1.905176000
H	-6.773325000	-0.766980000	0.651060000
C	-3.703132000	0.724313000	1.284333000
H	-3.546484000	0.309112000	2.286443000
H	-3.330392000	1.757165000	1.300452000

Optimized Cartesian coordinates for anion 9



9

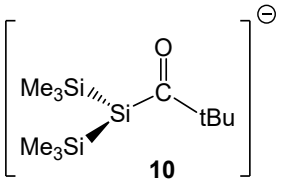
Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.360429 (Hartree/Particle)
Thermal correction to Energy= 0.383688
Thermal correction to Enthalpy= 0.384632
Thermal correction to Gibbs Free Energy= 0.310372
Sum of electronic and zero-point Energies= -1127.310716

Sum of electronic and thermal Energies= -1127.287457
Sum of electronic and thermal Enthalpies= -1127.286512
Sum of electronic and thermal Free Energies= -1127.360773
Number of imaginary frequencies = 0

Charge = -1 Multiplicity = 1

Si	0.250632000	1.794971000	0.012560000
Si	1.734154000	-1.062512000	-0.004968000
O	-0.660517000	-2.186098000	0.444934000
C	0.301239000	2.564208000	-1.739099000
H	1.152856000	2.144785000	-2.288960000
H	0.423079000	3.655476000	-1.699528000
H	-0.603231000	2.335976000	-2.313538000
C	2.223306000	-1.913438000	1.626041000
H	2.383283000	-1.162363000	2.410158000
H	3.148203000	-2.496470000	1.515844000
H	1.410374000	-2.575562000	1.936549000
C	-0.886436000	-0.969736000	0.166798000
C	-2.402226000	-0.640612000	-0.050789000
C	3.318595000	-0.081083000	-0.474034000
H	3.160423000	0.597155000	-1.321716000
H	3.726360000	0.500608000	0.358676000
H	4.081772000	-0.812438000	-0.773433000
C	1.697778000	-2.364887000	-1.396777000
H	1.699214000	-1.864524000	-2.373663000
H	2.588049000	-3.006606000	-1.343755000
H	0.803161000	-2.986711000	-1.315315000
C	1.826192000	2.494235000	0.846078000
H	2.073839000	1.940749000	1.759029000
H	2.698352000	2.468255000	0.187489000
H	1.647833000	3.542293000	1.120673000
C	-1.075103000	2.794431000	0.976505000
H	-1.017820000	2.546183000	2.043639000
H	-0.827126000	3.859229000	0.869757000
H	-2.111850000	2.662526000	0.656097000
C	-2.639181000	0.407916000	-1.142595000
H	-3.716639000	0.555089000	-1.305873000
H	-2.212352000	1.379103000	-0.897031000
H	-2.188286000	0.082695000	-2.086649000
C	-2.994182000	-0.187708000	1.294079000
H	-2.494360000	0.704181000	1.675898000
H	-4.067721000	0.031326000	1.196530000
H	-2.871096000	-0.984745000	2.035991000
C	-3.128289000	-1.925102000	-0.483089000
H	-4.201907000	-1.724360000	-0.610887000
H	-2.728869000	-2.296710000	-1.433500000
H	-2.991026000	-2.716492000	0.256755000
C	0.180410000	-0.035603000	0.056048000

Optimized Cartesian coordinates for anion 10



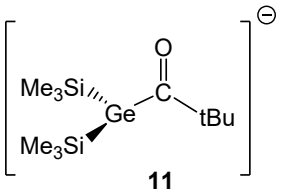
Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.355019 (Hartree/Particle)
Thermal correction to Energy= 0.379965
Thermal correction to Enthalpy= 0.380910
Thermal correction to Gibbs Free Energy= 0.302841
Sum of electronic and zero-point Energies= -1378.669808
Sum of electronic and thermal Energies= -1378.644862
Sum of electronic and thermal Enthalpies= -1378.643917
Sum of electronic and thermal Free Energies= -1378.721986
Number of imaginary frequencies: 0

Charge = -1 Multiplicity = 1

Si	0.278372000	2.023595000	-0.013448000
Si	2.042781000	-1.143903000	-0.089816000
O	-0.864808000	-2.004443000	0.734717000
C	-0.631696000	3.427490000	-0.944495000
H	-0.204522000	3.538800000	-1.948330000
H	-0.513729000	4.381525000	-0.411816000
H	-1.702134000	3.230437000	-1.061267000
C	2.230747000	-0.989750000	1.803751000
H	2.385515000	0.051804000	2.107817000
H	3.075708000	-1.586278000	2.175908000
H	1.309745000	-1.352274000	2.272681000
C	-1.158398000	-1.013613000	0.050088000
C	-2.694478000	-0.726429000	-0.074583000
C	3.694184000	-0.532960000	-0.843320000
H	3.678797000	-0.642209000	-1.934510000
H	3.893631000	0.519039000	-0.614998000
H	4.529373000	-1.130715000	-0.452422000
C	2.022413000	-3.014991000	-0.453929000
H	1.990738000	-3.202191000	-1.533929000
H	2.917528000	-3.502632000	-0.043017000
H	1.130889000	-3.457496000	0.000647000
C	2.079025000	2.660551000	0.063260000
H	2.686404000	2.060836000	0.749060000
H	2.553458000	2.627806000	-0.923928000
H	2.091137000	3.700877000	0.416243000
C	-0.338173000	2.108372000	1.794322000
H	0.186185000	1.358695000	2.396911000

H	-0.160997000	3.100964000	2.232373000
H	-1.409635000	1.890219000	1.862862000
C	-3.009044000	0.638366000	-0.683712000
H	-4.090192000	0.743024000	-0.849622000
H	-2.696917000	1.449528000	-0.019531000
H	-2.497253000	0.771654000	-1.643613000
C	-3.336950000	-0.836256000	1.313687000
H	-2.953946000	-0.055960000	1.981889000
H	-4.427305000	-0.722595000	1.244012000
H	-3.104872000	-1.806014000	1.762693000
C	-3.247975000	-1.832010000	-0.990689000
H	-4.337002000	-1.731288000	-1.101978000
H	-2.790557000	-1.771223000	-1.984918000
H	-3.025193000	-2.817813000	-0.569616000
Si	0.160681000	-0.089949000	-1.053423000

Optimized Cartesian coordinates for anion 11



11

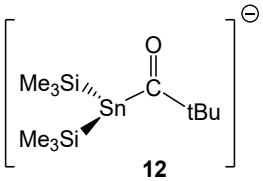
Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00Atm.
Zero-point correction= 0.354860 (Hartree/Particle)
Thermal correction to Energy= 0.379879
Thermal correction to Enthalpy= 0.380823
Thermal correction to Gibbs Free Energy= 0.302773
Sum of electronic and zero-point Energies= -3164.253612
Sum of electronic and thermal Energies= -3164.228594
Sum of electronic and thermal Enthalpies= -3164.227649
Sum of electronic and thermal Free Energies= -3164.305699
Number of imaginary frequencies: 0

Charge = -1 Multiplicity = 1

Si	0.431064000	2.025169000	0.114362000
Si	1.949485000	-1.246714000	0.037618000
O	-0.963628000	-1.505303000	1.301997000
C	-0.505912000	3.483994000	-0.691554000
H	-0.192537000	3.600378000	-1.735793000
H	-0.296111000	4.422781000	-0.159810000
H	-1.588756000	3.322163000	-0.685558000
C	2.327091000	-0.968307000	1.886362000
H	2.569271000	0.079583000	2.094851000
H	3.167061000	-1.591423000	2.224976000

H	1.432739000	-1.230943000	2.461016000
C	-1.252140000	-0.796713000	0.336118000
C	-2.769523000	-0.626416000	0.014734000
C	3.575349000	-0.905283000	-0.909598000
H	3.459588000	-1.157067000	-1.970616000
H	3.851481000	0.153672000	-0.850856000
H	4.404719000	-1.499668000	-0.501663000
C	1.617601000	-3.114712000	-0.132533000
H	1.457966000	-3.388379000	-1.182120000
H	2.448905000	-3.715092000	0.262849000
H	0.708668000	-3.359319000	0.427255000
C	2.258597000	2.574655000	0.056974000
H	2.896188000	1.883641000	0.617528000
H	2.624008000	2.601679000	-0.976202000
H	2.372691000	3.577217000	0.491706000
C	-0.083161000	2.020321000	1.950750000
H	0.407069000	1.190879000	2.470297000
H	0.161387000	2.962043000	2.461996000
H	-1.162832000	1.849152000	2.033861000
C	-3.068062000	0.788490000	-0.485130000
H	-4.126212000	0.880681000	-0.765320000
H	-2.857767000	1.531148000	0.292263000
H	-2.456489000	1.033132000	-1.360715000
C	-3.615183000	-0.939294000	1.250925000
H	-3.387870000	-0.239328000	2.063089000
H	-4.684392000	-0.858988000	1.013277000
H	-3.405239000	-1.946419000	1.621162000
C	-3.076771000	-1.637907000	-1.104572000
H	-4.137728000	-1.582051000	-1.387232000
H	-2.464121000	-1.429348000	-1.988004000
H	-2.860714000	-2.660066000	-0.772687000
Ge	0.112283000	-0.079968000	-0.993066000

Optimized Cartesian coordinates for anion 12



12

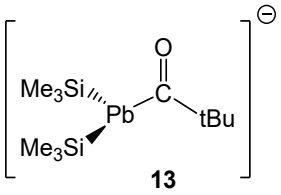
Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.352249 (Hartree/Particle)
Thermal correction to Energy= 0.378666
Thermal correction to Enthalpy= 0.379611
Thermal correction to Gibbs Free Energy= 0.295506
Sum of electronic and zero-point Energies= -1092.630678

Sum of electronic and thermal Energies= -1092.604260
Sum of electronic and thermal Enthalpies= -1092.603316
Sum of electronic and thermal Free Energies= -1092.687421
Number of imaginary frequencies: 0

Charge = -1 Multiplicity = 1

Sn	0.169149000	-0.081829000	-1.142091000
Si	0.314084000	2.176539000	0.250206000
Si	2.128801000	-1.229844000	0.238207000
O	-1.035175000	-1.829004000	1.202644000
C	-0.662539000	3.621718000	-0.540561000
H	-0.277611000	3.835530000	-1.544936000
H	-0.573462000	4.535061000	0.065120000
H	-1.726601000	3.378823000	-0.639413000
C	2.172318000	-0.926246000	2.121470000
H	2.412903000	0.117344000	2.354095000
H	2.922121000	-1.566587000	2.608540000
H	1.187127000	-1.156156000	2.540540000
C	-1.372388000	-1.004958000	0.359670000
C	-2.908818000	-0.739939000	0.199055000
C	3.861079000	-0.725953000	-0.407411000
H	3.960578000	-0.953617000	-1.475721000
H	4.032953000	0.349286000	-0.279135000
H	4.651667000	-1.265399000	0.133756000
C	2.041196000	-3.127035000	0.042084000
H	2.082692000	-3.417637000	-1.014627000
H	2.869125000	-3.621083000	0.570739000
H	1.093751000	-3.485391000	0.459611000
C	2.110980000	2.825023000	0.356215000
H	2.735208000	2.144651000	0.946018000
H	2.558618000	2.906138000	-0.641380000
H	2.142919000	3.816817000	0.829559000
C	-0.292269000	2.088699000	2.060836000
H	0.242213000	1.301688000	2.602707000
H	-0.134929000	3.044554000	2.581628000
H	-1.359642000	1.844941000	2.106808000
C	-3.182965000	0.662365000	-0.343552000
H	-4.257337000	0.800793000	-0.525630000
H	-2.859811000	1.430427000	0.366371000
H	-2.651837000	0.834638000	-1.286842000
C	-3.619810000	-0.934672000	1.541338000
H	-3.275763000	-0.192909000	2.271752000
H	-4.706098000	-0.823054000	1.423200000
H	-3.403734000	-1.925653000	1.950616000
C	-3.394870000	-1.790027000	-0.814644000
H	-4.471149000	-1.670503000	-1.001816000
H	-2.864466000	-1.684405000	-1.768175000
H	-3.217353000	-2.802394000	-0.434760000

Optimized Cartesian coordinates for anion 13



13

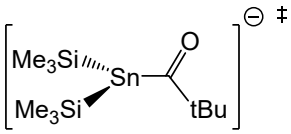
Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.351769 (Hartree/Particle)
Thermal correction to Energy= 0.378422
Thermal correction to Enthalpy= 0.379366
Thermal correction to Gibbs Free Energy= 0.294284
Sum of electronic and zero-point Energies= -1092.680238
Sum of electronic and thermal Energies= -1092.653585
Sum of electronic and thermal Enthalpies= -1092.652641
Sum of electronic and thermal Free Energies= -1092.737724
Number of imaginary frequencies: 0

Charge = -1 Multiplicity = 1

Si	0.352873000	2.223191000	0.431464000
Si	2.098788000	-1.277141000	0.472600000
O	-1.144080000	-1.678611000	1.517627000
C	-0.620420000	3.683862000	-0.340410000
H	-0.259333000	3.895712000	-1.354151000
H	-0.509088000	4.596939000	0.262515000
H	-1.689194000	3.450368000	-0.412240000
C	2.141265000	-0.884712000	2.339430000
H	2.415117000	0.160013000	2.525212000
H	2.866781000	-1.527008000	2.859900000
H	1.146579000	-1.062208000	2.761385000
C	-1.472102000	-0.954638000	0.588456000
C	-3.006152000	-0.707947000	0.368345000
C	3.868839000	-0.902232000	-0.164199000
H	3.975359000	-1.183508000	-1.219095000
H	4.095519000	0.167628000	-0.082335000
H	4.621615000	-1.455794000	0.415824000
C	1.913247000	-3.177241000	0.383410000
H	1.968950000	-3.536068000	-0.651613000
H	2.694282000	-3.684800000	0.968216000
H	0.934795000	-3.456872000	0.789978000
C	2.156413000	2.859046000	0.536337000
H	2.789471000	2.138902000	1.066933000
H	2.580340000	2.995797000	-0.465818000
H	2.210054000	3.820930000	1.066764000
C	-0.252271000	2.143104000	2.243315000

H	0.285782000	1.367630000	2.797505000
H	-0.103015000	3.106619000	2.752616000
H	-1.317943000	1.891774000	2.289352000
C	-3.258494000	0.718686000	-0.122016000
H	-4.327275000	0.871388000	-0.324562000
H	-2.946512000	1.454498000	0.626618000
H	-2.702385000	0.926318000	-1.042721000
C	-3.782327000	-0.967078000	1.662021000
H	-3.478506000	-0.260225000	2.442683000
H	-4.862118000	-0.854808000	1.494741000
H	-3.581527000	-1.974574000	2.037900000
C	-3.434674000	-1.710437000	-0.715647000
H	-4.499638000	-1.582262000	-0.953625000
H	-2.856066000	-1.563618000	-1.634905000
H	-3.277600000	-2.740633000	-0.375678000
Pb	0.160183000	-0.077810000	-1.025775000

Optimized Cartesian coordinates for TS of inversion at Sn in anion 12



TS-inversion

Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.352618 (Hartree/Particle)
Thermal correction to Energy= 0.378131
Thermal correction to Enthalpy= 0.379076
Thermal correction to Gibbs Free Energy= 0.296497
Sum of electronic and zero-point Energies= -1092.600288
Sum of electronic and thermal Energies= -1092.574775
Sum of electronic and thermal Enthalpies= -1092.573831
Sum of electronic and thermal Free Energies= -1092.656409
Number of imaginary frequencies: 1

Charge = -1 Multiplicity = 1

Sn	-0.166031000	-0.025722000	0.024425000
C	1.547336000	-1.363175000	0.041907000
Si	-0.290179000	2.518537000	0.002024000
Si	-2.293479000	-1.426625000	-0.011154000
O	1.371750000	-2.587775000	0.064117000
C	3.019333000	-0.855385000	-0.005785000
C	3.130104000	0.665274000	0.064727000
H	2.697428000	1.047621000	0.996094000
H	4.182227000	0.975924000	0.023775000

H	2.606822000	1.136408000	-0.775592000
C	3.762826000	-1.485581000	1.181405000
H	4.830191000	-1.226229000	1.154087000
H	3.342914000	-1.127846000	2.129156000
H	3.658738000	-2.574559000	1.153486000
C	3.618406000	-1.358462000	-1.328698000
H	3.083103000	-0.919688000	-2.179060000
H	4.680258000	-1.085644000	-1.404348000
H	3.525261000	-2.447253000	-1.392706000
C	-2.060353000	-2.959627000	-1.112809000
H	-1.129176000	-3.465779000	-0.835255000
H	-2.899512000	-3.661049000	-1.002695000
H	-1.980112000	-2.666802000	-2.165542000
C	-3.783447000	-0.441461000	-0.681623000
H	-4.686341000	-1.067717000	-0.689298000
H	-3.983099000	0.439802000	-0.061844000
H	-3.588723000	-0.097535000	-1.703438000
C	-2.840428000	-2.091450000	1.692139000
H	-3.049856000	-1.263951000	2.379397000
H	-3.742305000	-2.715175000	1.604295000
H	-2.039560000	-2.695684000	2.132672000
C	-2.126400000	3.025300000	0.085462000
H	-2.220012000	4.119734000	0.065837000
H	-2.688083000	2.614792000	-0.760363000
H	-2.587060000	2.656227000	1.008405000
C	0.424544000	3.361746000	-1.554697000
H	0.280746000	4.451406000	-1.512444000
H	1.498413000	3.163151000	-1.647520000
H	-0.063847000	2.973042000	-2.454444000
C	0.566046000	3.402408000	1.461231000
H	1.643282000	3.202140000	1.462813000
H	0.420941000	4.490647000	1.394807000
H	0.158326000	3.048029000	2.413799000

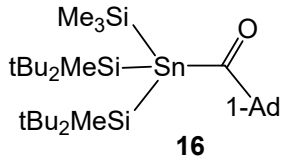
Optimized Cartesian coordinates for TS of rotation about the Sn-C bond in anion 12

Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.352196 (Hartree/Particle)
Thermal correction to Energy= 0.377774
Thermal correction to Enthalpy= 0.378718
Thermal correction to Gibbs Free Energy= 0.297149
Sum of electronic and zero-point Energies= -1092.626955
Sum of electronic and thermal Energies= -1092.601376
Sum of electronic and thermal Enthalpies= -1092.600432
Sum of electronic and thermal Free Energies= -1092.682001
Number of imaginary frequencies: 1

Charge = -1 Multiplicity = 1

Sn	-0.114531000	-0.059775000	-1.066500000
Si	-1.853769000	-1.603347000	0.220411000
Si	-0.785416000	2.166673000	0.213754000
O	1.285634000	-0.627209000	1.772144000
C	-1.492567000	-3.438255000	-0.194530000
H	-1.479838000	-3.599733000	-1.279015000
H	-2.250526000	-4.101020000	0.247430000
H	-0.511563000	-3.732286000	0.198233000
C	-0.983491000	2.066567000	2.109382000
H	-1.955674000	1.634165000	2.371209000
H	-0.916797000	3.063329000	2.568732000
H	-0.211009000	1.419343000	2.538081000
C	1.542693000	-0.447684000	0.589706000
C	3.042569000	-0.508800000	0.149309000
C	-2.424656000	2.901896000	-0.446800000
H	-2.366282000	3.075392000	-1.527966000
H	-3.259203000	2.214240000	-0.266036000
H	-2.656035000	3.857740000	0.044663000
C	0.515786000	3.542379000	-0.074360000
H	0.699411000	3.696268000	-1.144209000
H	0.179780000	4.494380000	0.361350000
H	1.470618000	3.274632000	0.392591000
C	-3.644049000	-1.302566000	-0.391398000
H	-3.982957000	-0.296920000	-0.114908000
H	-3.711420000	-1.387777000	-1.482593000
H	-4.336822000	-2.030382000	0.054837000
C	-1.949202000	-1.545247000	2.123102000
H	-2.440683000	-0.626807000	2.460914000
H	-2.516787000	-2.403642000	2.511216000
H	-0.939938000	-1.553111000	2.545855000
C	3.197378000	-1.721329000	-0.780699000
H	4.233779000	-1.796310000	-1.137434000
H	2.947299000	-2.651338000	-0.256214000
H	2.536453000	-1.634935000	-1.650228000
C	3.957984000	-0.659266000	1.366682000
H	3.714050000	-1.565809000	1.929580000
H	5.009287000	-0.709329000	1.052860000
H	3.837121000	0.186630000	2.051761000
C	3.383948000	0.776571000	-0.613690000
H	4.418391000	0.738602000	-0.981187000
H	2.717581000	0.913188000	-1.472875000
H	3.283473000	1.655766000	0.032653000

Optimized Cartesian coordinates for 16



16

Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.926381 (Hartree/Particle)
Thermal correction to Energy= 0.976278
Thermal correction to Enthalpy= 0.977222
Thermal correction to Gibbs Free Energy= 0.848820
Sum of electronic and zero-point Energies= -2205.107711
Sum of electronic and thermal Energies= -2205.057815
Sum of electronic and thermal Enthalpies= -2205.056871
Sum of electronic and thermal Free Energies= -2205.185273
Number of imaginary frequencies: 0

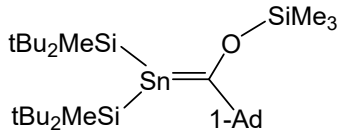
Charge = 0 Multiplicity = 1

Sn	0.410252000	0.014843000	0.191669000
Si	1.381712000	-2.379429000	-0.451359000
Si	1.511101000	2.242219000	-0.759807000
O	-1.231238000	-0.040175000	-2.349316000
C	2.497644000	-3.116607000	0.956556000
C	3.576736000	-2.122813000	1.407133000
H	4.237609000	-1.819787000	0.590231000
H	4.202493000	-2.571555000	2.192409000
H	3.134655000	-1.215024000	1.824404000
C	3.178649000	-4.420031000	0.507057000
H	2.461188000	-5.155078000	0.124278000
H	3.693450000	-4.881492000	1.362543000
H	3.933024000	-4.245196000	-0.265376000
C	1.600428000	-3.441553000	2.161016000
H	1.049769000	-2.563477000	2.507016000
H	2.211744000	-3.795721000	3.003882000
H	0.870965000	-4.226507000	1.933698000
C	2.214635000	-2.402928000	-2.200917000
C	3.616960000	-1.779588000	-2.152821000
H	3.601807000	-0.778763000	-1.707661000
H	4.023868000	-1.681664000	-3.169529000
H	4.321724000	-2.390240000	-1.578788000
C	1.341519000	-1.596558000	-3.174175000
H	0.333044000	-2.010834000	-3.269476000
H	1.797292000	-1.602059000	-4.175129000
H	1.224800000	-0.555852000	-2.870576000
C	2.312155000	-3.836968000	-2.757089000
H	2.948291000	-4.491977000	-2.157347000

H	2.743164000	-3.804236000	-3.768478000
H	1.326936000	-4.308049000	-2.844054000
C	-0.185570000	-3.450182000	-0.559580000
H	-0.804852000	-3.345563000	0.337301000
H	0.065789000	-4.511157000	-0.674249000
H	-0.791202000	-3.147840000	-1.420166000
C	3.039729000	2.737961000	0.333698000
C	2.603288000	3.389720000	1.653414000
H	3.475337000	3.557905000	2.301958000
H	1.901704000	2.757611000	2.208237000
H	2.123197000	4.360123000	1.496853000
C	3.965869000	3.698542000	-0.433995000
H	4.825489000	3.968282000	0.197066000
H	3.469368000	4.629034000	-0.720328000
H	4.364093000	3.236605000	-1.343728000
C	3.845465000	1.471723000	0.660070000
H	4.129755000	0.914000000	-0.239326000
H	3.287301000	0.791903000	1.308638000
H	4.772904000	1.734627000	1.189563000
C	0.162947000	3.641685000	-0.893197000
C	0.811485000	5.020100000	-1.110493000
H	1.390240000	5.355733000	-0.244925000
H	0.027398000	5.771437000	-1.285398000
H	1.469531000	5.033517000	-1.986817000
C	-0.721092000	3.704047000	0.359230000
H	-1.217767000	2.748033000	0.555668000
H	-1.507737000	4.462480000	0.234640000
H	-0.152011000	3.967729000	1.254934000
C	-0.728803000	3.352799000	-2.114175000
H	-0.171744000	3.426945000	-3.053861000
H	-1.542657000	4.091399000	-2.159199000
H	-1.184549000	2.362426000	-2.082066000
C	2.144236000	1.970818000	-2.525716000
H	3.002175000	1.293398000	-2.564352000
H	2.451864000	2.932466000	-2.954420000
H	1.356561000	1.555864000	-3.160575000
C	-1.455895000	-0.121182000	-1.156147000
C	-2.903806000	-0.283187000	-0.679359000
C	-3.001140000	-0.659962000	0.797485000
H	-2.502404000	0.108466000	1.399182000
H	-2.473755000	-1.604952000	0.977755000
C	-4.469061000	-0.770568000	1.229887000
H	-4.514527000	-1.048168000	2.291140000
C	-5.153889000	0.588957000	1.019612000
H	-6.202423000	0.537216000	1.341557000
H	-4.664499000	1.355540000	1.636137000
C	-5.077185000	0.977938000	-0.465382000
H	-5.562458000	1.950712000	-0.618836000

C	-3.605959000	1.079107000	-0.895171000
H	-3.095499000	1.858338000	-0.314299000
H	-3.527723000	1.359231000	-1.952352000
C	-5.172883000	-1.841408000	0.382100000
H	-6.221682000	-1.938042000	0.693231000
H	-4.697896000	-2.818982000	0.541489000
C	-5.094027000	-1.452037000	-1.102691000
H	-5.594081000	-2.216231000	-1.711902000
C	-5.781416000	-0.093355000	-1.313010000
H	-5.746986000	0.184880000	-2.374708000
H	-6.840533000	-0.159689000	-1.030030000
C	-3.621249000	-1.353042000	-1.528328000
H	-3.534257000	-1.089844000	-2.588070000
H	-3.122840000	-2.322135000	-1.391659000
Si	-0.047486000	0.161019000	2.797448000
C	-0.938824000	1.760142000	3.295837000
H	-1.173873000	1.699423000	4.366228000
H	-0.316176000	2.644818000	3.138325000
H	-1.878039000	1.910195000	2.754009000
C	1.569204000	0.137831000	3.795957000
H	1.321083000	0.359551000	4.842144000
H	2.057626000	-0.840645000	3.772582000
H	2.292574000	0.887135000	3.461693000
C	-1.122912000	-1.256684000	3.485130000
H	-0.810265000	-1.460479000	4.516763000
H	-2.176756000	-0.962744000	3.507592000
H	-1.051308000	-2.193373000	2.926063000

Optimized Cartesian coordinates for 17



17

Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.924788 (Hartree/Particle)
Thermal correction to Energy= 0.974842
Thermal correction to Enthalpy= 0.975786
Thermal correction to Gibbs Free Energy= 0.846676
Sum of electronic and zero-point Energies= -2205.071369
Sum of electronic and thermal Energies= -2205.021315
Sum of electronic and thermal Enthalpies= -2205.020371
Sum of electronic and thermal Free Energies= -2205.149481
Number of imaginary frequencies: 0

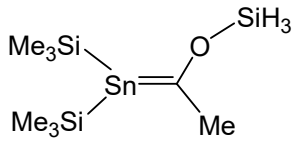
Charge = 0 Multiplicity = 1

Sn	-0.690269000	-0.202937000	-0.958449000
Si	-0.613020000	-2.539055000	0.403933000
Si	-2.444765000	1.675648000	-0.122162000
O	1.166484000	0.973849000	1.241258000
C	-1.288567000	-3.904459000	-0.803116000
C	-2.577919000	-3.469180000	-1.513716000
H	-3.390576000	-3.253456000	-0.812981000
H	-2.925874000	-4.267595000	-2.185451000
H	-2.415611000	-2.576242000	-2.128336000
C	-1.553533000	-5.227377000	-0.065945000
H	-0.681958000	-5.575006000	0.500375000
H	-1.804952000	-6.015300000	-0.791380000
H	-2.398284000	-5.146312000	0.626069000
C	-0.205113000	-4.140916000	-1.871679000
H	0.059328000	-3.212330000	-2.393033000
H	-0.571888000	-4.850761000	-2.627433000
H	0.710011000	-4.565412000	-1.443987000
C	-1.556918000	-2.392632000	2.101106000
C	-3.064011000	-2.241099000	1.875935000
H	-3.277407000	-1.401737000	1.208890000
H	-3.579480000	-2.049596000	2.828745000
H	-3.508700000	-3.141438000	1.438780000
C	-1.037133000	-1.136946000	2.816976000
H	0.033501000	-1.208985000	3.035874000
H	-1.559216000	-1.002869000	3.776498000
H	-1.193482000	-0.236006000	2.218643000
C	-1.293581000	-3.602292000	3.014371000
H	-1.639782000	-4.544241000	2.581274000
H	-1.828488000	-3.466748000	3.966477000
H	-0.230923000	-3.712888000	3.256006000
C	1.137435000	-3.098456000	0.912389000
H	1.855500000	-3.083194000	0.091361000
H	1.102268000	-4.123346000	1.301780000
H	1.522860000	-2.451924000	1.706784000
C	-4.098555000	1.334405000	-1.112763000
C	-3.909765000	1.562940000	-2.620539000
H	-4.817578000	1.263056000	-3.165311000
H	-3.074884000	0.977976000	-3.024386000
H	-3.726598000	2.616095000	-2.855918000
C	-5.260217000	2.211711000	-0.611788000
H	-6.178895000	1.961884000	-1.164224000
H	-5.078788000	3.279437000	-0.754120000
H	-5.467709000	2.045264000	0.451023000
C	-4.515273000	-0.129272000	-0.895228000
H	-4.731492000	-0.338071000	0.158023000
H	-3.752537000	-0.838837000	-1.231159000
H	-5.433138000	-0.349502000	-1.460849000

C	-1.658156000	3.409231000	-0.600676000
C	-2.714106000	4.526014000	-0.647769000
H	-3.410449000	4.401649000	-1.482334000
H	-2.221224000	5.501039000	-0.783645000
H	-3.299865000	4.585042000	0.276863000
C	-0.928110000	3.371937000	-1.953317000
H	-0.104764000	2.649940000	-1.953029000
H	-0.500797000	4.361245000	-2.177751000
H	-1.590161000	3.104250000	-2.781382000
C	-0.632009000	3.787333000	0.479984000
H	-1.108540000	3.940800000	1.454281000
H	-0.130968000	4.729922000	0.211334000
H	0.139963000	3.021742000	0.592980000
C	-2.960904000	1.818464000	1.706220000
H	-3.533859000	0.939422000	2.019409000
H	-3.584690000	2.705860000	1.870902000
H	-2.090925000	1.893379000	2.362526000
C	1.193595000	0.275672000	0.128699000
C	2.549066000	0.103442000	-0.533226000
C	2.521266000	-0.892218000	-1.710093000
H	1.739437000	-0.597356000	-2.421306000
H	2.254620000	-1.891487000	-1.354150000
C	3.881528000	-0.938318000	-2.421401000
H	3.823020000	-1.664018000	-3.242265000
C	4.207779000	0.452651000	-2.984211000
H	5.170985000	0.433581000	-3.511220000
H	3.443511000	0.751443000	-3.713336000
C	4.259161000	1.464467000	-1.830659000
H	4.477940000	2.466309000	-2.222917000
C	2.896795000	1.508529000	-1.121933000
H	2.111532000	1.802367000	-1.828672000
H	2.907719000	2.254890000	-0.320772000
C	4.973735000	-1.363560000	-1.429472000
H	5.947174000	-1.417477000	-1.935130000
H	4.757292000	-2.366168000	-1.036580000
C	5.030270000	-0.349751000	-0.280287000
H	5.802706000	-0.647179000	0.441035000
C	5.350443000	1.046832000	-0.834076000
H	5.412441000	1.773604000	-0.012309000
H	6.329913000	1.040346000	-1.330107000
C	3.674096000	-0.309508000	0.438169000
H	3.741331000	0.407578000	1.259188000
H	3.443384000	-1.287358000	0.874945000
Si	1.859552000	1.534063000	2.703083000
C	2.681428000	0.103086000	3.606793000
H	2.330922000	-0.859734000	3.225103000
H	3.771674000	0.121032000	3.519310000
H	2.422140000	0.153660000	4.670074000

C	3.031828000	2.952389000	2.344315000
H	3.942847000	2.638144000	1.827393000
H	2.533628000	3.715031000	1.736243000
H	3.325007000	3.420835000	3.291823000
C	0.416717000	2.152187000	3.711944000
H	-0.298527000	1.348545000	3.908002000
H	0.786349000	2.520128000	4.676787000
H	-0.106803000	2.972128000	3.215062000

Optimized Cartesian coordinates for 18



18

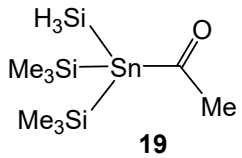
Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.296289 (Hartree/Particle)
Thermal correction to Energy= 0.321278
Thermal correction to Enthalpy= 0.322223
Thermal correction to Gibbs Free Energy= 0.239662
Sum of electronic and zero-point Energies= -1265.943022
Sum of electronic and thermal Energies= -1265.918033
Sum of electronic and thermal Enthalpies= -1265.917088
Sum of electronic and thermal Free Energies= -1265.999649
Number of imaginary frequencies: 0

Charge = 0 Multiplicity = 1

Sn	0.251153000	0.058145000	-0.821811000
Si	2.508041000	0.814934000	0.264898000
Si	-0.509025000	-2.238494000	0.166808000
O	-2.444143000	0.810941000	0.236343000
C	3.945614000	0.364996000	-0.883243000
C	2.749870000	-0.112356000	1.901623000
C	2.578692000	2.676791000	0.614806000
H	2.437522000	3.266527000	-0.297374000
H	3.560644000	2.934640000	1.031556000
H	1.815820000	2.975788000	1.341292000
C	0.820678000	-3.556548000	-0.133319000
C	-2.131524000	-2.803613000	-0.628067000
C	-0.783956000	-2.066461000	2.034367000
H	0.146660000	-1.798076000	2.545236000
H	-1.153231000	-3.007691000	2.462022000
H	-1.520132000	-1.281717000	2.237406000
C	-1.215781000	1.329048000	0.006679000
C	-1.129616000	2.819073000	0.125803000

Si	-3.979853000	1.514238000	0.273080000
H	-4.067031000	2.543324000	1.340899000
H	-4.288614000	2.132861000	-1.042668000
H	-4.887081000	0.381843000	0.558070000
H	-1.365696000	3.129492000	1.154871000
H	-0.129896000	3.180167000	-0.120032000
H	-1.845581000	3.327889000	-0.539246000
H	1.969211000	0.153255000	2.622158000
H	3.725003000	0.131015000	2.343098000
H	2.708481000	-1.196255000	1.748851000
H	3.962538000	-0.710277000	-1.093114000
H	4.902865000	0.633204000	-0.418724000
H	1.771701000	-3.275654000	0.332765000
H	0.507459000	-4.516656000	0.295734000
H	-2.025080000	-2.931265000	-1.710480000
H	-2.920600000	-2.066180000	-0.448526000
H	-2.452470000	-3.761436000	-0.199248000
H	3.870166000	0.892221000	-1.840256000
H	1.000692000	-3.706855000	-1.203353000

Optimized Cartesian coordinates for 19



19

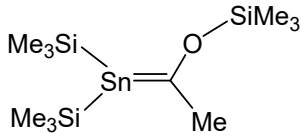
Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.294481 (Hartree/Particle)
Thermal correction to Energy= 0.320540
Thermal correction to Enthalpy= 0.321484
Thermal correction to Gibbs Free Energy= 0.235470
Sum of electronic and zero-point Energies= -1265.976733
Sum of electronic and thermal Energies= -1265.950675
Sum of electronic and thermal Enthalpies= -1265.949730
Sum of electronic and thermal Free Energies= -1266.035745
Number of imaginary frequencies: 0

Charge = 0 Multiplicity = 1

Sn	-0.013830000	0.441800000	0.218648000
Si	-2.101474000	-1.072994000	-0.088456000
Si	2.131241000	-1.003833000	0.012253000
O	0.284117000	1.248355000	-2.699413000
C	-3.679720000	-0.219585000	0.509995000
H	-3.614963000	0.041093000	1.571800000
H	-4.543291000	-0.882829000	0.375584000
H	-3.870716000	0.700323000	-0.052892000

C	1.877004000	-2.167733000	-1.456544000
H	1.056073000	-2.869327000	-1.270721000
H	2.785882000	-2.753467000	-1.642108000
H	1.641047000	-1.601560000	-2.363726000
C	0.063048000	1.765067000	-1.622021000
C	-0.154994000	3.254161000	-1.480976000
C	2.390075000	-2.015372000	1.590187000
H	2.556282000	-1.367717000	2.457718000
H	1.519152000	-2.645484000	1.801171000
H	3.264089000	-2.669869000	1.483752000
C	3.635083000	0.096047000	-0.306379000
H	3.804624000	0.793151000	0.521178000
H	4.537602000	-0.516353000	-0.424676000
H	3.499637000	0.679907000	-1.223058000
C	-1.834329000	-2.668873000	0.894503000
H	-0.928661000	-3.187196000	0.560882000
H	-1.732533000	-2.467152000	1.966235000
H	-2.683301000	-3.349779000	0.756686000
C	-2.243008000	-1.481778000	-1.927273000
H	-1.345124000	-1.997334000	-2.283092000
H	-3.107984000	-2.131310000	-2.109971000
H	-2.358669000	-0.574769000	-2.529192000
H	-1.115238000	3.441180000	-0.985370000
H	-0.128175000	3.748469000	-2.457428000
H	0.622345000	3.670950000	-0.828330000
Si	-0.123369000	1.919305000	2.344375000
H	-1.289825000	2.849839000	2.296439000
H	-0.262006000	1.091231000	3.578299000
H	1.103799000	2.754852000	2.500385000

Optimized Cartesian coordinates for 20



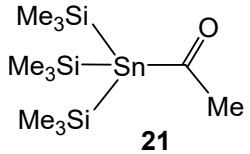
20

Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.383038 (Hartree/Particle)
Thermal correction to Energy= 0.413195
Thermal correction to Enthalpy= 0.414139
Thermal correction to Gibbs Free Energy= 0.320999
Sum of electronic and zero-point Energies= -1383.828496
Sum of electronic and thermal Energies= -1383.798339
Sum of electronic and thermal Enthalpies= -1383.797395
Sum of electronic and thermal Free Energies= -1383.890535
Number of imaginary frequencies: 0

Charge = 0 Multiplicity = 1

Sn	-0.888668000	-0.014892000	-0.921007000
Si	-2.845852000	-1.208855000	0.344575000
Si	-0.498329000	2.326345000	0.180608000
O	1.920451000	-0.258610000	0.093122000
C	-4.480063000	-0.808743000	-0.528127000
C	-2.973113000	-0.581609000	2.132080000
C	-2.656959000	-3.096234000	0.410277000
H	-2.525030000	-3.528982000	-0.587260000
H	-3.558658000	-3.538731000	0.852708000
H	-1.803367000	-3.390288000	1.030265000
C	-2.110205000	3.325290000	0.224465000
C	0.798246000	3.303846000	-0.797664000
C	0.142242000	2.116541000	1.953007000
H	-0.611271000	1.638774000	2.587579000
H	0.403675000	3.086799000	2.395019000
H	1.034638000	1.482220000	1.949903000
C	0.832595000	-0.994769000	-0.142754000
C	1.018688000	-2.479524000	-0.053856000
Si	3.610686000	-0.517342000	0.162837000
H	1.285490000	-2.757125000	0.976005000
H	0.105626000	-3.008312000	-0.330346000
H	1.831367000	-2.832469000	-0.705245000
H	-2.056609000	-0.804524000	2.688605000
H	-3.816292000	-1.058866000	2.648709000
H	-3.128278000	0.502361000	2.163993000
H	-4.651702000	0.272771000	-0.568108000
H	-5.321740000	-1.264754000	0.008347000
H	-2.883880000	2.805110000	0.800049000
H	-1.942116000	4.303346000	0.692680000
H	0.472645000	3.477571000	-1.828849000
H	1.742197000	2.749706000	-0.830023000
H	0.988194000	4.277221000	-0.327696000
H	-4.482941000	-1.187538000	-1.555799000
H	-2.499441000	3.495430000	-0.785370000
C	4.251409000	1.175114000	0.627057000
H	4.004309000	1.911397000	-0.144231000
H	3.802436000	1.510982000	1.567566000
H	5.339834000	1.163105000	0.752229000
C	4.030399000	-1.785721000	1.480957000
H	3.778098000	-2.804313000	1.171096000
H	5.105716000	-1.757216000	1.693713000
H	3.500549000	-1.568320000	2.414692000
C	4.192182000	-1.054150000	-1.536159000
H	3.829432000	-0.360394000	-2.301669000
H	5.287471000	-1.066594000	-1.579404000
H	3.835855000	-2.057183000	-1.791757000

Optimized Cartesian coordinates for 21



21

Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.381699 (Hartree/Particle)
Thermal correction to Energy= 0.413003
Thermal correction to Enthalpy= 0.413947
Thermal correction to Gibbs Free Energy= 0.316635
Sum of electronic and zero-point Energies= -1383.848936
Sum of electronic and thermal Energies= -1383.817632
Sum of electronic and thermal Enthalpies= -1383.816688
Sum of electronic and thermal Free Energies= -1383.914000
Number of imaginary frequencies: 0

Charge = 0 Multiplicity = 1

Sn	-0.033450000	-0.031812000	0.236898000
Si	0.585117000	2.381416000	-0.489818000
Si	1.837187000	-1.643244000	-0.540678000
O	1.262880000	-0.219592000	2.997048000
C	-0.919674000	3.528706000	-0.393976000
H	-1.721752000	3.184671000	-1.056341000
H	-0.645766000	4.547335000	-0.695664000
H	-1.320409000	3.574962000	0.624467000
C	3.506847000	-0.838610000	-0.166583000
H	3.636514000	0.089752000	-0.733600000
H	4.332103000	-1.513177000	-0.426295000
H	3.577961000	-0.599148000	0.899769000
C	0.164397000	-0.075876000	2.496247000
C	-1.077792000	0.078106000	3.347830000
C	1.678912000	-1.961983000	-2.401576000
H	0.725317000	-2.446516000	-2.638584000
H	1.733079000	-1.028172000	-2.971712000
H	2.486277000	-2.618556000	-2.748973000
C	1.713103000	-3.284606000	0.391889000
H	0.757090000	-3.783374000	0.199266000
H	2.518533000	-3.962376000	0.082596000
H	1.801752000	-3.120843000	1.471164000
C	1.200979000	2.326962000	-2.281036000
H	2.085221000	1.686668000	-2.371852000
H	0.431296000	1.934778000	-2.954918000
H	1.474493000	3.331735000	-2.626333000
C	1.960598000	3.046921000	0.623474000
H	2.840424000	2.395921000	0.592460000

H	2.264258000	4.050482000	0.300426000
H	1.632926000	3.108064000	1.666571000
H	-1.610327000	0.993650000	3.063512000
H	-0.824734000	0.099221000	4.412904000
H	-1.757271000	-0.758500000	3.141858000
Si	-2.414455000	-0.692633000	-0.542373000
C	-2.731315000	-2.530059000	-0.210228000
H	-3.742586000	-2.810858000	-0.529663000
H	-2.017520000	-3.156521000	-0.756193000
H	-2.635415000	-2.764620000	0.855562000
C	-2.562546000	-0.368733000	-2.404252000
H	-3.549407000	-0.679074000	-2.769631000
H	-2.438369000	0.695858000	-2.631529000
H	-1.803639000	-0.922727000	-2.967268000
C	-3.727357000	0.335748000	0.356509000
H	-3.570788000	1.407040000	0.189770000
H	-4.729116000	0.078240000	-0.009325000
H	-3.707478000	0.156386000	1.436649000

Optimized Cartesian coordinates for TS of the 1,3 silyl shift in Eq. 3

Thermochemistry
Temperature 298.15 Kelvin. Pressure 1.00 Atm.
Zero-point correction= 0.925803 (Hartree/Particle)
Thermal correction to Energy= 0.974653
Thermal correction to Enthalpy= 0.975597
Thermal correction to Gibbs Free Energy= 0.849796
Sum of electronic and zero-point Energies= -2205.060197
Sum of electronic and thermal Energies= -2205.011347
Sum of electronic and thermal Enthalpies= -2205.010403
Sum of electronic and thermal Free Energies= -2205.136204
Number of imaginary frequencies: 1

Charge = 0 Multiplicity = 1

Sn	-0.694855000	-0.083614000	0.575916000
Si	-1.027208000	2.547423000	0.123137000
Si	-1.528575000	-1.751795000	-1.374910000
O	1.773260000	-1.257218000	1.638261000
C	-2.337657000	3.090569000	1.462927000
C	-3.570139000	2.173751000	1.474657000
H	-4.074561000	2.132572000	0.504184000
H	-4.302371000	2.531855000	2.213167000
H	-3.302166000	1.149941000	1.761580000
C	-2.806590000	4.539549000	1.254763000
H	-1.970313000	5.245103000	1.190591000
H	-3.432522000	4.853878000	2.103147000
H	-3.413826000	4.649039000	0.350514000

C	-1.663939000	2.996964000	2.844480000
H	-1.255003000	1.996898000	3.028543000
H	-2.400274000	3.203848000	3.634905000
H	-0.850881000	3.721626000	2.959607000
C	-1.444545000	3.140921000	-1.682405000
C	-2.856313000	2.700898000	-2.087763000
H	-2.975687000	1.617067000	-2.000815000
H	-3.059163000	2.973431000	-3.133866000
H	-3.629049000	3.172905000	-1.472002000
C	-0.433058000	2.507381000	-2.651269000
H	0.584797000	2.873462000	-2.474038000
H	-0.690638000	2.766462000	-3.688925000
H	-0.418220000	1.417538000	-2.574949000
C	-1.325211000	4.668666000	-1.829821000
H	-2.056224000	5.213290000	-1.228142000
H	-1.495251000	4.950879000	-2.879733000
H	-0.327387000	5.029821000	-1.557549000
C	0.574710000	3.463683000	0.598259000
H	1.001991000	3.078287000	1.528407000
H	0.364897000	4.530295000	0.746090000
H	1.333468000	3.382665000	-0.185902000
C	-3.413957000	-2.109352000	-1.038016000
C	-3.595911000	-2.995281000	0.202593000
H	-4.665112000	-3.114284000	0.431921000
H	-3.117899000	-2.552192000	1.083542000
H	-3.183323000	-3.999301000	0.060766000
C	-4.081713000	-2.777912000	-2.253822000
H	-5.148465000	-2.944136000	-2.042477000
H	-3.646611000	-3.749118000	-2.499084000
H	-4.024485000	-2.148189000	-3.148569000
C	-4.144694000	-0.782092000	-0.786890000
H	-4.053651000	-0.093010000	-1.632869000
H	-3.776449000	-0.273068000	0.108141000
H	-5.218383000	-0.964741000	-0.632807000
C	-0.439778000	-3.372705000	-1.377604000
C	-1.103935000	-4.504917000	-2.178132000
H	-1.997086000	-4.892728000	-1.679244000
H	-0.401713000	-5.345483000	-2.281729000
H	-1.386581000	-4.192441000	-3.189767000
C	-0.133269000	-3.884760000	0.037059000
H	0.463418000	-3.163170000	0.600670000
H	0.452776000	-4.814200000	-0.015147000
H	-1.037072000	-4.097964000	0.614275000
C	0.893722000	-3.027885000	-2.057001000
H	0.769123000	-2.772279000	-3.114420000
H	1.583526000	-3.882871000	-2.002190000
H	1.381922000	-2.183033000	-1.562872000
C	-1.422268000	-1.059998000	-3.143383000

H	-2.131311000	-0.240754000	-3.297829000
H	-1.649720000	-1.845502000	-3.874797000
H	-0.421740000	-0.676550000	-3.362702000
C	1.538737000	-0.518223000	0.635729000
C	2.770348000	-0.073798000	-0.110185000
C	2.410270000	0.558277000	-1.461299000
H	1.690725000	1.364641000	-1.293797000
H	1.913695000	-0.180181000	-2.101952000
C	3.668344000	1.096667000	-2.152328000
H	3.388452000	1.533955000	-3.119158000
C	4.310599000	2.172501000	-1.263545000
H	5.203182000	2.585176000	-1.751887000
H	3.609969000	3.005208000	-1.116192000
C	4.693450000	1.557025000	0.091192000
H	5.142074000	2.325530000	0.734042000
C	3.438792000	1.009446000	0.788836000
H	2.730568000	1.819989000	0.986536000
H	3.700375000	0.556356000	1.752661000
C	4.659569000	-0.057388000	-2.369504000
H	5.556899000	0.307973000	-2.886495000
H	4.207276000	-0.825237000	-3.011562000
C	5.047126000	-0.666142000	-1.011886000
H	5.755678000	-1.490237000	-1.165528000
C	5.694454000	0.413697000	-0.131567000
H	5.996924000	-0.016958000	0.832268000
H	6.602840000	0.799411000	-0.613058000
C	3.794032000	-1.214884000	-0.311380000
H	4.051134000	-1.649496000	0.660569000
H	3.347739000	-2.012483000	-0.915054000
Si	0.512238000	-1.602749000	3.062095000
C	1.622360000	-3.055952000	3.556284000
H	1.338307000	-3.421052000	4.550217000
H	1.508004000	-3.891375000	2.855022000
H	2.680536000	-2.777581000	3.572682000
C	-1.217050000	-2.290538000	3.450701000
H	-1.191977000	-2.759837000	4.445757000
H	-1.967002000	-1.495646000	3.432667000
H	-1.510970000	-3.058403000	2.729744000
C	0.887536000	-0.091763000	4.123436000
H	1.269024000	-0.419679000	5.098753000
H	1.647347000	0.546160000	3.662201000
H	-0.011426000	0.507677000	4.288828000

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