

Supporting Information for

Fast Kinetics Studies of the Lewis Acid-Base Complexation of Transient Stannylenes with σ - and π -Donors in Solution

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Figure S1. (a) Transient UV-vis spectra from laser flash photolysis (lfp) of **1** in hexanes containing 0.025 M Et₂O at 25 °C, recorded 0.32-0.42 μ s (○) and 17.3-17.5 μ s (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [Et₂O]; the solid line is the least squares fit of the data to eq. 6. S6

Figure S2. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 0.025 M Et₂O, recorded 0.96-1.60 μ s (○) and 22.6-23.4 μ s (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [Et₂O]; the solid line is the least squares fit of the data to eq. 6. S6

Figure S3. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 0.025 M THF, recorded 0.51-0.70 μ s (○) and 34.7-35.0 μ s (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plots of $(\Delta A_0)_0 / (\Delta A_{res})_Q$ (●) and k_{decay} (□) vs. [THF]; the solid lines are the least squares fits of the data to eq. 7 and 5, respectively. S7

Figure S4. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 1.2 mM THF, recorded 0.64-1.28 μ s (○) and 34.7-35.4 μ s (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plots of k_{decay} vs. [THF]; the solid line is the least squares fit of the data to eq. 5. S7

Figure S5. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 0.025 M EtOAc, recorded 0.51-0.70 μ s (○) and 34.7-35.0 μ s (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [EtOAc]; the solid line is the least squares fit of the data to eq. 6. S8

Figure S6. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 0.025 M acetone, recorded 0.26-0.45 μ s (○) and 33.7-34.0 μ s (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [acetone]; the solid line is the least squares fit of the data to eq. 6. S8

Figure S7. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 0.025 M acetone, recorded 0.48-0.80 μ s (○) and 85-86 μ s (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plots of k_{decay} (○) and $(\Delta A_0)_0 / (\Delta A_{res})_Q$ (□) vs. [acetone]; the solid lines are the least squares fits of the data to eq. 5 and 7, respectively. S9

Figure S8. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 1.0 mM Et₂S, recorded 0.16-0.48 μ s (○) and 11.2-11.8 μ s (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. The absorption at ~460 nm is due to the distannene, formed during the laser pulse as a result of the intensity being too high. S9

(b) Plot of k_{decay} vs. $[\text{Et}_2\text{S}]$; the solid line is the least squares fit of the data to eq. 5.

Figure S9. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 1.0 mM Et_2S , recorded 0.32-0.64 μs ($\circ$) and 85.9-86.7 μs ($\square$) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of k_{decay} vs. $[\text{Et}_2\text{S}]$; the solid line is the least squares fit of the data to eq. 5. S10

Figure S10. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 1.0 mM THT, recorded 0.26-0.38 μs ($\circ$) and 35.7-35.9 μs ($\square$) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of k_{decay} vs. $[\text{THT}]$; the solid line is the least squares fit of the data to eq. 5. S10

Figure S11. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 0.6 mM THT, recorded 2.2-3.2 μs ($\circ$) and 172-173 μs ($\square$) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of k_{decay} vs. $[\text{THT}]$; the solid line is the least squares fit of the data to eq. 5. S11

Figure S12. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 1.0 mM $n\text{-BuNH}_2$, recorded 0.16-0.32 μs ($\circ$), 1.60-2.08 μs ($\square$) and 26.7-27.5 μs (Δ) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of k_{decay} vs. $[n\text{-BuNH}_2]$; the solid line is the least squares fit of the data to eq. 5. S11

Figure S13. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 0.5 mM $n\text{-BuNH}_2$, recorded 3.2-4.5 μs ($\circ$) and 81-83 μs ($\square$) after the laser pulse; the inset shows representative absorbance-time profiles at 340 and 400 nm. (b) Plot of k_{decay} vs. $[n\text{-BuNH}_2]$; the solid line is the least squares fit of the data to eq. 5. S12

Figure S14. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 5.0 mM Et_2NH , recorded 1.9-3.2 μs ($\circ$), 21.8-23.0 μs ($\square$), and 88-91 μs (Δ) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of k_{decay} vs. $[\text{Et}_2\text{NH}]$; the solid line is the least squares fit of the data to eq. 5. S12

Figure S15. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 1.0 mM Et_3N , recorded 4.0-4.2 μs ($\circ$), 10.3-10.5 μs ($\square$), and 34.4-34.6 μs (Δ) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of k_{decay} vs. $[\text{Et}_3\text{N}]$; the solid line is the least squares fit of the data to eq. 5. S13

Figure S16. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 1.0 mM Et_3N , recorded 4.5-5.8 μs ($\circ$) and 344-347 μs ($\square$) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of k_{decay} vs. $[\text{Et}_3\text{N}]$; the solid line is the least squares fit of the data to eq. 5. S13

Figure S17. Plots of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [1-hexene] for complexation of (a) SnMe_2 and (b) SnPh_2 with 1-hexene in hexanes at 25 $^\circ\text{C}$. The solid lines are the least squares fits of the data to eq. 6. S14

Figure S18. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 0.5 M cyclohexene, recorded 0.32-0.64 μs ($\circ$), 5.9-6.4 μs ($\square$), and 89-90 μs (Δ) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [cyclohexene]; the solid line is the least squares fit of the data to eq. 6. S14

Figure S19. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 0.5 M cyclohexene, recorded 0.32-0.64 μs ($\circ$), 5.9-6.4 μs ($\square$), and 89-90 μs (Δ) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [cyclohexene]; the solid line is the least squares fit of the data to eq. 6. S15

Figure S20. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 0.25 M 1-hexyne, recorded 0.16-0.48 μs ($\circ$), 4.3-4.8 μs ($\square$), and 89-90 μs (Δ) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [1-hexyne]; the solid line is the least squares fit of the data to eq. 6. S15

Figure S21. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 0.25 M 1-hexyne, recorded 0.64-0.96 μs ($\circ$), 5.9-6.2 μs ($\square$), and 89-90 μs (Δ) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [1-hexyne]; the solid line is the least squares fit of the data to eq. 6. S16

Figure S22. (a) Transient UV-vis spectra from lfp of (GeMe₂ photoprecursor) 1,1-dimethyl-3-phenylgermacyclopent-3-ene⁴ in hexanes containing 5.0 mM EtOAc, recorded 0.80-1.44 μs ($\bullet$), 5.92-6.88 μs ($\circ$), and 85.9-86.7 μs ($\square$) after the laser pulse; the inset shows representative absorbance-time profiles at 300 nm and 360 nm. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [EtOAc]; the solid line is the least squares fit of the data to eq. 6. S16

Figure S23. (a) Transient UV-vis spectra from lfp of (GeMe₂ photoprecursor) 1,1-dimethyl-3-phenylgermacyclopent-3-ene⁴ in hexanes containing 11.4 mM acetone, recorded 0.16-0.64 μs ($\bullet$), 4.3-5.3 μs ($\circ$), and 53.9-54.7 μs ($\square$) after the laser pulse; the inset shows representative absorbance-time profiles at 300 and 360 nm. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [acetone]; the solid line is the least squares fit of the data to eq. 6. S17

Figure S24. (a) Transient UV-vis spectra from lfp of (GePh₂ photoprecursor) 3,4-dimethyl-1,1-diphenylgermacyclopent-3-ene⁵ in hexanes containing 10.0 mM acetone, recorded 0.13-0.45 μs ($\bullet$), 5.6-6.0 μs ($\circ$), and 28.0-28.3 μs ($\square$) after the laser pulse; the inset shows representative absorbance-time profiles at 350 and 440 nm. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [acetone]; the solid line is the least squares fit of the data to eq. 6. S17

Computational Studies S18

Table S1. Calculated Electronic Energies, Enthalpies (298.15 K), and Free Energies (298.15 K) of the (1+2)-Cycloadducts of SnMe₂ and SnPh₂ with Propene, Propyne, and Isoprene, Calculated at the ω B97XD/def2-TZVP Level of Theory (energies in kcal mol⁻¹). ^a S18

Optimized Structures and Energies (ω B97XD/def2-TZVP) S19

Dimethylstannylene (SnMe₂) S19

	S4
Diphenylstannylene (SnPh ₂)	S19
Methanol (MeOH; 5)	S20
Dimethyl ether (Me ₂ O; 6')	S20
Diethyl ether (Et ₂ O; 6)	S21
Tetrahydrofuran (THF; 7)	S21
Ethyl acetate (EtOAc; 8)	S22
Acetone (Me ₂ CO; 9)	S22
Dimethylsulfide (Me ₂ S; 10')	S23
Diethylsulfide (Et ₂ S; 10)	S23
Tetrahydrothiophene (THT; 11)	S24
Methylamine (MeNH ₂ ; 12')	S24
Dimethylamine (Me ₂ NH; 13')	S25
Trimethylamine (NMe ₃ ; 14')	S25
Propene (15')	S26
Cyclohexene (16)	S26
Propyne (17')	S27
Isoprene (18)	S27
SnMe ₂ -MeOH Complex (5a)	S27
SnMe ₂ -Me ₂ O Complex (6a')	S28
SnMe ₂ -Et ₂ O Complex (6a)	S29
SnMe ₂ -THF Complex (7a)	S30
SnMe ₂ -EtOAc Complex (8a)	S31
SnMe ₂ -Me ₂ CO Complex (9a)	S32
SnMe ₂ -Me ₂ S Complex (10a')	S33
SnMe ₂ -Et ₂ S Complex (10a)	S34
SnMe ₂ -THT Complex (11a)	S35
SnMe ₂ -MeNH ₂ Complex (12a')	S36
SnMe ₂ -Me ₂ NH Complex (13a')	S37
SnMe ₂ -NMe ₃ Complex (14a')	S38
SnMe ₂ -propene Complex (15a')	S39
1,1,2-Trimethylstannirane (19a)	S40
SnMe ₂ -cyclohexene Complex (16a)	S41

SnMe ₂ -propyne Complex (17a')	S42
1,1,2-Trimethylstannirene (20a)	S42
SnMe ₂ -isoprene C ₁ -C ₂ Complex (18a)	S43
1,1-Dimethyl-2-(methylethenyl)stannirene (21a)	S44
SnPh ₂ -MeOH Complex (5b)	S45
SnPh ₂ -Et ₂ O Complex (6b)	S46
SnPh ₂ -THF Complex (7b)	S47
SnPh ₂ -EtOAc Complex (8b)	S48
SnPh ₂ -Me ₂ CO Complex (9b)	S49
SnPh ₂ -Et ₂ S Complex (10b)	S50
SnPh ₂ -THT Complex (11b)	S51
SnPh ₂ -MeNH ₂ Complex (12b')	S52
SnPh ₂ -Me ₂ NH Complex (13b')	S53
SnPh ₂ -NMe ₃ Complex (14b')	S54
SnPh ₂ -propene Complex (15b')	S55
2-Methyl-1,1-diphenylstannirane (19b)	S56
SnPh ₂ -cyclohexene Complex (16b)	S57
SnPh ₂ -propyne Complex (17b')	S58
2-Methyl-1,1-diphenylstannirene (20b)	S59
SnPh ₂ -isoprene C ₁ -C ₂ Complex (18b)	S60
2-Methylethenyl-1,1-diphenylstannirane (21b)	S61
Me ₂ O-Sn ₂ Me ₄ Complex (22a)	S62
Me ₂ S-Sn ₂ Me ₄ Complex (22b)	S63
Me ₂ NH-Sn ₂ Me ₄ Complex (22c)	S64

References

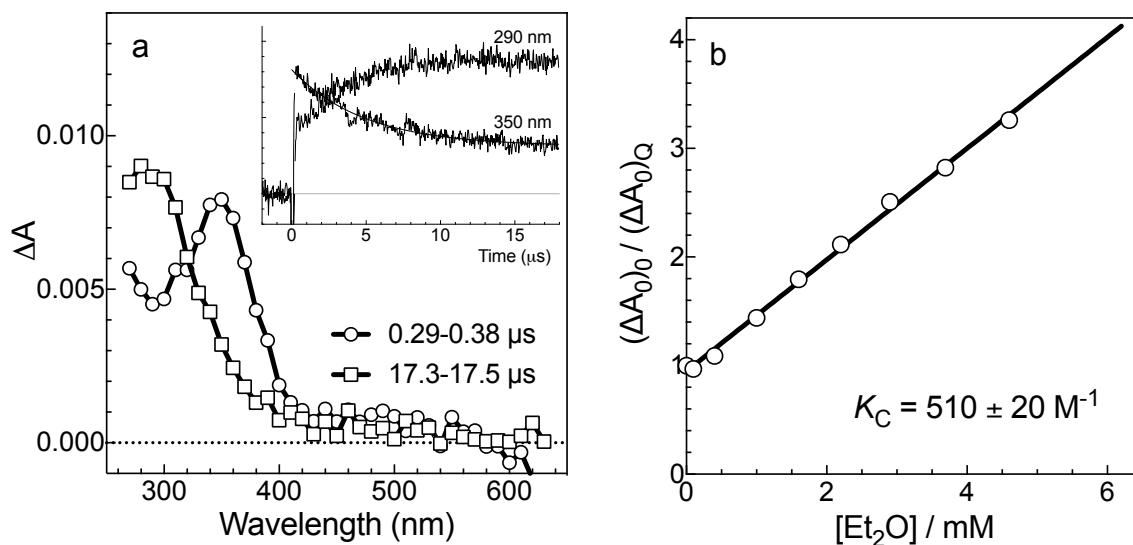


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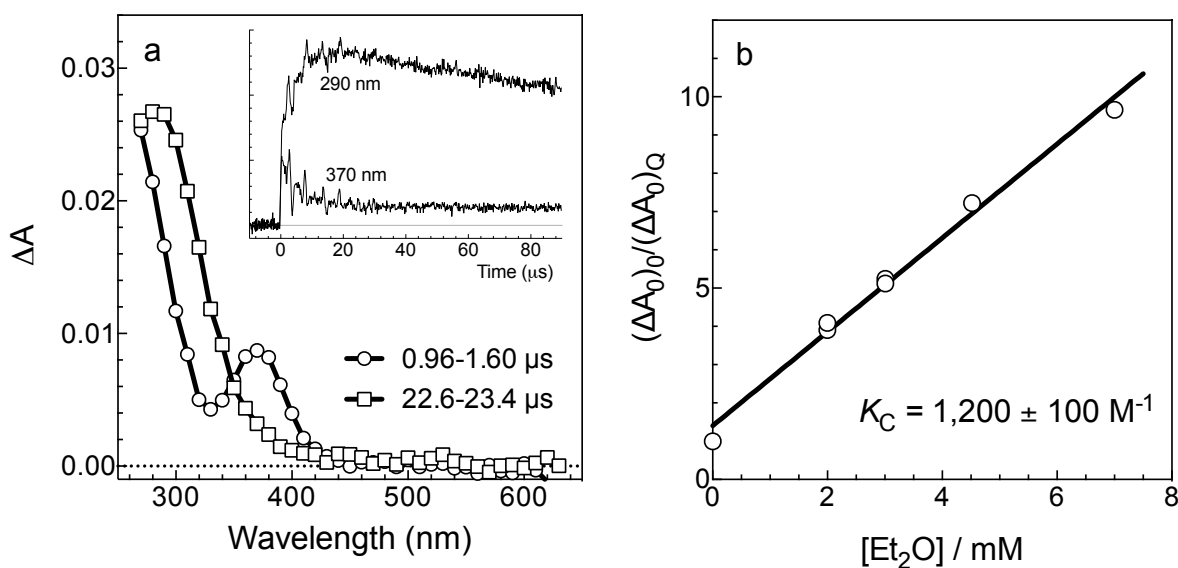


Figure S2. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 0.025 M Et₂O, recorded 0.96-1.60 μs (○) and 22.6-23.4 μs (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [Et₂O]; the solid line is the least squares fit of the data to eq. 6.

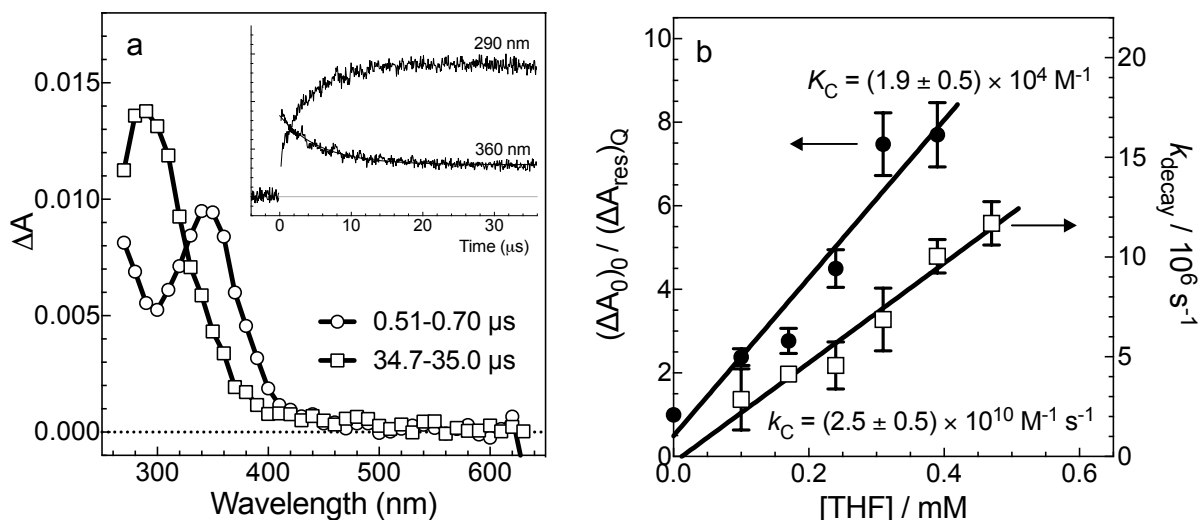


Figure S3. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 0.025 M THF, recorded 0.51-0.70 μs (○) and 34.7-35.0 μs (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plots of $(\Delta A_0)_0 / (\Delta A_{\text{res}})_Q$ (●) and k_{decay} (□) vs. [THF]; the solid lines are the least squares fits of the data to eq. 7 and 5, respectively.

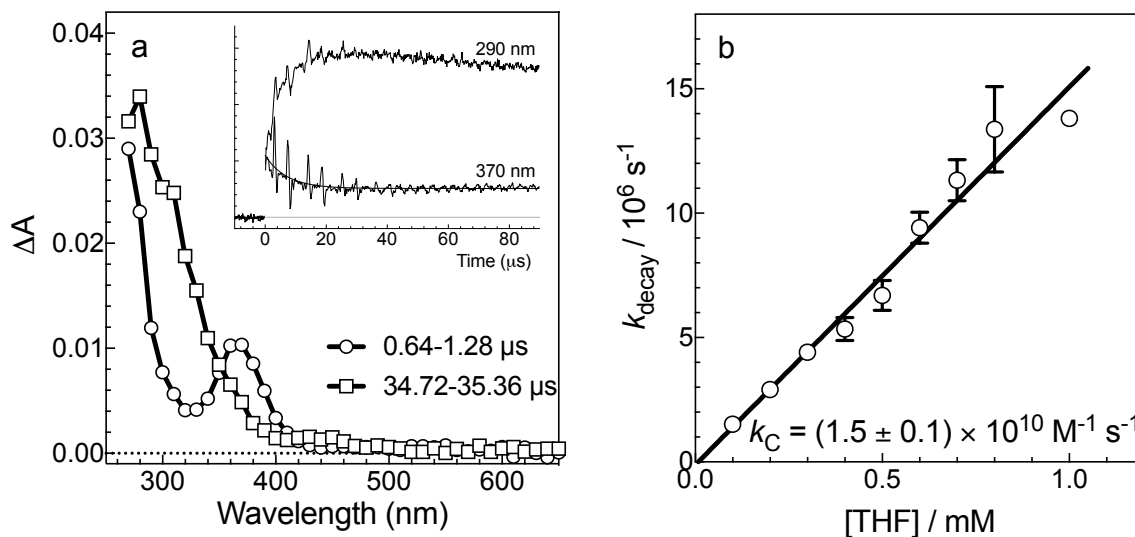


Figure S4. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 1.2 mM THF, recorded 0.64-1.28 μs (○) and 34.7-35.4 μs (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plots of k_{decay} vs. [THF]; the solid line is the least squares fit of the data to eq. 5.

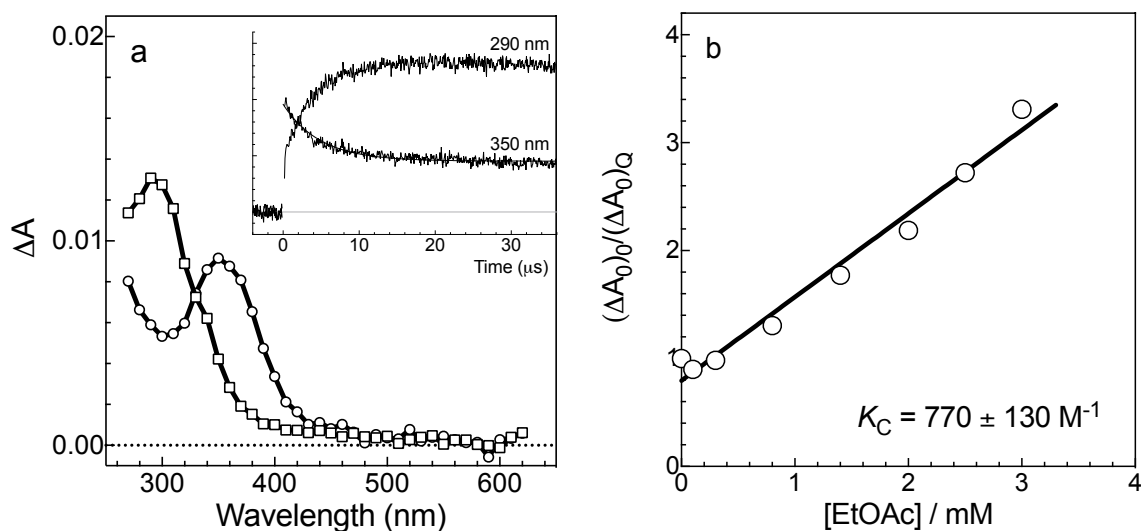


Figure S5. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 0.025 M EtOAc, recorded 0.51-0.70 μs (○) and 34.7-35.0 μs (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_\infty$ vs. [EtOAc]; the solid line is the least squares fit of the data to eq. 6.

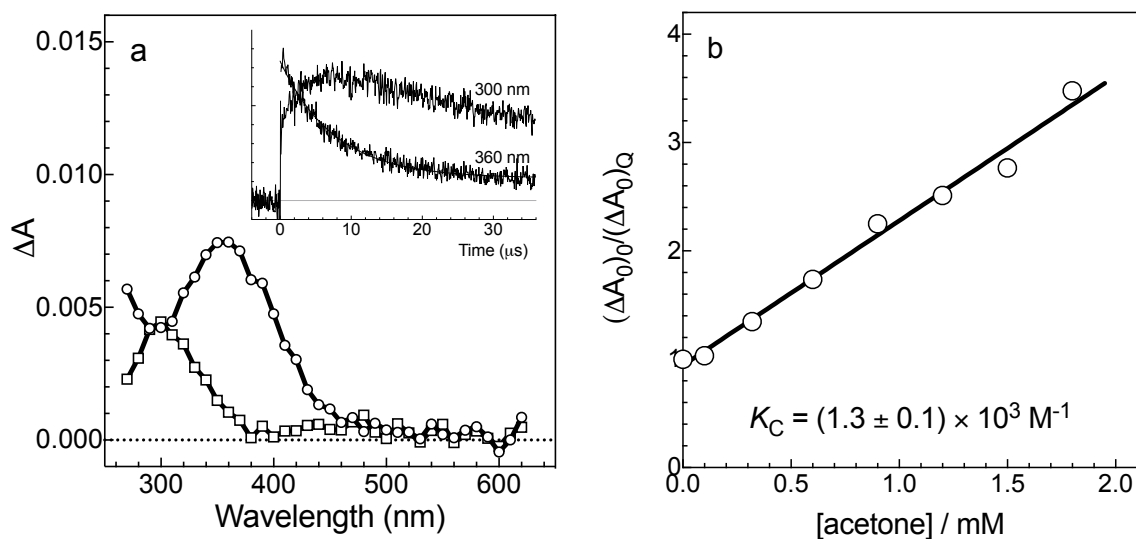


Figure S6. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 0.025 M acetone, recorded 0.26-0.45 μs (○) and 33.7-34.0 μs (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_\infty$ vs. [acetone]; the solid line is the least squares fit of the data to eq. 6.

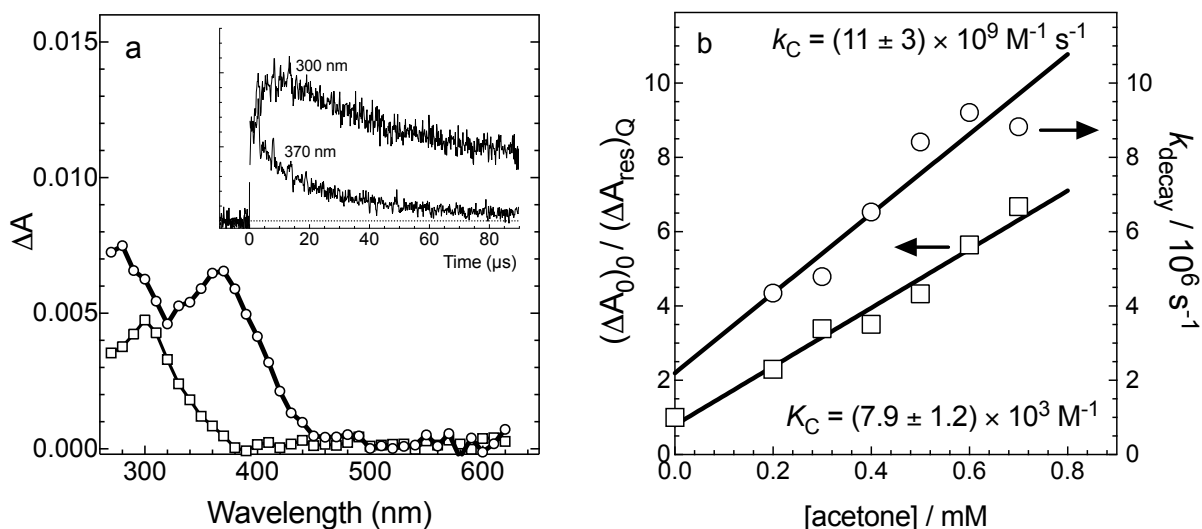


Figure S7. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 0.025 M acetone, recorded 0.48-0.80 μs (○) and 85-86 μs (□) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plots of k_{decay} (○) and $(\Delta A_0)_0 / (\Delta A_{\text{res}})_Q$ (□) vs. [acetone]; the solid lines are the least squares fits of the data to eq. 5 and 7, respectively.

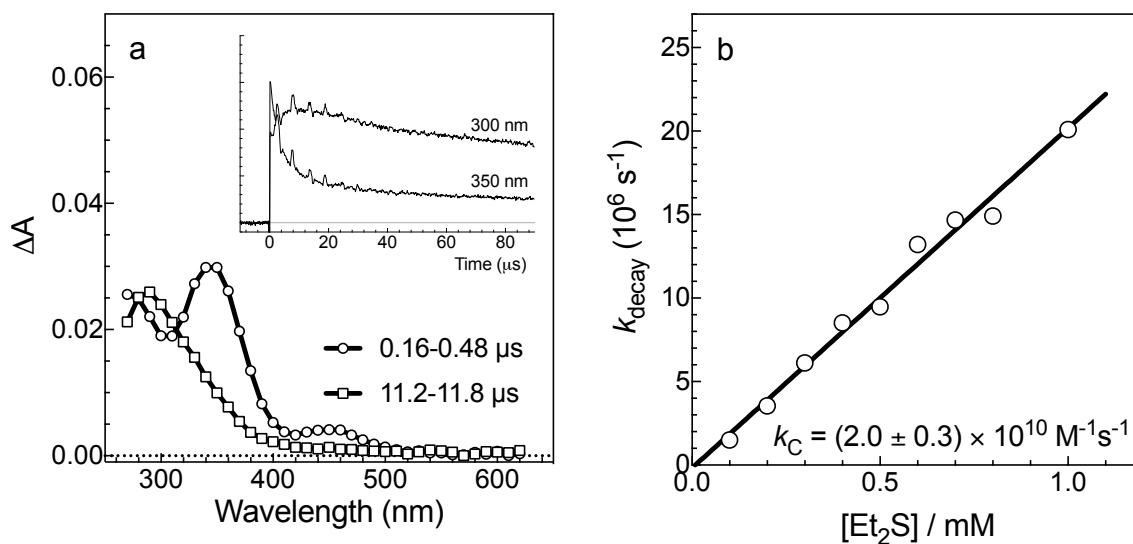


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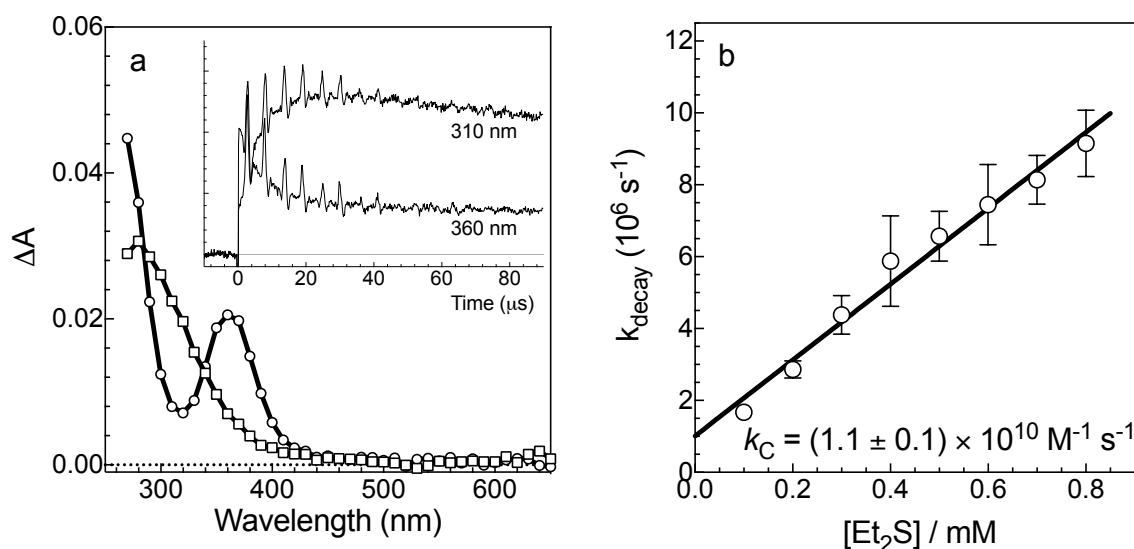


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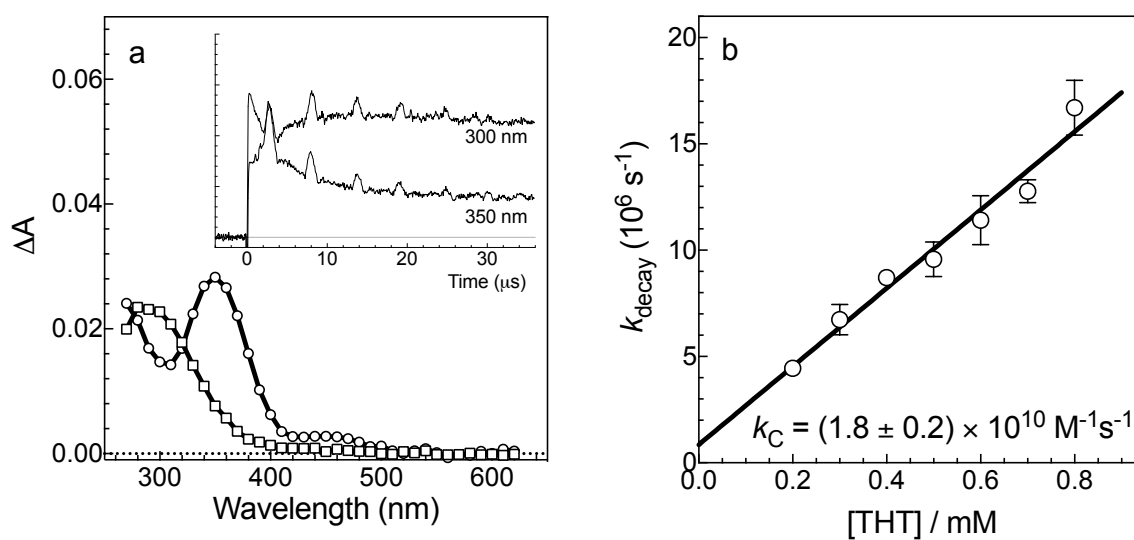


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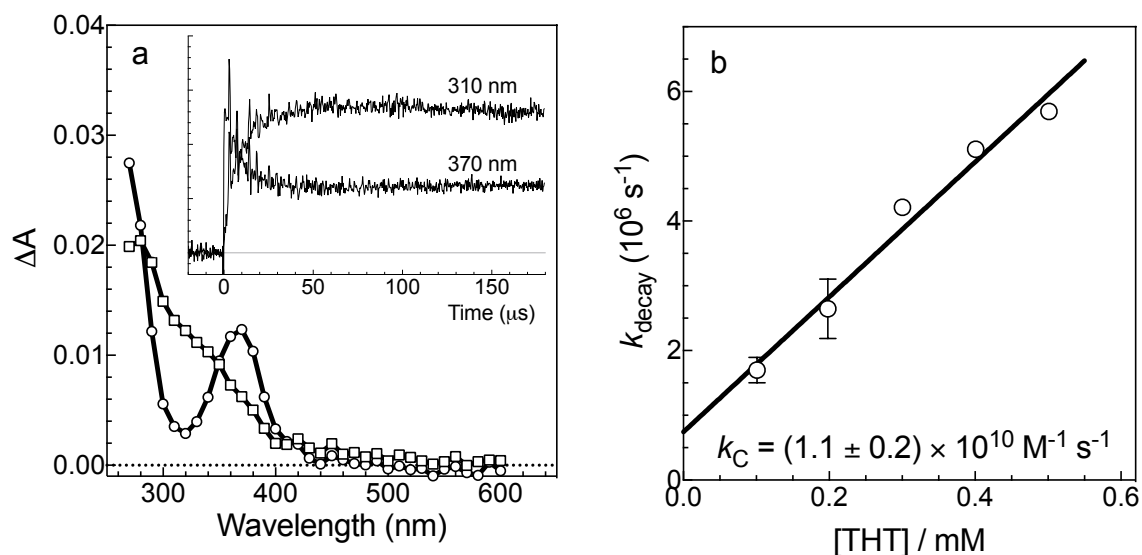


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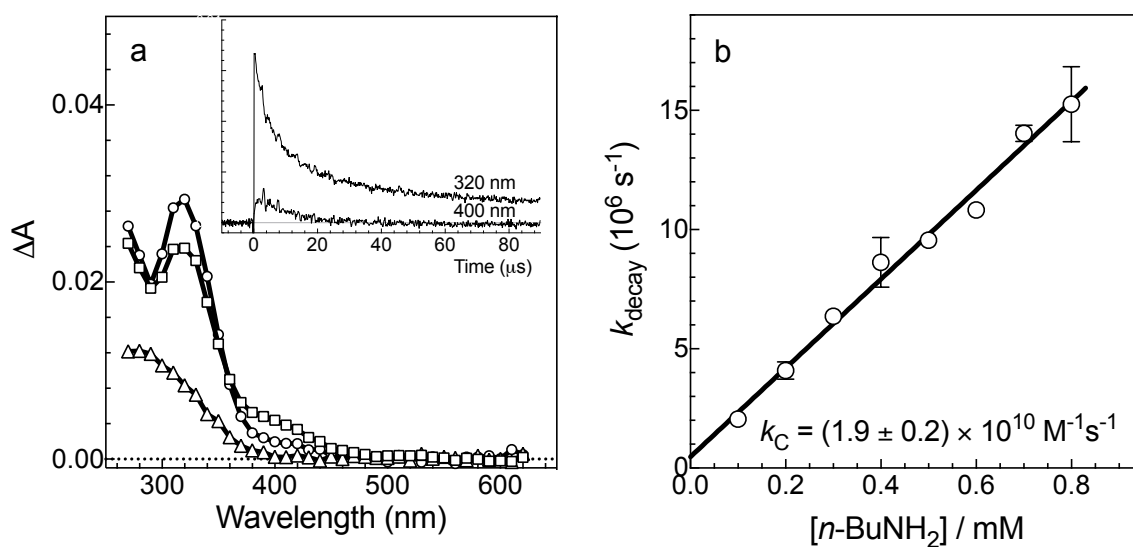


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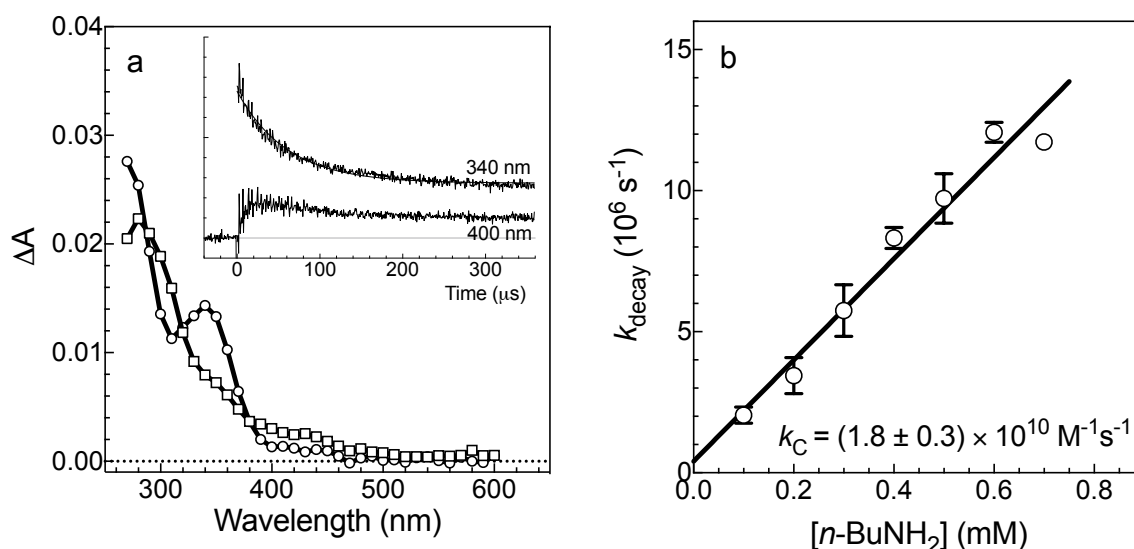


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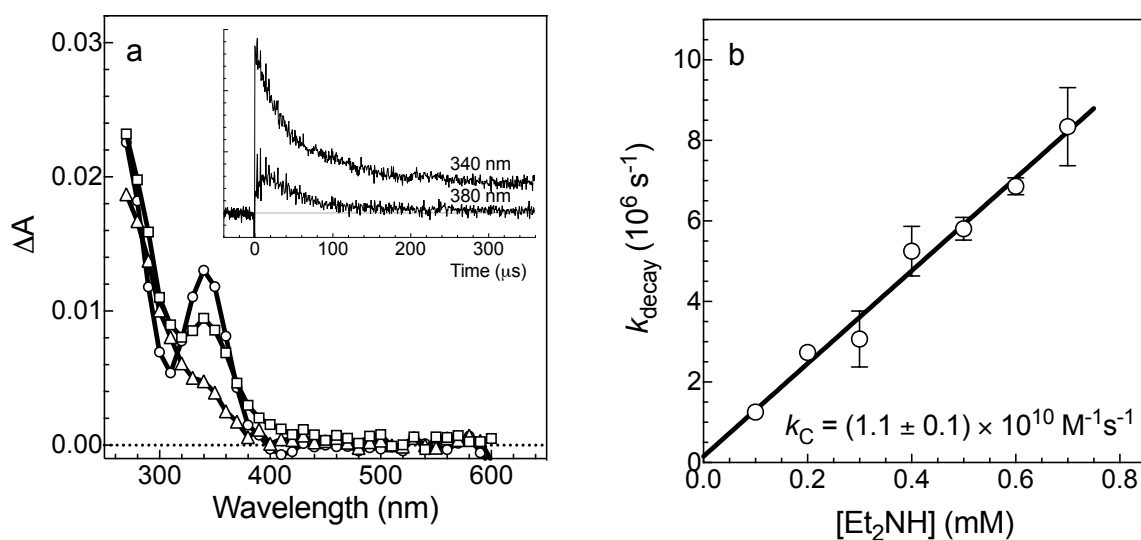


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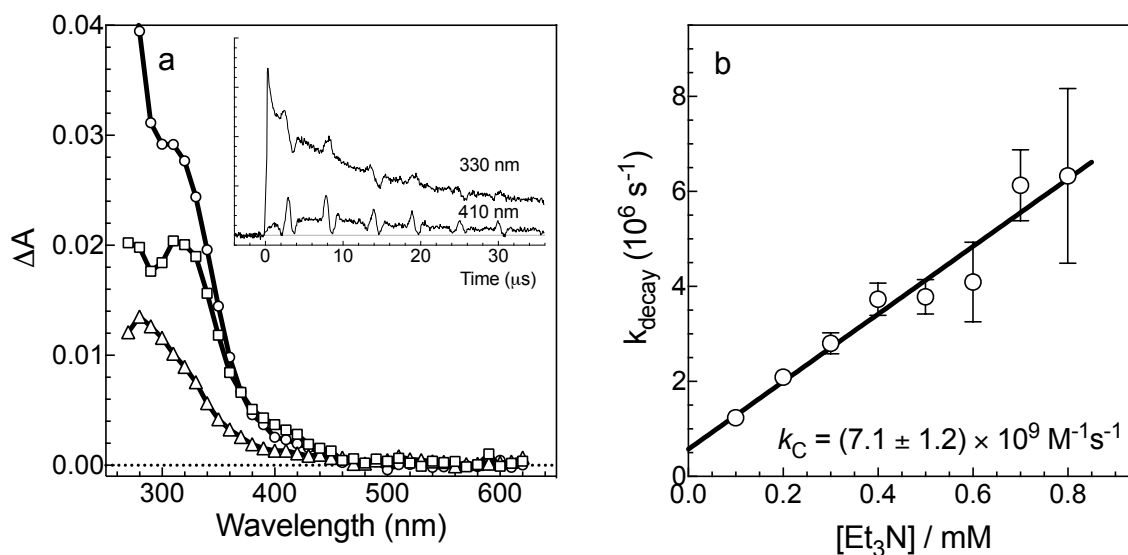


Figure S15. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 1.0 mM Et₃N, recorded 4.0-4.2 μs (○), 10.3-10.5 μs (□), and 34.4-34.6 μs (Δ) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of k_{decay} vs. [Et₃N]; the solid line is the least squares fit of the data to eq. 5.

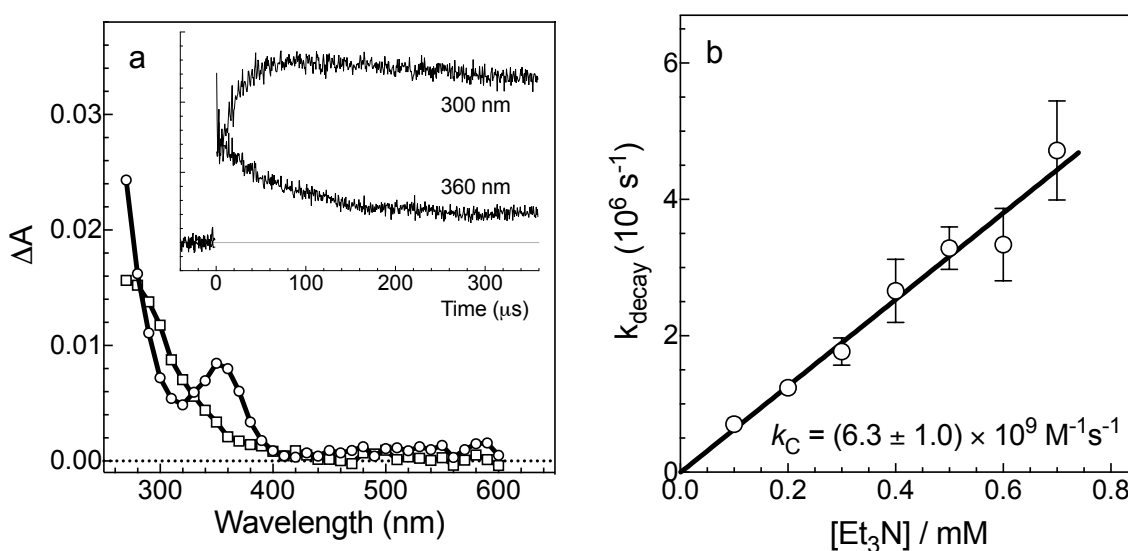


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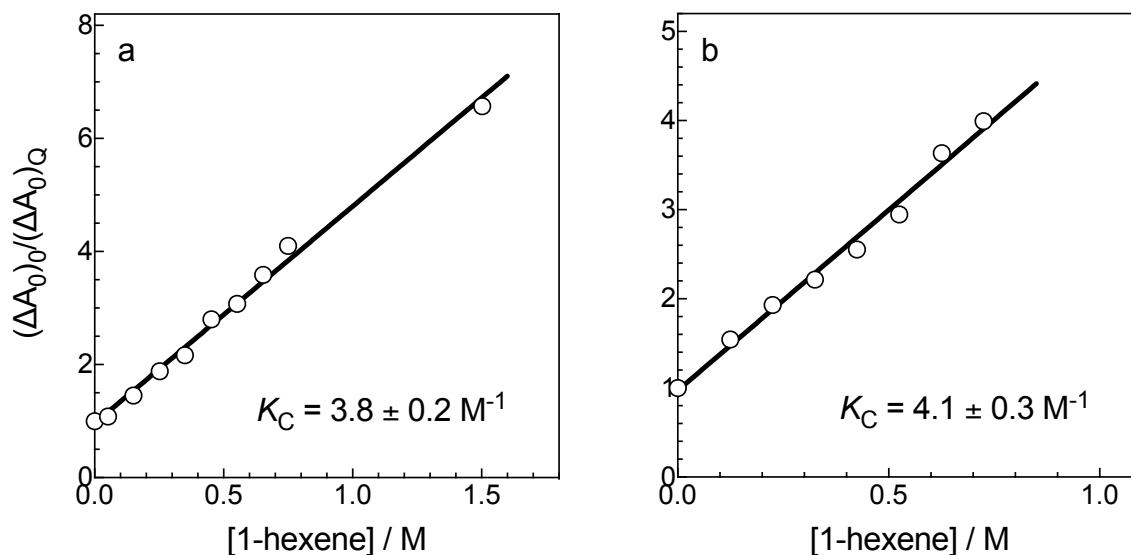


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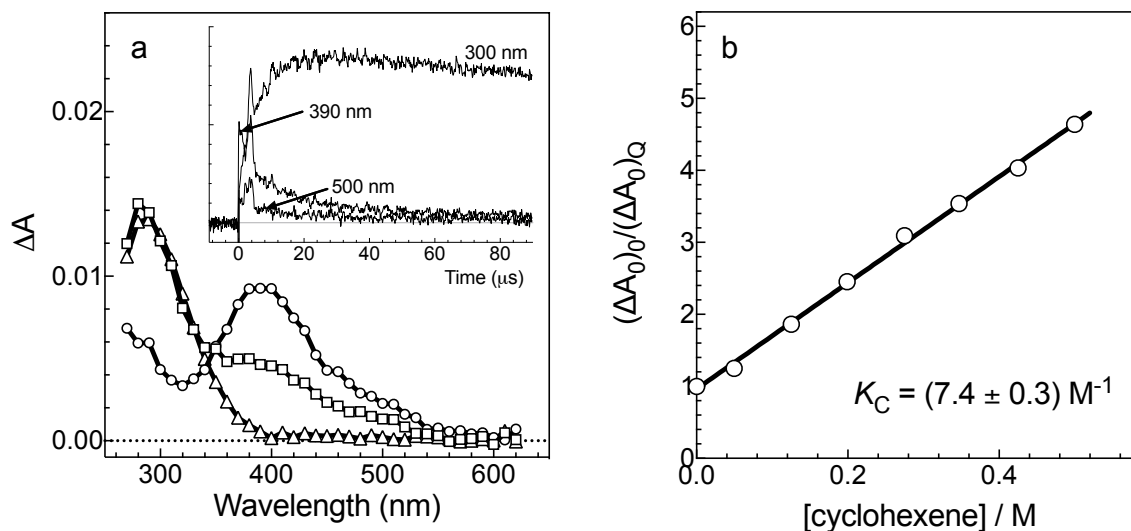


Figure S18. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 0.5 M cyclohexene, recorded 0.32-0.64 μs ($\circ$), 5.9-6.4 μs ($\square$), and 89-90 μs (Δ) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0/(\Delta A_0)_Q$ vs. [cyclohexene]; the solid line is the least squares fit of the data to eq. 6.

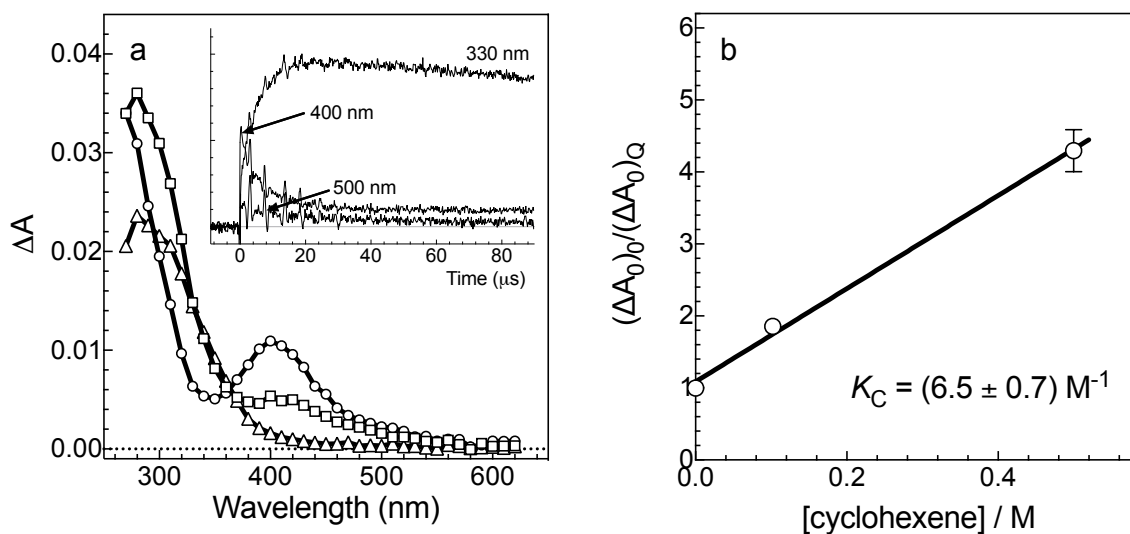


Figure S19. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 0.5 M cyclohexene, recorded 0.32-0.64 μs ($\circ$), 5.9-6.4 μs ($\square$), and 89-90 μs (Δ) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [cyclohexene]; the solid line is the least squares fit of the data to eq. 6.

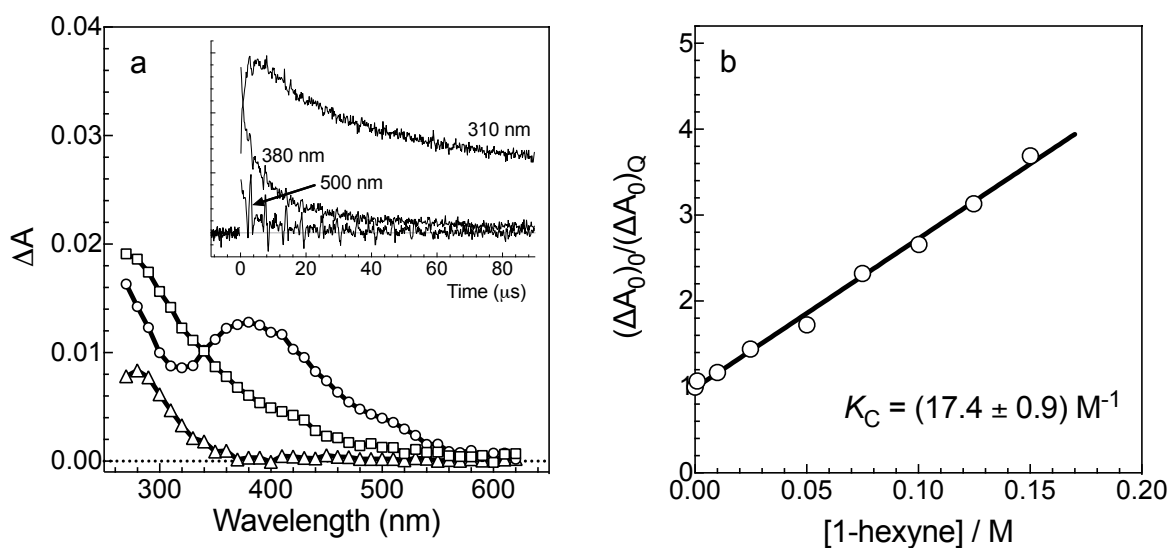


Figure S20. (a) Transient UV-vis spectra from lfp of **1** in hexanes containing 0.25 M 1-hexyne, recorded 0.16-0.48 μs ($\circ$), 4.3-4.8 μs ($\square$), and 89-90 μs (Δ) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [1-hexyne]; the solid line is the least squares fit of the data to eq. 6.

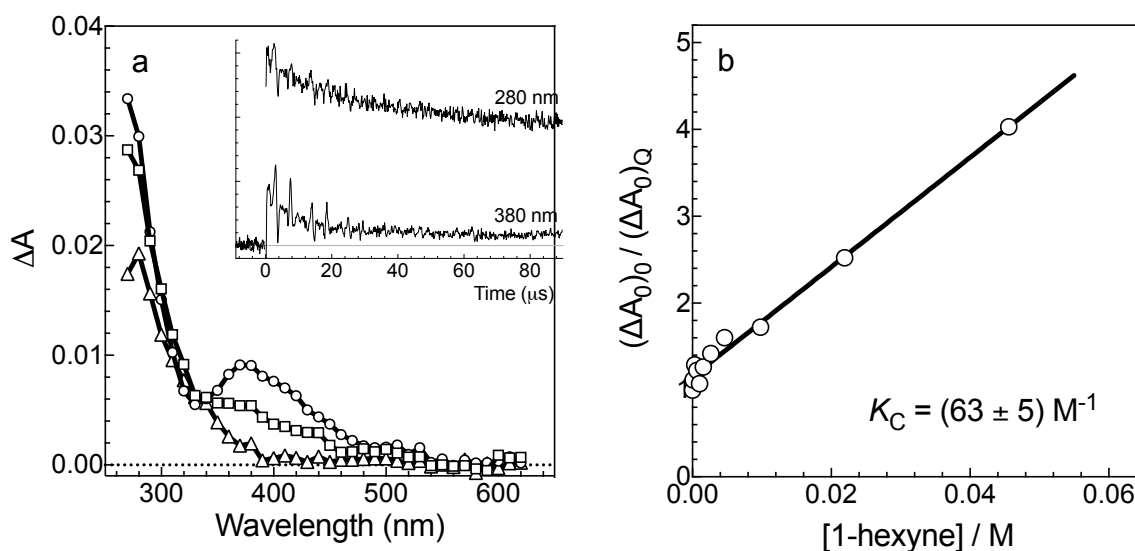


Figure S21. (a) Transient UV-vis spectra from lfp of **2** in hexanes containing 0.25 M 1-hexyne, recorded 0.64-0.96 μs ($\circ$), 5.9-6.2 μs ($\square$), and 89-90 μs ($\triangle$) after the laser pulse; the inset shows representative absorbance-time profiles at selected wavelengths. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [1-hexyne]; the solid line is the least squares fit of the data to eq. 6.

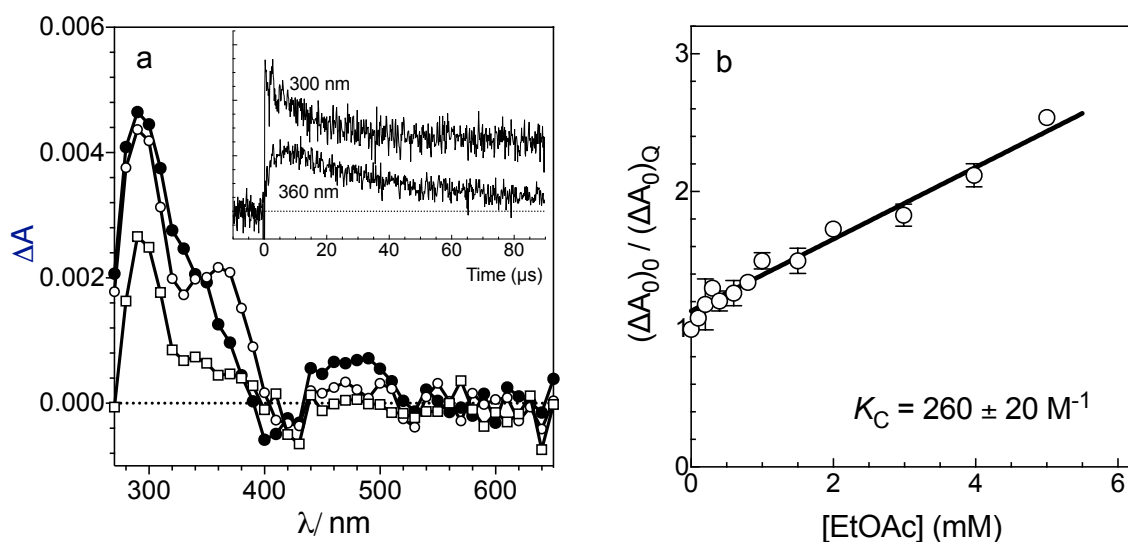


Figure S22. (a) Transient UV-vis spectra from lfp of (GeMe₂ photoprecursor) 1,1-dimethyl-3-phenylgermacyclopent-3-ene⁴ in hexanes containing 5.0 mM EtOAc, recorded 0.80-1.44 μs ($\bullet$), 5.92-6.88 μs ($\circ$), and 85.9-86.7 μs ($\square$) after the laser pulse; the inset shows representative absorbance-time profiles at 300 nm and 360 nm. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [EtOAc]; the solid line is the least squares fit of the data to eq. 6.

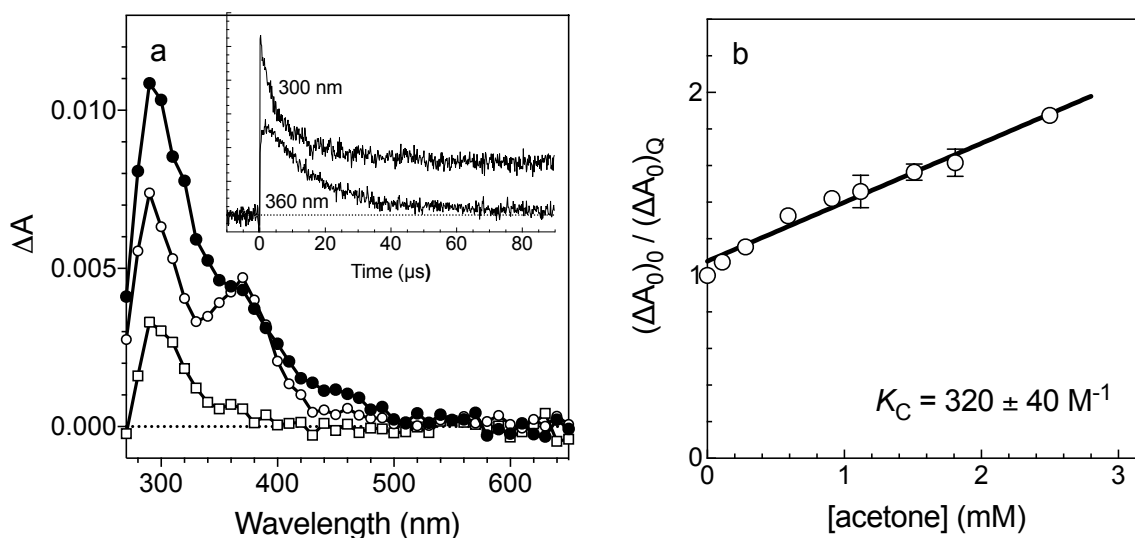


Figure S23. (a) Transient UV-vis spectra from lfp of (GeMe₂ photoprecursor) 1,1-dimethyl-3-phenylgermacyclopent-3-ene⁴ in hexanes containing 11.4 mM acetone, recorded recorded 0.16-0.64 μ s (●), 4.3-5.3 μ s (○), and 53.9-54.7 μ s (□) after the laser pulse; the inset shows representative absorbance-time profiles at 300 and 360 nm. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [acetone]; the solid line is the least squares fit of the data to eq. 6.

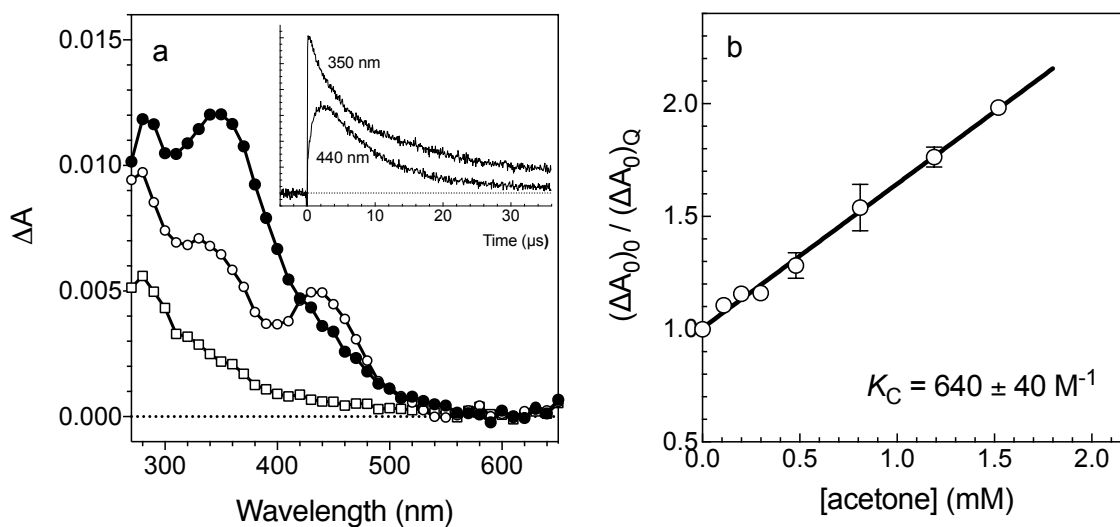


Figure S24. (a) Transient UV-vis spectra from lfp of (GePh₂ photoprecursor) 3,4-dimethyl-1,1-diphenylgermacyclopent-3-ene⁵ in hexanes containing 10.0 mM acetone, recorded recorded 0.13-0.45 μ s (●), 5.6-6.0 μ s (○), and 28.0-28.3 μ s (□) after the laser pulse; the inset shows representative absorbance-time profiles at 350 and 440 nm. (b) Plot of $(\Delta A_0)_0 / (\Delta A_0)_Q$ vs. [acetone]; the solid line is the least squares fit of the data to eq. 6.

Computational Studies

Geometry optimizations, frequency calculations, and Natural Bond Orbital calculations were performed using Gaussian 09, Revision E.01.⁶ Density functional theory (DFT) with the ω B97XD functional⁷ was used in conjunction with the def2-TZVP basis set⁸ for all calculations. Unless noted otherwise, final geometry optimizations were carried out with tight convergence criteria and “ultrafine” numerical integration grid. Energy minima were identified by the absence of negative eigenvalues of the Hessian matrix from a frequencies calculation on the optimized geometry. Vibrational frequencies were not scaled. Basis set superposition errors (BSSEs) were assessed using the counterpoise correction method, and found to be less than 1 kcal mol⁻¹ in all cases.⁹ Electronic spectral and Natural Transition Orbital calculations were carried out using the time-dependent (TD) extension of the ω B97XD functional and the same basis set as was employed for the geometry optimizations.

Table S1. Calculated Electronic Energies, Enthalpies (298.15 K), and Free Energies (298.15 K) of the (1+2)-Cycloadducts of SnMe₂ and SnPh₂ with Propene, Propyne, and Isoprene, Calculated at the ω B97XD/def2-TZVP Level of Theory (energies in kcal mol⁻¹). ^a

Species	ΔE_{elec}	ΔH°	ΔG°
1,1,2-trimethylstannirane (19a)	+3.0	+4.8	+17.6
1,1,2-trimethylstannirene (20a)	-4.8	-2.7	+9.6
1,1-dimethyl-2-(methylethenyl)stannirane (21a)	+9.6	+11.0	+23.9
2-methyl-1,1-diphenylstannirane (19b)	+6.4	+7.1	+18.7
2-methyl-1,1-diphenylstannirene (20b)	-1.4	-0.3	+10.8
2-methylethenyl-1,1-diphenylstannirane (21b)	+7.9	+8.4	+19.9

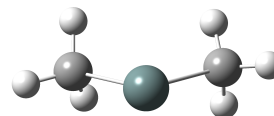
- a. Electronic and standard energies were computed at 298.15 K and 1 atm from unscaled vibrational frequencies, relative to the isolated reactants, and are not corrected for Basis Set Superposition Errors (BSSEs). Tight optimization criteria were employed for all species.

Optimized Structures and Energies (ω B97XD/def2-TZVP)

Dimethylstannylene (SnMe_2)

Opt=(verytight,nosymm) int=ultrafine

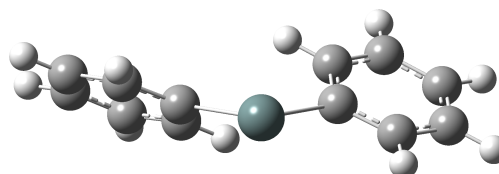
Zero-point correction= 0.069684 (Hartree/Particle)
 Thermal correction to Energy= 0.075865
 Thermal correction to Enthalpy= 0.076809
 Thermal correction to Gibbs Free Energy= 0.038474
 Sum of electronic and zero-point Energies= -294.108274
 Sum of electronic and thermal Energies= -294.102093
 Sum of electronic and thermal Enthalpies= -294.101149
 Sum of electronic and thermal Free Energies= -294.139484



Sn	0.002429	0.413509	0.200736
C	-1.586590	-1.092490	0.085415
C	1.584320	-1.076999	-0.086150
H	1.431118	-1.589791	-1.040644
H	1.516173	-1.837252	0.697796
H	-1.522736	-1.617889	-0.872247
H	-2.586488	-0.671892	0.189829
H	-1.435414	-1.840798	0.869399
H	2.586350	-0.648773	-0.074793

Diphenylstannylene (SnPh_2)

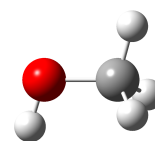
Zero-point correction= 0.181123 (Hartree/Particle)
 Thermal correction to Energy= 0.192757
 Thermal correction to Enthalpy= 0.193702
 Thermal correction to Gibbs Free Energy= 0.141044
 Sum of electronic and zero-point Energies= -677.461199
 Sum of electronic and thermal Energies= -677.449565
 Sum of electronic and thermal Enthalpies= -677.448621
 Sum of electronic and thermal Free Energies= -677.501278



C	-0.000000	1.642356	0.009600
C	-0.000000	-1.642356	0.009600
C	-0.584521	1.578572	-1.259446
C	-0.610888	2.683920	-2.096644
C	-0.038257	3.879386	-1.686441
C	0.545255	3.969823	-0.431977
C	0.549004	2.865254	0.407675
C	0.584521	-1.578572	-1.259446
C	-0.549004	-2.865254	0.407675
C	0.610888	-2.683920	-2.096644
C	0.038257	-3.879386	-1.686441
C	-0.545255	-3.969823	-0.431977
H	-1.075495	2.612839	-3.072737
H	0.988032	4.902783	-0.104971
H	0.990637	2.966517	1.395146
H	-0.990637	-2.966517	1.395146
H	1.075495	-2.612839	-3.072737
H	-1.029488	0.651766	-1.604507
H	-0.052032	4.741173	-2.342292
H	1.029488	-0.651766	-1.604507
H	0.052032	-4.741173	-2.342292
H	-0.988032	-4.902783	-0.104971
Sn	0.000000	-0.000000	1.442910

Methanol (MeOH, 5)

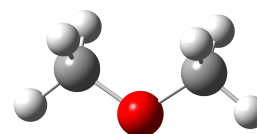
Zero-point correction= 0.051686 (Hartree/Particle)
 Thermal correction to Energy= 0.055016
 Thermal correction to Enthalpy= 0.055960
 Thermal correction to Gibbs Free Energy= 0.028942
 Sum of electronic and zero-point Energies= -115.683260
 Sum of electronic and thermal Energies= -115.679930
 Sum of electronic and thermal Enthalpies= -115.678986
 Sum of electronic and thermal Free Energies= -115.706004



C	0.662764	-0.020690	0.000003
H	1.081898	0.987035	-0.000546
H	1.024622	-0.545125	0.894269
O	-0.744853	0.122105	0.000003
H	-1.148812	-0.748583	0.000000
H	1.024533	-0.546031	-0.893767

Dimethyl ether (Me₂O, 6')

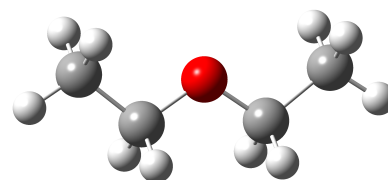
Zero-point correction= 0.080145 (Hartree/Particle)
 Thermal correction to Energy= 0.084447
 Thermal correction to Enthalpy= 0.085391
 Thermal correction to Gibbs Free Energy= 0.054770
 Sum of electronic and zero-point Energies= -154.958166
 Sum of electronic and thermal Energies= -154.953863
 Sum of electronic and thermal Enthalpies= -154.952919
 Sum of electronic and thermal Free Energies= -154.983540



C	-1.163882	-0.193140	0.000067
H	-2.015478	0.485811	-0.000029
H	-1.219210	-0.834562	-0.890211
H	-1.219160	-0.834244	0.890578
C	1.163882	-0.193140	0.000003
H	1.219147	-0.834585	-0.890263
H	2.015478	0.485810	-0.000173
H	1.219223	-0.834221	0.890526
O	0.000000	0.585458	-0.000106

Diethyl ether (Et₂O, 6)

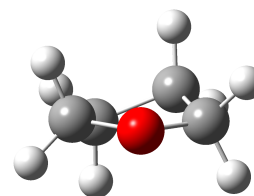
Zero-point correction= 0.137306 (Hartree/Particle)
 Thermal correction to Energy= 0.144089
 Thermal correction to Enthalpy= 0.145033
 Thermal correction to Gibbs Free Energy= 0.107231
 Sum of electronic and zero-point Energies= -233.542952
 Sum of electronic and thermal Energies= -233.536170
 Sum of electronic and thermal Enthalpies= -233.535225
 Sum of electronic and thermal Free Energies= -233.573027



C	-1.173340	-0.513856	-0.000001
C	1.173340	-0.513856	0.000000
H	-1.191921	-1.167191	0.884913
H	-1.191922	-1.167189	-0.884916
H	1.191921	-1.167190	-0.884914
H	1.191922	-1.167190	0.884915
O	0.000000	0.259702	0.000000
C	-2.369857	0.409141	0.000001
H	-3.294342	-0.170427	0.000000
H	-2.360271	1.047144	0.884384
H	-2.360271	1.047147	-0.884380
C	2.369857	0.409141	-0.000000
H	2.360271	1.047146	0.884381
H	3.294342	-0.170427	-0.000000
H	2.360271	1.047145	-0.884383

Tetrahydrofuran (THF, 7)

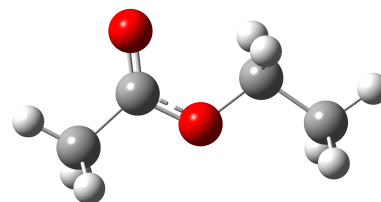
Zero-point correction= 0.117706 (Hartree/Particle)
 Thermal correction to Energy= 0.122596
 Thermal correction to Enthalpy= 0.123540
 Thermal correction to Gibbs Free Energy= 0.089457
 Sum of electronic and zero-point Energies= -232.349555
 Sum of electronic and thermal Energies= -232.344665
 Sum of electronic and thermal Enthalpies= -232.343721
 Sum of electronic and thermal Free Energies= -232.377804



C	1.157651	-0.428609	-0.131659
C	-1.157635	-0.428655	0.131652
C	-0.729062	0.989633	-0.226485
C	0.729022	0.989658	0.226488
H	1.937931	-0.818881	0.524763
H	1.521536	-0.479148	-1.165083
H	-1.937888	-0.818955	-0.524785
H	-1.521535	-0.479213	1.165069
H	-0.790561	1.145636	-1.305714
H	-1.337119	1.748975	0.263810
H	1.337048	1.749027	-0.263802
H	0.790516	1.145657	1.305718
O	0.000027	-1.240657	0.000006

Ethyl acetate (EtOAc, 8)

Zero-point correction= 0.118773 (Hartree/Particle)
 Thermal correction to Energy= 0.126208
 Thermal correction to Enthalpy= 0.127152
 Thermal correction to Gibbs Free Energy= 0.086177
 Sum of electronic and zero-point Energies= -307.614593
 Sum of electronic and thermal Energies= -307.607158
 Sum of electronic and thermal Enthalpies= -307.606214
 Sum of electronic and thermal Free Energies= -307.647189

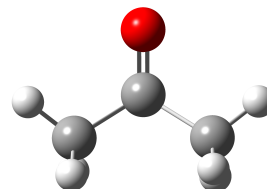


O	-1.197000	1.334685	0.000004
C	-1.031705	0.145290	-0.000002
O	0.176352	-0.433855	-0.000007
C	1.304810	0.449143	-0.000005
H	1.251101	1.091789	0.880578
H	1.251111	1.091782	-0.880593
C	-2.125594	-0.884657	0.000002
H	-2.033028	-1.522480	-0.879461
H	-2.033024	-1.522478	0.879466
H	-3.091488	-0.387951	0.000004
C	2.552995	-0.398702	0.000006
H	2.592038	-1.034549	-0.884992
H	3.433414	0.245345	0.000009
H	2.592027	-1.034543	0.885008

Acetone (Me₂CO, 9)

Opt=verytight,nosymm int=ultrafine

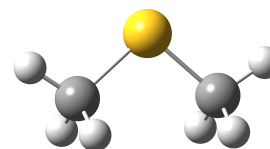
Zero-point correction= 0.083949 (Hartree/Particle)
 Thermal correction to Energy= 0.089401
 Thermal correction to Enthalpy= 0.090345
 Thermal correction to Gibbs Free Energy= 0.054532
 Sum of electronic and zero-point Energies= -193.085942
 Sum of electronic and thermal Energies= -193.080490
 Sum of electronic and thermal Enthalpies= -193.079546
 Sum of electronic and thermal Free Energies= -193.115359



C	-0.00148200	0.18678900	-0.01181400
C	1.28167500	-0.60641200	0.06609300
C	-1.28109600	-0.61447400	-0.05966200
O	-0.00415300	1.39104000	-0.03449500
H	1.30153600	-1.18518500	0.99278100
H	1.33609800	-1.32159300	-0.75773600
H	2.13834700	0.06249000	0.03474700
H	-2.14073900	0.05130800	-0.05300400
H	-1.29852000	-1.22746500	-0.96413100
H	-1.33216500	-1.29866500	0.79027500

Dimethylsulfide (Me₂S, 10')

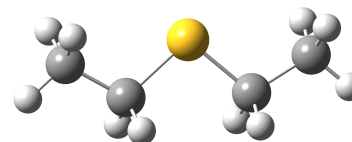
Zero-point correction= 0.076079 (Hartree/Particle)
 Thermal correction to Energy= 0.080923
 Thermal correction to Enthalpy= 0.081867
 Thermal correction to Gibbs Free Energy= 0.049109
 Sum of electronic and zero-point Energies= -477.953576
 Sum of electronic and thermal Energies= -477.948732
 Sum of electronic and thermal Enthalpies= -477.947788
 Sum of electronic and thermal Free Energies= -477.980546



C	0.000000	-0.508599	1.372224
C	0.000000	-0.508599	-1.372224
H	0.891493	-1.136519	1.354141
H	-0.000000	0.074405	2.292214
H	-0.891492	-1.136520	1.354140
H	-0.000000	0.074405	-2.292214
H	-0.891492	-1.136520	-1.354140
H	0.891493	-1.136519	-1.354141
S	-0.000000	0.656279	0.000000

Diethylsulfide (Et₂S, 10)

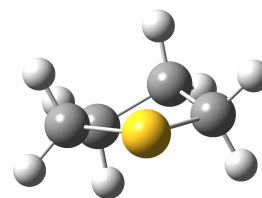
Zero-point correction= 0.133813 (Hartree/Particle)
 Thermal correction to Energy= 0.141284
 Thermal correction to Enthalpy= 0.142228
 Thermal correction to Gibbs Free Energy= 0.101968
 Sum of electronic and zero-point Energies= -556.528592
 Sum of electronic and thermal Energies= -556.521122
 Sum of electronic and thermal Enthalpies= -556.520177
 Sum of electronic and thermal Free Energies= -556.560438



C	-0.000001	-0.614838	1.382818
C	-0.000001	-0.614838	-1.382818
H	0.883476	-1.252065	1.305180
H	-0.883479	-1.252063	1.305179
H	-0.883479	-1.252063	-1.305179
H	0.883476	-1.252065	-1.305180
S	0.000002	0.552638	-0.000000
C	-0.000001	0.134457	2.705555
H	-0.883328	0.768151	2.797628
H	-0.000002	-0.570989	3.537994
H	0.883328	0.768149	2.797629
C	-0.000001	0.134457	-2.705555
H	-0.000002	-0.570989	-3.537994
H	-0.883328	0.768151	-2.797628
H	0.883328	0.768149	-2.797629

Tetrahydrothiophene (THT, 11)

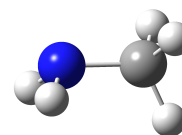
Zero-point correction= 0.114763 (Hartree/Particle)
 Thermal correction to Energy= 0.119846
 Thermal correction to Enthalpy= 0.120790
 Thermal correction to Gibbs Free Energy= 0.086178
 Sum of electronic and zero-point Energies= -555.341866
 Sum of electronic and thermal Energies= -555.336783
 Sum of electronic and thermal Enthalpies= -555.335838
 Sum of electronic and thermal Free Energies= -555.370451



C	0.056777	-1.330337	0.136774
C	0.056761	1.330342	-0.136754
C	-1.274972	0.711458	0.273101
C	-1.274957	-0.711474	-0.273111
H	0.346787	-2.159131	-0.506918
H	0.023382	-1.686275	1.167006
H	0.346767	2.159122	0.506956
H	0.023369	1.686299	-1.166980
H	-1.349742	0.686215	1.363223
H	-2.114413	1.297827	-0.105049
H	-2.114402	-1.297853	0.105014
H	-1.349682	-0.686228	-1.363236
S	1.300392	0.000006	-0.000005

Methylamine (MeNH₂, 12')

Zero-point correction= 0.064435 (Hartree/Particle)
 Thermal correction to Energy= 0.067862
 Thermal correction to Enthalpy= 0.068806
 Thermal correction to Gibbs Free Energy= 0.041519
 Sum of electronic and zero-point Energies= -95.801528
 Sum of electronic and thermal Energies= -95.798102
 Sum of electronic and thermal Enthalpies= -95.797157
 Sum of electronic and thermal Free Energies= -95.824444

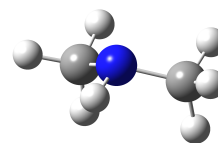


C	0.049082	0.702042	0.000000
H	-0.946127	1.166588	0.000000
H	0.587561	1.062631	-0.877771
H	0.587561	1.062631	0.877771
N	0.049082	-0.754248	-0.000000
H	-0.433528	-1.112184	-0.812497
H	-0.433528	-1.112184	0.812497

Dimethylamine (Me₂NH, 13')

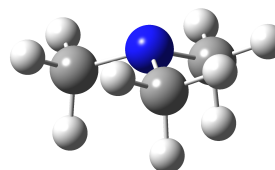
Zero-point correction= 0.092958 (Hartree/Particle)
 Thermal correction to Energy= 0.097346
 Thermal correction to Enthalpy= 0.098291
 Thermal correction to Gibbs Free Energy= 0.067510
 Sum of electronic and zero-point Energies= -135.080179
 Sum of electronic and thermal Energies= -135.075790
 Sum of electronic and thermal Enthalpies= -135.074846
 Sum of electronic and thermal Free Energies= -135.105626

C	-1.206939	-0.221609	0.020072
H	-2.082274	0.424077	-0.059810
H	-1.270106	-0.966079	-0.777467
H	-1.258087	-0.759926	0.980675
N	0.000000	0.561256	-0.147177
H	0.000000	1.334370	0.502579
C	1.206939	-0.221609	0.020072
H	1.270106	-0.966079	-0.777467
H	2.082274	0.424077	-0.059810
H	1.258086	-0.759926	0.980675

**Trimethylamine (NMe₃, 14')**

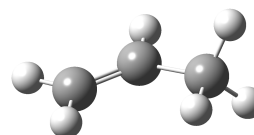
Zero-point correction= 0.120858 (Hartree/Particle)
 Thermal correction to Energy= 0.126258
 Thermal correction to Enthalpy= 0.127202
 Thermal correction to Gibbs Free Energy= 0.094627
 Sum of electronic and zero-point Energies= -174.362590
 Sum of electronic and thermal Energies= -174.357190
 Sum of electronic and thermal Enthalpies= -174.356246
 Sum of electronic and thermal Free Energies= -174.388821

C	0.000000	1.379384	-0.060075
C	1.194582	-0.689692	-0.060075
C	-1.194582	-0.689692	-0.060075
H	0.000000	1.479262	-1.161021
H	0.883663	1.890594	0.325627
H	-0.883663	1.890594	0.325627
H	1.281078	-0.739631	-1.161021
H	2.079134	-0.180023	0.325627
H	1.195471	-1.710571	0.325627
H	-1.281078	-0.739631	-1.161021
H	-2.079134	-0.180023	0.325627
H	-1.195471	-1.710571	0.325627
N	0.000000	0.000000	0.372951



Propene (15')

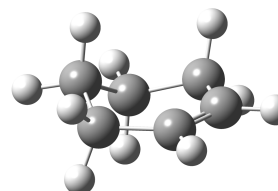
Zero-point correction= 0.080121 (Hartree/Particle)
 Thermal correction to Energy= 0.084191
 Thermal correction to Enthalpy= 0.085135
 Thermal correction to Gibbs Free Energy= 0.055126
 Sum of electronic and zero-point Energies= -117.829946
 Sum of electronic and thermal Energies= -117.825876
 Sum of electronic and thermal Enthalpies= -117.824932
 Sum of electronic and thermal Free Energies= -117.854941



C	1.274021	0.220368	-0.000002
H	2.231011	-0.286096	0.000035
H	1.290743	1.305178	-0.000012
C	0.134196	-0.452774	0.000000
H	0.167842	-1.539256	0.000034
C	-1.228244	0.162008	-0.000005
H	-1.797704	-0.154461	-0.877677
H	-1.797661	-0.154339	0.877741
H	-1.174071	1.251362	-0.000080

Cyclohexene (16)

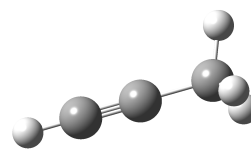
Zero-point correction= 0.147448 (Hartree/Particle)
 Thermal correction to Energy= 0.152898
 Thermal correction to Enthalpy= 0.153843
 Thermal correction to Gibbs Free Energy= 0.119522
 Sum of electronic and zero-point Energies= -234.510154
 Sum of electronic and thermal Energies= -234.504703
 Sum of electronic and thermal Enthalpies= -234.503759
 Sum of electronic and thermal Free Energies= -234.538080



C	0.005482	1.492556	0.045405
C	-0.005482	0.663424	1.298104
C	0.005482	-0.663424	1.298104
C	-0.005482	-1.492556	0.045405
C	-0.373075	-0.665231	-1.184213
C	0.373075	0.665231	-1.184213
H	0.020706	-1.195473	2.243843
H	-0.020706	1.195473	2.243843
H	-0.981104	1.951037	-0.091548
H	0.704793	2.324655	0.164281
H	0.981104	-1.951037	-0.091548
H	-0.704793	-2.324655	0.164281
H	-0.158506	-1.227789	-2.095016
H	-1.450195	-0.469716	-1.177336
H	1.450195	0.469716	-1.177336
H	0.158506	1.227789	-2.095016

Propyne (17')

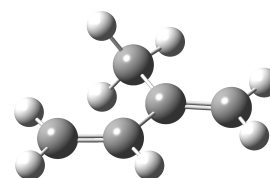
Zero-point correction= 0.056094 (Hartree/Particle)
 Thermal correction to Energy= 0.059986
 Thermal correction to Enthalpy= 0.060930
 Thermal correction to Gibbs Free Energy= 0.031938
 Sum of electronic and zero-point Energies= -116.598816
 Sum of electronic and thermal Energies= -116.594924
 Sum of electronic and thermal Enthalpies= -116.593980
 Sum of electronic and thermal Free Energies= -116.622972



C	-1.236676	-0.000005	-0.000011
H	-1.622009	-0.841447	-0.577514
H	-1.622085	-0.079433	1.017417
H	-1.622044	0.920835	-0.439961
C	1.415780	0.000002	0.000006
H	2.479059	-0.000051	-0.000082
C	0.218743	0.000019	0.000028

Isoprene (18)

Zero-point correction= 0.114283 (Hartree/Particle)
 Thermal correction to Energy= 0.120058
 Thermal correction to Enthalpy= 0.121003
 Thermal correction to Gibbs Free Energy= 0.085869
 Sum of electronic and zero-point Energies= -195.198672
 Sum of electronic and thermal Energies= -195.192896
 Sum of electronic and thermal Enthalpies= -195.191952
 Sum of electronic and thermal Free Energies= -195.227086



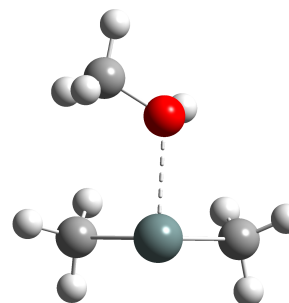
C	-1.97008800	0.00686000	0.00001500
H	-2.92628700	-0.49988800	-0.00004000
H	-1.99211400	1.08991800	0.00000800
C	-0.83160100	-0.67864800	-0.00000600
H	-0.87262500	-1.76410400	-0.00000500
C	0.51653300	-0.09992500	-0.00000300
C	1.57973900	-0.90349400	0.00000400
H	1.46998100	-1.98153200	0.00000700
H	2.58903700	-0.51077600	0.00000000
C	0.65317800	1.39450700	-0.00000500
H	0.17223900	1.82955700	-0.87945000
H	0.17224300	1.82955600	0.87944600
H	1.70096600	1.69146700	0.00001000

SnMe₂-MeOH complex (5a)

Zero-point correction= 0.124038 (Hartree/Particle)
 Thermal correction to Energy= 0.134347
 Thermal correction to Enthalpy= 0.135291
 Thermal correction to Gibbs Free Energy= 0.087457
 Sum of electronic and zero-point Energies= -409.810352
 Sum of electronic and thermal Energies= -409.800043
 Sum of electronic and thermal Enthalpies= -409.799099
 Sum of electronic and thermal Free Energies= -409.846933

$r_{\text{Sn-O}} = 2.443$

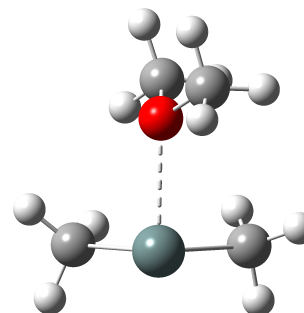
Sn	-0.553682	0.115822	-0.440911
C	2.772882	-0.033391	-0.018804
H	2.802464	0.349500	-1.036842
H	2.703698	0.804618	0.677688
H	3.678593	-0.610536	0.173654
O	1.622356	-0.870829	0.067557
C	-1.282609	-1.382818	1.009845
H	-1.217011	-2.398355	0.614077
H	-0.749457	-1.333573	1.964127
H	-2.337243	-1.183838	1.222544
C	-0.092235	1.609127	1.126338
H	0.524666	2.432079	0.759868
H	-1.034286	2.039021	1.481258
H	0.399003	1.152900	1.990719
H	1.546592	-1.233784	0.953718

**SnMe₂-Me₂O complex (6a')**

Zero-point correction= 0.152616 (Hartree/Particle)
 Thermal correction to Energy= 0.164106
 Thermal correction to Enthalpy= 0.165051
 Thermal correction to Gibbs Free Energy= 0.113630
 Sum of electronic and zero-point Energies= -449.085618
 Sum of electronic and thermal Energies= -449.074128
 Sum of electronic and thermal Enthalpies= -449.073184
 Sum of electronic and thermal Free Energies= -449.124604

$r_{\text{Sn-O}} = 2.459$

Sn	0.78019500	-0.33170100	-0.29590500
C	-2.45996200	-0.91130200	-0.42289700
H	-2.01046400	-1.61726900	-1.11868900
H	-2.55001800	-1.37642500	0.56412800
H	-3.45163900	-0.62236700	-0.78206200
C	-2.11513000	1.23453600	0.49065800
H	-2.20226800	0.86324700	1.51615000
H	-1.41245100	2.06324600	0.46156500
H	-3.09457200	1.56959000	0.13751200
O	-1.61435100	0.22336900	-0.36594700
C	1.22214600	1.82632100	-0.17683700
H	0.72849600	2.37053000	-0.98597200
H	0.94024200	2.26946200	0.78063700
H	2.29885100	1.96887000	-0.30823900
C	0.53607100	-0.60391400	1.88316500
H	-0.05096700	-1.49224200	2.12688400
H	1.52812100	-0.74011900	2.32547500
H	0.08296100	0.26771600	2.36088500

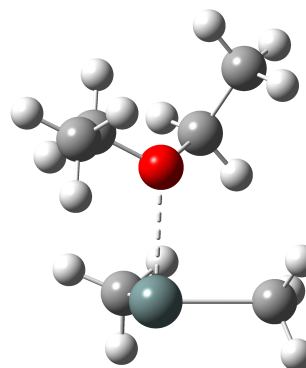


SnMe₂-Et₂O complex (6a)

Zero-point correction= 0.209598 (Hartree/Particle)
 Thermal correction to Energy= 0.223764
 Thermal correction to Enthalpy= 0.224709
 Thermal correction to Gibbs Free Energy= 0.166587
 Sum of electronic and zero-point Energies= -527.668932
 Sum of electronic and thermal Energies= -527.654766
 Sum of electronic and thermal Enthalpies= -527.653821
 Sum of electronic and thermal Free Energies= -527.711943

$r_{\text{Sn-O}} = 2.464$

Sn	-1.198419	0.350790	-0.179292
C	1.963705	1.110038	0.509419
H	1.456206	1.472229	1.410251
H	2.961234	0.774134	0.801788
C	1.664954	-1.273725	0.497234
H	1.851093	-1.188875	1.572381
H	0.825507	-1.952367	0.359331
O	1.233656	-0.007318	-0.005913
C	-1.335618	-1.630270	-1.145302
H	-0.525856	-1.753905	-1.869500
H	-1.309090	-2.460822	-0.436588
H	-2.273815	-1.690330	-1.703461
C	-1.335708	-0.399948	1.894300
H	-0.888631	0.292554	2.611228
H	-2.395912	-0.491038	2.151770
H	-0.881362	-1.385006	2.019915
C	2.880240	-1.784099	-0.247441
H	3.738875	-1.120363	-0.133776
H	3.162646	-2.764918	0.138747
H	2.656609	-1.882015	-1.309939
C	2.062747	2.190474	-0.540882
H	2.608233	3.044995	-0.137138
H	2.591603	1.821248	-1.420081
H	1.072419	2.528694	-0.846988

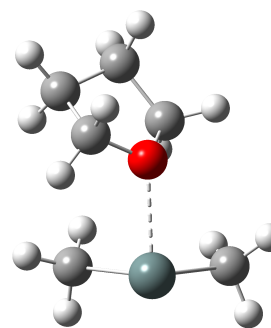


SnMe₂-THF complex (7a)

Zero-point correction= 0.190202 (Hartree/Particle)
 Thermal correction to Energy= 0.202197
 Thermal correction to Enthalpy= 0.203142
 Thermal correction to Gibbs Free Energy= 0.150661
 Sum of electronic and zero-point Energies= -526.480190
 Sum of electronic and thermal Energies= -526.468195
 Sum of electronic and thermal Enthalpies= -526.467251
 Sum of electronic and thermal Free Energies= -526.519731

$r_{\text{Sn-O}} = 2.426$

C	1.873129	-0.919665	-0.811011
C	1.692610	1.260554	0.072012
C	3.105185	0.747144	0.311055
C	2.907148	-0.766971	0.287231
H	1.251710	-1.809818	-0.713938
H	2.329766	-0.912766	-1.804642
H	1.650449	2.187637	-0.498283
H	1.148806	1.397188	1.007849
H	3.770226	1.055824	-0.497664
H	3.516782	1.113168	1.250161
H	3.821797	-1.319104	0.077374
H	2.496664	-1.114973	1.236930
O	1.026683	0.235429	-0.690438
C	-1.602015	1.840485	0.336026
H	-1.255893	2.523582	-0.443557
H	-2.674180	2.017417	0.462187
H	-1.107547	2.092662	1.276223
C	-0.639364	-0.957218	1.721426
H	-0.129041	-1.922082	1.672087
H	0.016000	-0.234430	2.214450
H	-1.518926	-1.087012	2.359879
Sn	-1.311005	-0.261934	-0.271520

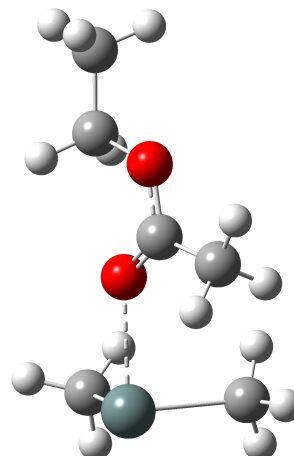


SnMe₂-EtOAc complex (8a)

Zero-point correction= 0.190939 (Hartree/Particle)
 Thermal correction to Energy= 0.205582
 Thermal correction to Enthalpy= 0.206526
 Thermal correction to Gibbs Free Energy= 0.146929
 Sum of electronic and zero-point Energies= -601.742608
 Sum of electronic and thermal Energies= -601.727965
 Sum of electronic and thermal Enthalpies= -601.727021
 Sum of electronic and thermal Free Energies= -601.786618

$r_{\text{Sn-O}} = 2.419$

Sn	-1.698350	-0.060954	-0.380245
O	0.709473	-0.164427	-0.172396
C	1.517334	0.745641	-0.119838
O	2.811354	0.520269	-0.023525
C	1.158396	2.194949	-0.143852
H	0.652248	2.436434	0.792034
H	2.037352	2.821963	-0.261939
H	0.446307	2.369920	-0.951242
C	-1.717697	-2.029230	0.597420
H	-2.734759	-2.248151	0.937100
H	-1.413607	-2.826148	-0.083033
H	-1.062518	-2.035357	1.470790
C	-1.743240	1.040408	1.541044
H	-0.913824	0.730639	2.182887
H	-1.720151	2.125594	1.422300
H	-2.669868	0.783015	2.062933
C	3.236221	-0.857357	0.032375
H	2.746614	-1.334960	0.881695
H	2.899124	-1.358853	-0.875361
C	4.737778	-0.866210	0.162173
H	5.054292	-0.355179	1.071554
H	5.089857	-1.897342	0.207056
H	5.207066	-0.379795	-0.693102

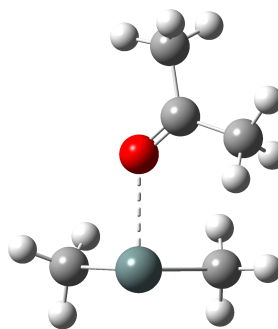


SnMe₂-Me₂CO complex (9a)

Zero-point correction= 0.156343 (Hartree/Particle)
 Thermal correction to Energy= 0.168793
 Thermal correction to Enthalpy= 0.169738
 Thermal correction to Gibbs Free Energy= 0.116320
 Sum of electronic and zero-point Energies= -487.213459
 Sum of electronic and thermal Energies= -487.201008
 Sum of electronic and thermal Enthalpies= -487.200064
 Sum of electronic and thermal Free Energies= -487.253481

$r_{\text{Sn-O}} = 2.420$

O	-1.166229	0.761480	-0.037154
C	-2.236912	0.181414	-0.021168
C	-2.333636	-1.301488	-0.217901
H	-2.052119	-1.784085	0.721665
H	-3.341514	-1.614431	-0.484504
H	-1.617687	-1.626081	-0.974403
Sn	1.059770	-0.112832	-0.409031
C	1.776728	1.606936	0.753416
H	2.813251	1.422872	1.052505
H	1.754395	2.529814	0.172122
H	1.183270	1.741243	1.659671
C	0.771778	-1.380872	1.384585
H	0.125940	-0.882738	2.112874
H	0.364212	-2.368236	1.158476
H	1.746067	-1.524208	1.861306
C	-3.503029	0.944918	0.214325
H	-4.125506	0.885431	-0.682408
H	-4.069906	0.480258	1.024156
H	-3.288618	1.984453	0.447760

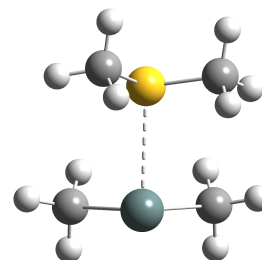


SnMe₂-Me₂S complex (10a')

Zero-point correction= 0.148055 (Hartree/Particle)
 Thermal correction to Energy= 0.160329
 Thermal correction to Enthalpy= 0.161274
 Thermal correction to Gibbs Free Energy= 0.107750
 Sum of electronic and zero-point Energies= -772.084291
 Sum of electronic and thermal Energies= -772.072016
 Sum of electronic and thermal Enthalpies= -772.071072
 Sum of electronic and thermal Free Energies= -772.124595

$r_{\text{Sn-S}} = 2.790$

Sn	0.89110800	-0.06887000	-0.46738000
C	-2.31102700	1.41246500	-0.09647600
H	-1.82310400	2.24875100	0.40090900
H	-2.07604000	1.43966800	-1.16051500
H	-3.38719600	1.47404700	0.05792600
C	-2.49897300	-1.33576100	-0.34140100
H	-2.26611400	-1.19747700	-1.39671700
H	-2.12593400	-2.30563400	-0.01641500
H	-3.57437200	-1.28906500	-0.17562500
S	-1.66396700	-0.08979800	0.65198200
C	1.59803100	-1.38435500	1.15835000
H	1.27436900	-2.41825900	1.02366800
H	2.69208300	-1.37922600	1.14857200
H	1.27103700	-1.03207400	2.13833600
C	1.23208700	1.80158300	0.66688300
H	0.79073900	2.67341400	0.17987200
H	0.85998000	1.73463400	1.69180400
H	2.31192900	1.96791700	0.72134500

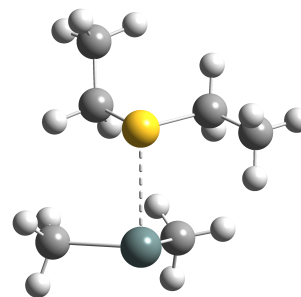


SnMe₂-Et₂S complex (10a)

Zero-point correction= 0.206257 (Hartree/Particle)
 Thermal correction to Energy= 0.220762
 Thermal correction to Enthalpy= 0.221706
 Thermal correction to Gibbs Free Energy= 0.163809
 Sum of electronic and zero-point Energies= -850.661877
 Sum of electronic and thermal Energies= -850.647372
 Sum of electronic and thermal Enthalpies= -850.646428
 Sum of electronic and thermal Free Energies= -850.704325

$r_{\text{Sn-S}} = 2.825$

Sn	1.45992100	0.14952400	-0.23151100
C	-1.94594900	1.35530500	0.31466900
H	-1.58850100	1.19380300	1.33243100
H	-3.03439400	1.30076900	0.31164400
C	-1.86027300	-1.44368200	0.23605000
H	-1.45739900	-1.35280800	1.24560200
H	-1.35320500	-2.28331600	-0.23924500
S	-1.32002900	-0.00118000	-0.71371400
C	1.02923800	0.39551200	1.93134200
H	0.71551800	1.41070900	2.18402200
H	1.96211700	0.20074000	2.46967200
H	0.28677000	-0.31200100	2.30899400
C	1.50232500	-2.06267900	-0.15421000
H	1.16280800	-2.51028400	-1.09123100
H	0.91796600	-2.47063100	0.67270500
H	2.54257300	-2.36871900	-0.01069900
C	-1.47670100	2.69668400	-0.22287200
H	-1.89250500	3.49941700	0.38721800
H	-0.38939500	2.77832700	-0.19535700
H	-1.80366900	2.84815600	-1.25238900
C	-3.36514200	-1.65039200	0.24632700
H	-3.60478000	-2.57305400	0.77797400
H	-3.88210900	-0.83523300	0.75352300
H	-3.75838200	-1.72766000	-0.76772800

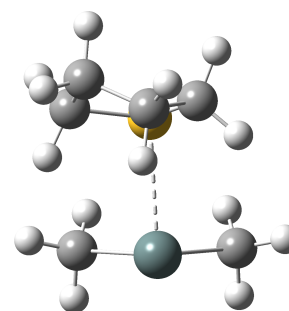


SnMe₂-THT complex (11a)

Zero-point correction= 0.187101 (Hartree/Particle)
 Thermal correction to Energy= 0.199326
 Thermal correction to Enthalpy= 0.200271
 Thermal correction to Gibbs Free Energy= 0.147479
 Sum of electronic and zero-point Energies= -849.474905
 Sum of electronic and thermal Energies= -849.462679
 Sum of electronic and thermal Enthalpies= -849.461735
 Sum of electronic and thermal Free Energies= -849.514527

$r_{\text{Sn-S}} = 2.779$

C	-1.83370700	1.41801300	0.08525500
C	-2.07053900	-1.16809800	-0.58384700
C	-3.25436800	-0.57818500	0.17189700
C	-2.70316100	0.57071600	1.00877900
H	-1.04715700	1.95343700	0.61346100
H	-2.42369500	2.13206400	-0.48808400
H	-2.36023700	-1.72435600	-1.47256800
H	-1.46800200	-1.81219000	0.05670300
H	-3.99789000	-0.20436500	-0.53627700
H	-3.73464000	-1.33914900	0.78850700
H	-3.49788100	1.17402000	1.44945100
H	-2.09232100	0.17429100	1.82115900
S	-1.05909400	0.26168000	-1.09908100
C	1.98696500	1.73813400	-0.21672300
H	2.96493600	1.86387400	0.25704900
H	2.07273300	2.08809300	-1.24696000
H	1.28011300	2.37669300	0.31829200
C	0.68842400	-0.28725900	1.96778100
H	0.22476500	0.67436300	2.19979700
H	-0.01187500	-1.09187000	2.20411100
H	1.54841600	-0.40457700	2.63435400
Sn	1.45213100	-0.40414300	-0.11225100

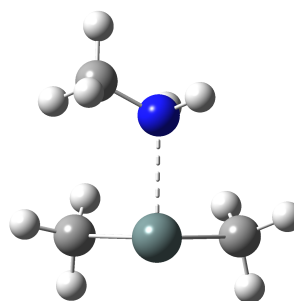


SnMe₂-MeNH₂ complex (12a')

Zero-point correction= 0.137980 (Hartree/Particle)
 Thermal correction to Energy= 0.148014
 Thermal correction to Enthalpy= 0.148958
 Thermal correction to Gibbs Free Energy= 0.102011
 Sum of electronic and zero-point Energies= -389.939954
 Sum of electronic and thermal Energies= -389.929920
 Sum of electronic and thermal Enthalpies= -389.928976
 Sum of electronic and thermal Free Energies= -389.975923

$r_{\text{Sn-N}} = 2.418$

Sn	0.50463600	0.09211200	-0.45752500
C	1.45908700	-1.26897100	1.00752100
H	1.41388100	-2.31280900	0.68722400
H	2.51653900	-1.00711600	1.10280100
H	1.01214900	-1.18363200	2.00235400
C	0.13588900	1.68531000	1.03735400
H	-0.51728400	2.47535100	0.66079700
H	-0.29000400	1.28469700	1.96246600
H	1.09218200	2.14832600	1.29712600
C	-2.76480600	-0.03546300	0.00549000
H	-2.62535400	0.93311200	0.48293300
H	-2.84392800	0.12502400	-1.06917400
H	-3.69242300	-0.48289000	0.36911700
N	-1.58858000	-0.86834400	0.27757900
H	-1.46628500	-1.00683000	1.27408300
H	-1.69222700	-1.78568900	-0.13874000

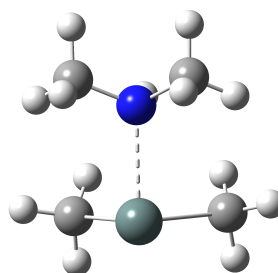


SnMe₂-Me₂NH complex (13a')

Zero-point correction= 0.166413 (Hartree/Particle)
 Thermal correction to Energy= 0.177586
 Thermal correction to Enthalpy= 0.178530
 Thermal correction to Gibbs Free Energy= 0.129109
 Sum of electronic and zero-point Energies= -429.221236
 Sum of electronic and thermal Energies= -429.210063
 Sum of electronic and thermal Enthalpies= -429.209118
 Sum of electronic and thermal Free Energies= -429.258540

$r_{\text{Sn-N}} = 2.411$

Sn	-0.68753300	0.00000100	-0.46525200
C	-1.09492000	1.61457600	0.99869500
H	-0.79268000	2.59886500	0.63459900
H	-2.17217000	1.65266300	1.18384200
H	-0.61024000	1.43075800	1.96262600
C	-1.09492200	-1.61457800	0.99868900
H	-0.79270100	-2.59887000	0.63458400
H	-0.61022600	-1.43077200	1.96261500
H	-2.17217000	-1.65265100	1.18385100
C	2.29007900	-1.21789300	0.01536400
H	1.73381600	-2.08634200	0.36519500
H	2.36528000	-1.27042900	-1.07147900
H	3.29919300	-1.23921700	0.43955900
N	1.56897000	0.00000000	0.38312900
H	1.40553600	0.00000200	1.38340900
C	2.29008400	1.21789000	0.01536100
H	2.36528100	1.27042600	-1.07148300
H	1.73382700	2.08634100	0.36519400
H	3.29920000	1.23920900	0.43955200

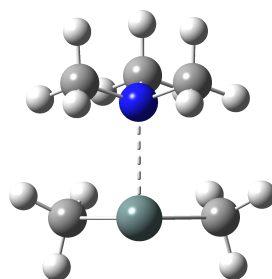


SnMe₂-NMe₃ complex (14a')

Zero-point correction= 0.194514 (Hartree/Particle)
 Thermal correction to Energy= 0.206711
 Thermal correction to Enthalpy= 0.207655
 Thermal correction to Gibbs Free Energy= 0.155537
 Sum of electronic and zero-point Energies= -468.502561
 Sum of electronic and thermal Energies= -468.490364
 Sum of electronic and thermal Enthalpies= -468.489420
 Sum of electronic and thermal Free Energies= -468.541537

$r_{\text{Sn-N}} = 2.466$

Sn	-0.87628100	0.00000000	-0.46344400
C	2.10019700	-1.20075800	-0.56737100
H	1.65588700	-2.08628300	-0.11417600
H	1.87475000	-1.20474600	-1.63370000
H	3.18830000	-1.23872200	-0.43073800
C	2.10019300	1.20077100	-0.56735200
H	1.87474500	1.20477500	-1.63368100
H	1.65588200	2.08628800	-0.11414200
H	3.18829700	1.23873500	-0.43072000
N	1.53533700	0.00000100	0.04954800
C	1.79754500	-0.00001000	1.48870500
H	1.35214300	0.88442400	1.94079800
H	1.35214400	-0.88445300	1.94078400
H	2.87668100	-0.00001100	1.68931100
C	-1.19055900	1.63111300	0.99957600
H	-0.64057800	2.53832500	0.73637900
H	-2.25308100	1.89167100	0.98962800
H	-0.93288000	1.34033400	2.02040700
C	-1.19055400	-1.63111600	0.99957500
H	-0.64055500	-2.53831900	0.73638600
H	-0.93289300	-1.34033100	2.02040800
H	-2.25307300	-1.89169100	0.98961300

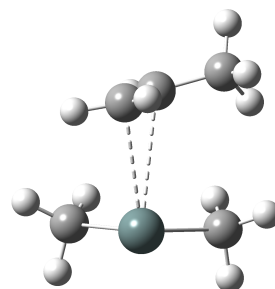


SnMe₂-propene complex (15a')

Zero-point correction= 0.152583 (Hartree/Particle)
 Thermal correction to Energy= 0.163690
 Thermal correction to Enthalpy= 0.164635
 Thermal correction to Gibbs Free Energy= 0.114359
 Sum of electronic and zero-point Energies= -411.952069
 Sum of electronic and thermal Energies= -411.940962
 Sum of electronic and thermal Enthalpies= -411.940017
 Sum of electronic and thermal Free Energies= -411.990293

$r_{\text{Sn-C1}} = 2.793$; $r_{\text{Sn-C2}} = 3.032$

Sn	-0.81623800	0.00064500	-0.39678100
C	1.59617700	-1.40160600	-0.52236900
H	1.03266700	-2.28922000	-0.26130700
H	1.86872100	-1.28065700	-1.56450600
C	2.04848800	-0.56556200	0.41845800
H	1.78369300	-0.75911800	1.45385400
C	2.94177800	0.60037600	0.16653400
H	2.54002600	1.50756800	0.62105600
H	3.91954100	0.42042900	0.62140900
H	3.08417900	0.77472000	-0.90019800
C	-1.25075700	-0.91739900	1.56311300
H	-1.19575400	-2.00720100	1.52465200
H	-0.59519600	-0.55317100	2.35598400
H	-2.27741100	-0.65451700	1.83642000
C	-0.17632400	1.94008900	0.44097000
H	0.31020300	1.84801300	1.41339800
H	0.47121900	2.49245100	-0.24172900
H	-1.08616700	2.53307700	0.57975300

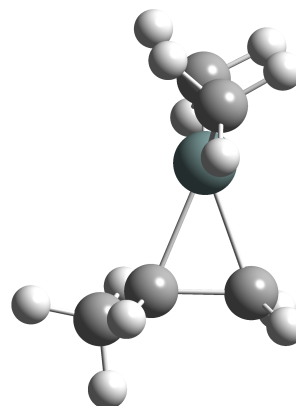


1,1,2-trimethylstannirane (19a)

Zero-point correction= 0.153534 (Hartree/Particle)
 Thermal correction to Energy= 0.163834
 Thermal correction to Enthalpy= 0.164778
 Thermal correction to Gibbs Free Energy= 0.116907
 Sum of electronic and zero-point Energies= -411.929709
 Sum of electronic and thermal Energies= -411.919409
 Sum of electronic and thermal Enthalpies= -411.918464
 Sum of electronic and thermal Free Energies= -411.966336

$r_{\text{Sn-C2}} = 2.137$; $r_{\text{Sn-C3}} = 2.136$

C	-1.58413000	-0.69140300	-0.29130400
C	-1.18214900	-0.78668900	1.19053600
H	-1.65330300	-1.65883400	-0.78191100
H	-1.08924100	-1.78508800	1.60575400
H	-1.71629600	-0.11540500	1.85745100
Sn	0.40668100	0.02213900	0.01358500
C	0.72145500	2.13443900	0.13147100
H	1.37193700	2.37797300	0.96997500
H	1.17126900	2.50573600	-0.78809600
H	-0.24003800	2.62527900	0.27729500
C	2.08264400	-1.23205500	-0.42287900
H	2.50822300	-0.97831900	-1.39251300
H	2.84957500	-1.12241800	0.34234100
H	1.74938800	-2.26882900	-0.44323200
C	-2.73291600	0.22698800	-0.63565700
H	-2.83093400	0.36272900	-1.71388800
H	-3.67965400	-0.17453900	-0.25579900
H	-2.60439500	1.21707300	-0.18962400

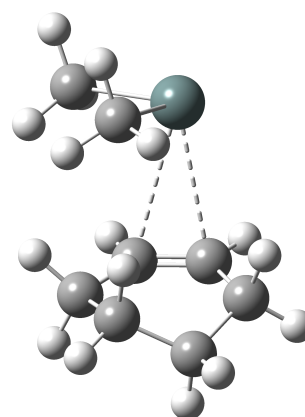


SnMe₂-cyclohexene complex (16a)

Zero-point correction= 0.219850 (Hartree/Particle)
 Thermal correction to Energy= 0.232474
 Thermal correction to Enthalpy= 0.233418
 Thermal correction to Gibbs Free Energy= 0.179435
 Sum of electronic and zero-point Energies= -528.633960
 Sum of electronic and thermal Energies= -528.621336
 Sum of electronic and thermal Enthalpies= -528.620392
 Sum of electronic and thermal Free Energies= -528.674374

$r_{\text{Sn-C1}} = 2.951$, $r_{\text{Sn-C2}} = 3.031$

C	-2.19756200	-1.42138500	0.20161900
C	-1.26639900	-0.73634400	1.16412200
C	-1.13663000	0.59395200	1.22848000
C	-1.86775900	1.54421900	0.33051400
C	-2.60285400	0.84170000	-0.80993000
C	-3.25001700	-0.45597000	-0.33840100
H	-0.51594800	1.03008900	2.00375400
H	-0.75581500	-1.35538600	1.89370200
H	-1.62351000	-1.85579700	-0.62411800
H	-2.67352500	-2.26378900	0.70840600
H	-2.57388900	2.11126900	0.94815800
H	-1.16449800	2.28351700	-0.06439200
H	-3.35161900	1.51233400	-1.23466300
H	-1.89442100	0.61307800	-1.60876100
H	-3.97413100	-0.23657100	0.45269600
H	-3.80303300	-0.92402400	-1.15447400
Sn	1.41198700	-0.44745200	-0.04008100
C	0.78377600	0.51375300	-1.92014000
H	0.15858600	-0.12635100	-2.54422600
H	0.28356000	1.47079900	-1.76173000
H	1.70595900	0.71521500	-2.47664700
C	2.04408500	1.45785400	0.87766300
H	1.37117600	2.28010800	0.62637400
H	2.14011400	1.38852100	1.96247900
H	3.03177900	1.70292600	0.47391800

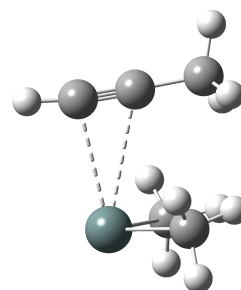


SnMe₂-propyne complex (17a')

Zero-point correction= 0.127697 (Hartree/Particle)
 Thermal correction to Energy= 0.139021
 Thermal correction to Enthalpy= 0.139965
 Thermal correction to Gibbs Free Energy= 0.088987
 Sum of electronic and zero-point Energies= -410.721229
 Sum of electronic and thermal Energies= -410.709905
 Sum of electronic and thermal Enthalpies= -410.708961
 Sum of electronic and thermal Free Energies= -410.759939

$r_{\text{Sn-C1}} = 2.789$; $r_{\text{Sn-C1}} = 2.955$

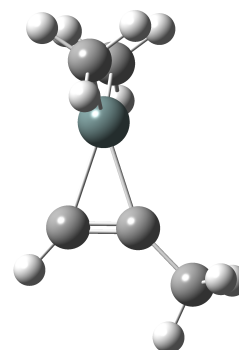
Sn	-0.85322100	-0.26886500	-0.00005500
C	2.73553000	0.75377700	0.00011100
H	2.44516100	1.32039000	0.88532900
H	3.81936600	0.63148500	0.00037800
H	2.44559900	1.32041900	-0.88523000
C	1.57718700	-1.63713100	-0.00021400
H	1.24349800	-2.64793400	-0.00034700
C	2.08893600	-0.54683200	-0.00006900
C	-0.33935600	1.11014100	1.64544900
H	0.24321700	0.59608900	2.41366900
H	0.20753500	1.99204500	1.30682400
H	-1.26613300	1.44836400	2.11749200
C	-0.33929300	1.11069300	-1.64507100
H	0.24292900	0.59681700	-2.41367200
H	-1.26609400	1.44940900	-2.11671700
H	0.20793900	1.99228800	-1.30618900

**1,1,3-trimethylstannirene (20a)**

Zero-point correction= 0.129880 (Hartree/Particle)
 Thermal correction to Energy= 0.140072
 Thermal correction to Enthalpy= 0.141016
 Thermal correction to Gibbs Free Energy= 0.093344
 Sum of electronic and zero-point Energies= -410.710575
 Sum of electronic and thermal Energies= -410.700383
 Sum of electronic and thermal Enthalpies= -410.699439
 Sum of electronic and thermal Free Energies= -410.747111

$r_{\text{Sn-C2}} = 2.106$; $r_{\text{Sn-C3}} = 2.097$

C	1.704621	0.000000	-0.004961
C	1.301231	0.000000	1.261236
H	1.853734	0.000000	2.197690
Sn	-0.401289	0.000000	0.036527
C	-1.499619	-1.816051	-0.253752
H	-2.347810	-1.857799	0.428601
H	-1.866697	-1.880862	-1.277307
H	-0.839522	-2.658990	-0.055544
C	-1.499619	1.816051	-0.253752
H	-1.866697	1.880862	-1.277307
H	-2.347810	1.857799	0.428601
H	-0.839522	2.658990	-0.055544
C	3.028178	0.000000	-0.683573
H	3.132006	0.877553	-1.325196
H	3.845995	0.000000	0.043652
H	3.132006	-0.877553	-1.325196

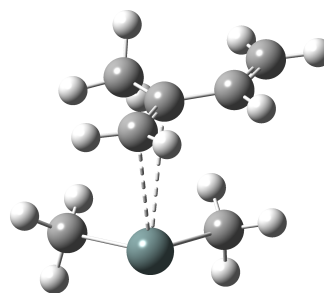


SnMe₂-isoprene complex (18a)

Zero-point correction= 0.186608 (Hartree/Particle)
 Thermal correction to Energy= 0.199466
 Thermal correction to Enthalpy= 0.200410
 Thermal correction to Gibbs Free Energy= 0.146901
 Sum of electronic and zero-point Energies= -489.322701
 Sum of electronic and thermal Energies= -489.309843
 Sum of electronic and thermal Enthalpies= -489.308899
 Sum of electronic and thermal Free Energies= -489.362408

$r_{\text{Sn-C1}} = 2.768$; $r_{\text{Sn-C2}} = 3.102$

Sn	1.25098600	-0.24246500	-0.29531000
C	-0.89992100	1.07446100	-1.43587500
H	-0.37644700	2.02274200	-1.41587400
H	-0.87362400	0.51838700	-2.36454900
C	-1.70332800	0.69680200	-0.42009300
C	1.54067600	1.32370800	1.22947200
H	1.56831100	2.32429800	0.79289900
H	0.78472600	1.29477600	2.01583700
H	2.51485600	1.14936900	1.69773800
C	0.23315400	-1.63367200	1.07657500
H	-0.48021200	-1.12894700	1.73083300
H	-0.27581000	-2.44418300	0.55506600
H	1.01316300	-2.07259800	1.70754800
C	-2.47939300	-0.53858500	-0.53851200
H	-2.32409600	-1.10496800	-1.45172000
C	-3.32904400	-0.99919200	0.37290600
H	-3.51563800	-0.47901100	1.30419700
H	-3.86879000	-1.92315000	0.21364500
C	-1.86025200	1.53244900	0.81227300
H	-2.89329900	1.87638800	0.90189000
H	-1.62960200	0.95438500	1.71002900
H	-1.20418700	2.39993300	0.78750300

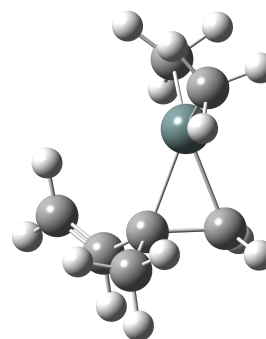


1,1-dimethyl-2-(methylethenyl)stannirane (21a)

Zero-point correction= 0.186401 (Hartree/Particle)
 Thermal correction to Energy= 0.198977
 Thermal correction to Enthalpy= 0.199921
 Thermal correction to Gibbs Free Energy= 0.146976
 Sum of electronic and zero-point Energies= -489.289135
 Sum of electronic and thermal Energies= -489.276559
 Sum of electronic and thermal Enthalpies= -489.275615
 Sum of electronic and thermal Free Energies= -489.328560

$r_{\text{Sn-C2}} = 2.144$; $r_{\text{Sn-C3}} = 2.137$

C	1.33091100	-0.57844100	0.09882900
C	0.68270200	-0.64642900	1.50220600
H	1.05878100	0.07341500	2.22383000
H	0.57778000	-1.64082300	1.92763400
Sn	-0.71110800	0.07267000	0.05010900
C	-2.19605300	-1.29322300	-0.66183400
H	-2.99966700	-1.39349600	0.06598300
H	-2.61188800	-0.94342100	-1.60559100
H	-1.73623100	-2.26831700	-0.81750800
C	-1.17974900	2.15738100	0.08637500
H	-1.36417500	2.52629100	-0.92160800
H	-2.05941200	2.34436200	0.70044100
H	-0.32746000	2.68730700	0.50897800
C	1.68358900	-1.93396400	-0.48387000
H	1.92943400	-1.85922400	-1.54395700
H	2.54959900	-2.36079800	0.03799700
H	0.86099100	-2.64558700	-0.37612000
C	2.44331900	0.40265700	-0.01013100
H	3.32713800	0.14879500	0.58016200
C	2.46774700	1.51362600	-0.73166500
H	1.61875900	1.80858400	-1.33971600
H	3.33696000	2.15978300	-0.74541700

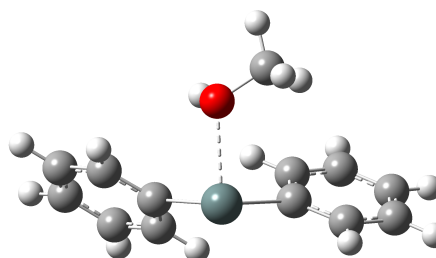


SnPh₂-MeOH complex (5b)

Zero-point correction= 0.235050 (Hartree/Particle)
 Thermal correction to Energy= 0.251012
 Thermal correction to Enthalpy= 0.251956
 Thermal correction to Gibbs Free Energy= 0.188605
 Sum of electronic and zero-point Energies= -793.167634
 Sum of electronic and thermal Energies= -793.151672
 Sum of electronic and thermal Enthalpies= -793.150728
 Sum of electronic and thermal Free Energies= -793.214080

$r_{\text{Sn-O}} = 2.432$

C	1.56355200	0.29852600	-0.30190000
C	-1.71729700	0.15052600	-0.28727500
C	1.41399800	1.34284700	0.61488300
C	2.47606200	2.16601300	0.96048500
C	3.72312200	1.96750700	0.38411100
C	3.89873500	0.94254200	-0.53190500
C	2.82990500	0.11823400	-0.86143800
C	-1.74535100	1.51172100	-0.60091200
C	-2.85754100	-0.39095700	0.31310900
C	-2.85442100	2.29832600	-0.32210500
C	-3.96598400	1.74013000	0.29203200
C	-3.96551500	0.39138300	0.61261300
H	2.33123300	2.96766300	1.67524000
H	4.86897300	0.78200700	-0.98674300
H	2.99631400	-0.68661200	-1.57214200
H	-2.89255800	-1.45030900	0.55357700
H	-2.84995900	3.35068500	-0.58036100
H	0.44466800	1.52930900	1.06746500
H	4.55351800	2.61084900	0.64805800
H	-0.88239500	1.97697900	-1.06643400
H	-4.83035300	2.35314200	0.51576200
H	-4.83268100	-0.05439300	1.08534100
Sn	-0.01619600	-1.16501400	-0.78632400
C	1.08156100	-1.83779500	2.33569900
H	1.55264800	-2.70474900	1.87708600
H	1.75923100	-0.98459200	2.27158000
H	0.84801400	-2.06420100	3.37691300
O	-0.12026600	-1.59284500	1.60544800
H	-0.57969800	-0.82631300	1.96290800

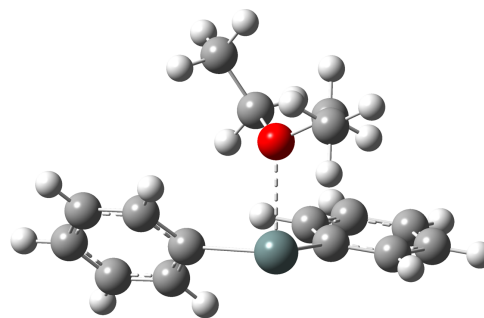


SnPh₂-Et₂O complex (6b)

Zero-point correction= 0.321135
 (Hartree/Particle)
 Thermal correction to Energy= 0.340828
 Thermal correction to Enthalpy= 0.341773
 Thermal correction to Gibbs Free Energy= 0.269879
 Sum of electronic and zero-point Energies= -911.020853
 Sum of electronic and thermal Energies= -911.001160
 Sum of electronic and thermal Enthalpies= -911.000216
 Sum of electronic and thermal Free Energies= -911.072109

$r_{\text{Sn-O}} = 2.461$

Sn	-0.09048400	0.28213000	-1.33913300
C	-1.29017800	2.67905300	0.58459200
H	-2.19164600	2.08409200	0.40021300
H	-1.38866500	3.13391800	1.57253400
C	0.11352200	1.23686600	1.88845200
H	-0.83151200	0.95584400	2.36175100
H	0.67835900	0.32563500	1.70529900
O	-0.16089600	1.79824300	0.59788500
C	0.92425800	2.18730800	2.74176000
H	0.39933800	3.12605900	2.92665000
H	1.13153200	1.72360700	3.70758700
H	1.87487500	2.40894900	2.25598700
C	-1.10154800	3.74986300	-0.46334700
H	-1.96682000	4.41470000	-0.46457300
H	-0.20877300	4.33910100	-0.25150400
H	-1.00268100	3.31605300	-1.45874200
C	1.75439300	-0.55542100	-0.48197900
C	1.96120400	-1.92762200	-0.33062400
C	2.81468900	0.29252900	-0.15241400
C	3.16605100	-2.43272800	0.14154200
H	1.16835500	-2.62649400	-0.57883100
C	4.01677400	-0.20033700	0.33435600
H	2.70317500	1.36700200	-0.26978900
C	4.19495800	-1.56843800	0.48199900
H	3.29973500	-3.50280700	0.24765900
H	4.81920800	0.48136800	0.59091000
H	5.13360200	-1.95858800	0.85576900
C	-1.54070600	-0.95515500	-0.22794300
C	-2.87491600	-0.87647500	-0.63527500
C	-1.26162900	-1.74981600	0.88692800
C	-3.88709600	-1.55198300	0.03491600
H	-3.13946100	-0.27428500	-1.50062400
C	-2.26375500	-2.42888800	1.56487300
H	-0.24071300	-1.84612000	1.24010900
C	-3.58130900	-2.33020000	1.13987500
H	-4.91245100	-1.47241900	-0.30636800
H	-2.01745200	-3.03877800	2.42623100
H	-4.36489600	-2.86061600	1.66703000

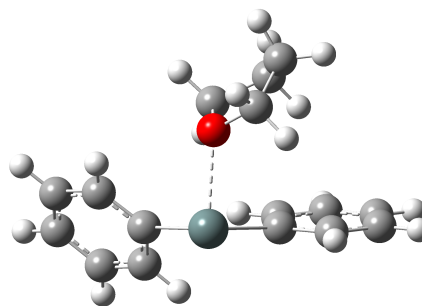


SnPh₂-THF complex (7b)

Zero-point correction= 0.301201 (Hartree/Particle)
 Thermal correction to Energy= 0.318847
 Thermal correction to Enthalpy= 0.319791
 Thermal correction to Gibbs Free Energy= 0.252886
 Sum of electronic and zero-point Energies= -909.838529
 Sum of electronic and thermal Energies= -909.820883
 Sum of electronic and thermal Enthalpies= -909.819938
 Sum of electronic and thermal Free Energies= -909.886843

$r_{\text{Sn-O}} = 2.419$

C	-1.73785700	2.47689400	-0.14000200
C	-0.41988500	1.54439800	1.58135100
C	-1.86916800	1.47450300	2.01377600
C	-2.49289300	2.59044900	1.17793000
H	-1.54235300	3.43603400	-0.61902100
H	-2.26288800	1.82792100	-0.84436400
H	0.12901200	0.61288100	1.69416500
H	0.12380300	2.34313800	2.09384800
H	-2.29007400	0.50429500	1.74282700
H	-1.98925300	1.62409200	3.08566900
H	-3.56620400	2.47337600	1.03864300
H	-2.31193900	3.56155400	1.64243400
O	-0.46949800	1.86470700	0.17635000
Sn	0.25918000	0.25288500	-1.47342600
C	2.02031700	-0.14822500	-0.21655900
C	2.76141400	0.89940700	0.33365600
C	2.50134800	-1.44415600	-0.02045300
C	3.91558800	0.66676400	1.06827900
H	2.43293700	1.92548000	0.19425600
C	3.66182000	-1.68773500	0.70270900
H	1.96198000	-2.29266300	-0.43173100
C	4.36955200	-0.63085400	1.25405200
H	4.46645400	1.49886800	1.49088900
H	4.01182300	-2.70424900	0.83848400
H	5.27259900	-0.81671900	1.82233100
C	-1.13571600	-1.10928200	-0.42816700
C	-0.86047400	-1.80454500	0.75168500
C	-2.44868900	-1.15783900	-0.90338600
C	-1.84906800	-2.50074100	1.43323500
H	0.14464400	-1.79817200	1.15958300
C	-3.44846900	-1.84609700	-0.22757600
H	-2.70743200	-0.64426400	-1.82596600
C	-3.14912800	-2.51736100	0.94775400
H	-1.60638900	-3.02929200	2.34770400
H	-4.45872200	-1.86141800	-0.61930700
H	-3.92315000	-3.05624700	1.48034200

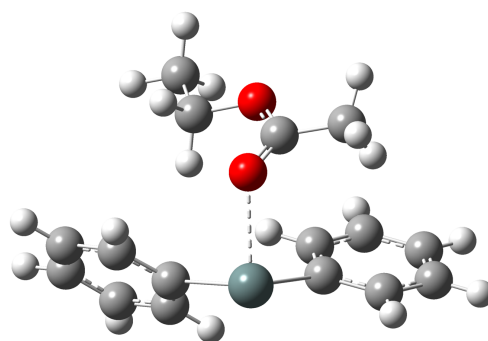


SnPh₂-EtOAc complex (8b)

Zero-point correction= 0.301456 (Hartree/Particle)
 Thermal correction to Energy= 0.321976
 Thermal correction to Enthalpy= 0.322920
 Thermal correction to Gibbs Free Energy= 0.248180
 Sum of electronic and zero-point Energies= -985.101756
 Sum of electronic and thermal Energies= -985.081236
 Sum of electronic and thermal Enthalpies= -985.080292
 Sum of electronic and thermal Free Energies= -985.155032

$r_{\text{Sn-O}} = 2.445$

C	-1.61900900	-0.73552700	0.52933200
C	1.64892000	-1.04803600	0.16736400
C	-1.32425300	0.28457300	1.43818900
C	-2.31171600	0.88484200	2.20655500
C	-3.63072700	0.46846600	2.09005500
C	-3.95062700	-0.54944900	1.20497100
C	-2.95353000	-1.13607500	0.43511200
C	1.75996600	-1.09714100	1.55780800
C	2.78332000	-0.66414600	-0.55181000
C	2.94090300	-0.75565200	2.20548300
C	4.04427600	-0.35222900	1.46918100
C	3.96451800	-0.31011700	0.08427800
H	-2.05354700	1.67902100	2.89726300
H	-4.97734400	-0.88240500	1.10964500
H	-3.23319200	-1.91882300	-0.26461400
H	2.74635100	-0.62235900	-1.63675600
H	2.99815600	-0.80127700	3.28670100
H	-0.30159800	0.62988400	1.54806600
H	-4.40428200	0.93454200	2.68795500
H	0.90704100	-1.39610200	2.15874000
H	4.96490800	-0.08046300	1.97099300
H	4.82620200	-0.00737600	-0.49924800
Sn	-0.18675800	-1.55921000	-0.94403500
O	-0.08258200	0.74526000	-1.75406700
C	-0.69874200	1.74162100	-1.41289600
O	-0.12206800	2.74451800	-0.79036900
C	-2.16189500	1.94151400	-1.63061500
H	-2.67846600	1.56368000	-0.74396100
H	-2.40163800	2.99547300	-1.75072900
H	-2.48653500	1.36284700	-2.49150100
C	1.26491700	2.58020400	-0.41670400
H	1.36637400	1.65212600	0.14511300
H	1.85700400	2.48251000	-1.32733500
C	1.66434900	3.78220700	0.39802500
H	2.70728800	3.67712500	0.69866800
H	1.55986200	4.70321900	-0.17616000
H	1.05450800	3.86030700	1.29840800

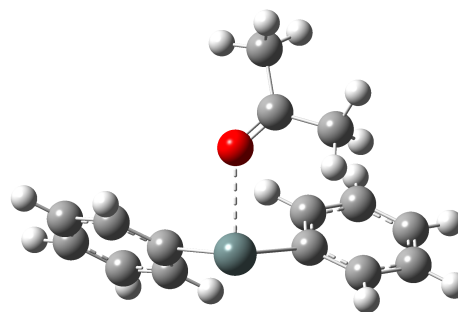


SnPh₂-Me₂CO complex (9b)

Zero-point correction= 0.266958 (Hartree/Particle)
 Thermal correction to Energy= 0.285203
 Thermal correction to Enthalpy= 0.286147
 Thermal correction to Gibbs Free Energy= 0.217066
 Sum of electronic and zero-point Energies= -870.570524
 Sum of electronic and thermal Energies= -870.552279
 Sum of electronic and thermal Enthalpies= -870.551335
 Sum of electronic and thermal Free Energies= -870.620415

$r_{\text{Sn-O}} = 2.414$

C	-1.26190900	-0.95205000	-0.27145600
C	1.94188500	-0.26366100	-0.19821600
C	-1.16175300	-1.17774200	1.10398900
C	-2.17395500	-1.81163200	1.81140400
C	-3.31448600	-2.24881500	1.15102400
C	-3.43196300	-2.05035000	-0.21596300
C	-2.41664600	-1.40446800	-0.91092600
C	2.13234200	-1.55121600	0.30569300
C	2.96157400	0.66628800	0.01189800
C	3.28729300	-1.89626500	0.99571700
C	4.27921000	-0.95054000	1.20434800
C	4.11305100	0.33584600	0.71215300
H	-2.07209600	-1.97111400	2.87866700
H	-4.31622700	-2.39392800	-0.73974500
H	-2.54118000	-1.24251400	-1.97826300
H	2.86003700	1.67732900	-0.37185100
H	3.41055600	-2.90400000	1.37481200
H	-0.27582700	-0.84917500	1.63804000
H	-4.10490000	-2.74640800	1.69959600
H	1.36315600	-2.30503200	0.17017100
H	5.17923800	-1.21479000	1.74604700
H	4.88529000	1.07988500	0.86878100
Sn	0.18579900	0.28254900	-1.39663100
O	-0.20435000	1.96128100	0.29325900
C	-1.22167000	2.39779900	0.80340900
C	-2.58757100	2.04458100	0.30383300
H	-2.88717900	1.10915100	0.78737700
H	-3.31584900	2.81431600	0.55537800
H	-2.57214200	1.86281000	-0.76963700
C	-1.12757600	3.30520300	1.99074500
H	-1.49841500	4.29544800	1.71389100
H	-1.77601200	2.93451400	2.78762500
H	-0.10058000	3.37791400	2.33865700

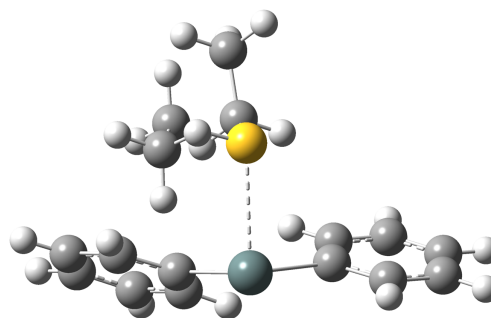


SnPh₂-Et₂S complex (10b)

Zero-point correction= 0.316807 (Hartree/Particle)
 Thermal correction to Energy= 0.337330
 Thermal correction to Enthalpy= 0.338274
 Thermal correction to Gibbs Free Energy= 0.263578
 Sum of electronic and zero-point Energies= -1234.018240
 Sum of electronic and thermal Energies= -1233.997718
 Sum of electronic and thermal Enthalpies= -1233.996774
 Sum of electronic and thermal Free Energies= -1234.071470

$r_{\text{Sn-S}} = 2.820$

C	-1.52532100	-0.75246500	-0.29790500
C	1.77989100	-0.54883300	-0.28733500
C	-1.42123300	-1.35994600	0.95682400
C	-2.48930100	-2.03897800	1.52534300
C	-3.69385800	-2.13448200	0.84308600
C	-3.82191300	-1.54626900	-0.40548900
C	-2.74884600	-0.86018000	-0.96126600
C	1.78175500	-1.91916400	-0.02149300
C	2.95860700	0.15398900	-0.02985500
C	2.90287300	-2.55662300	0.49261100
C	4.05330900	-1.83121700	0.76185000
C	4.07996500	-0.46973900	0.49882100
H	-2.38108200	-2.49743000	2.50124900
H	-4.75889100	-1.61866300	-0.94494700
H	-2.87851600	-0.39530200	-1.93457800
H	3.01681400	1.21736000	-0.24990200
H	2.87628000	-3.62244100	0.68686800
H	-0.48776600	-1.30257300	1.50689600
H	-4.52934300	-2.66475200	1.28349400
H	0.89017000	-2.50742600	-0.21138000
H	4.92694800	-2.32422400	1.17015300
H	4.97829000	0.10272000	0.69811500
Sn	0.06322400	0.50349900	-1.17730700
C	0.61359700	3.49739600	0.86170600
H	1.68373500	3.30370100	0.91528600
H	0.36057000	3.86005900	-0.13418800
H	0.34559600	4.23635900	1.61545800
C	-1.93980600	2.43898900	1.02391300
H	-2.11380000	2.86690000	0.03660900
H	-2.53858900	1.53640200	1.13580200
H	-2.20090700	3.15634200	1.80028100
S	-0.22056400	1.94019600	1.20157800

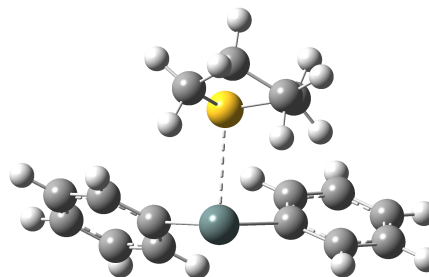


SnPh₂-THT complex (11b)

Zero-point correction= 0.297587 (Hartree/Particle)
 Thermal correction to Energy= 0.315827
 Thermal correction to Enthalpy= 0.316772
 Thermal correction to Gibbs Free Energy= 0.247510
 Sum of electronic and zero-point Energies= -1232.831733
 Sum of electronic and thermal Energies= -1232.813493
 Sum of electronic and thermal Enthalpies= -1232.812549
 Sum of electronic and thermal Free Energies= -1232.881811

$r_{\text{Sn-S}} = 2.820$

C	-2.22508100	-2.48498500	-0.42109100
C	-1.22026900	-1.34175300	1.78442000
C	-2.65125300	-1.84713100	1.90993500
C	-3.23835300	-1.81548700	0.50380400
H	-2.27836900	-2.12288100	-1.44647100
H	-2.33465700	-3.56858500	-0.42658100
H	-0.57982500	-1.63861800	2.61205800
H	-1.19307700	-0.25797800	1.67008300
H	-2.65642100	-2.86752300	2.30095600
H	-3.21745900	-1.21991200	2.59976000
H	-4.20185100	-2.32379000	0.44906500
H	-3.38463500	-0.77837000	0.19873900
S	-0.56927500	-2.10536800	0.25969400
Sn	0.42940600	-0.11969800	-1.42859500
C	2.16919800	0.05055000	-0.08304300
C	3.43454300	0.02727500	-0.67247500
C	2.11990600	0.14361600	1.31029500
C	4.59639500	0.10659700	0.08471300
H	3.52676900	-0.05844700	-1.75160200
C	3.27324200	0.21091200	2.07848900
H	1.16255600	0.17372700	1.81941800
C	4.51751700	0.19602400	1.46505200
H	5.56347400	0.09277600	-0.40376300
H	3.20220200	0.27864800	3.15781800
H	5.42005700	0.25231500	2.06110600
C	-0.89231400	1.35019200	-0.44071900
C	-2.22588500	1.40115000	-0.85450900
C	-0.50082700	2.24683300	0.55544300
C	-3.13905500	2.27524000	-0.28098900
H	-2.56833200	0.74482400	-1.65109200
C	-1.40328500	3.13263800	1.13092400
H	0.52960900	2.26249600	0.89212700
C	-2.72784400	3.14247900	0.72039100
H	-4.16800900	2.28786100	-0.62130000
H	-1.07046200	3.81851000	1.90113900
H	-3.43330100	3.83084300	1.16934400

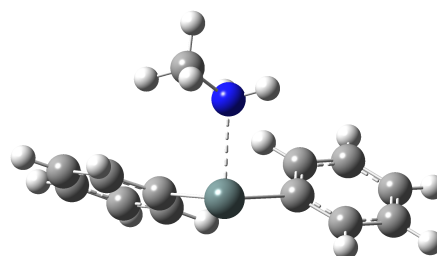


SnPh₂-MeNH₂ complex (12b')

Zero-point correction= 0.248478 (Hartree/Particle)
 Thermal correction to Energy= 0.264410
 Thermal correction to Enthalpy= 0.265354
 Thermal correction to Gibbs Free Energy= 0.201230
 Sum of electronic and zero-point Energies= -773.296631
 Sum of electronic and thermal Energies= -773.280699
 Sum of electronic and thermal Enthalpies= -773.279755
 Sum of electronic and thermal Free Energies= -773.343879

$r_{\text{Sn-N}} = 2.413$

C	1.68956000	0.24385900	-0.16969000
C	-1.60031100	0.38655100	-0.33309900
C	1.59502400	1.17321300	0.87049100
C	2.69609700	1.90043400	1.30129400
C	3.92820800	1.72032500	0.68913900
C	4.04964500	0.80911300	-0.34821200
C	2.94265600	0.07954900	-0.76325700
C	-1.47933800	1.77051900	-0.47112700
C	-2.83471800	-0.10379700	0.10028200
C	-2.53495900	2.62498900	-0.18160100
C	-3.74393600	2.11231600	0.26469600
C	-3.89324000	0.74115800	0.40708700
H	2.59190900	2.61487400	2.10960000
H	5.00789500	0.66428800	-0.83298200
H	3.06628600	-0.63517500	-1.57199400
H	-2.99018200	-1.17682100	0.19371600
H	-2.41228500	3.69512600	-0.30060700
H	0.63672700	1.35182000	1.34962400
H	4.78860700	2.29004200	1.01822700
H	-0.53923700	2.19888700	-0.80344300
H	-4.56704800	2.77736700	0.49525300
H	-4.83705200	0.33014800	0.74591500
Sn	0.01504700	-1.04357100	-0.82530700
C	-0.55840800	-3.04671100	1.80258300
H	-1.54187600	-3.22448600	1.36929800
H	0.14126400	-3.74198900	1.34096800
H	-0.60346500	-3.24329500	2.87595400
N	-0.14324100	-1.67483300	1.49813100
H	0.76726700	-1.46592800	1.89241500
H	-0.79613800	-1.00157900	1.88499000

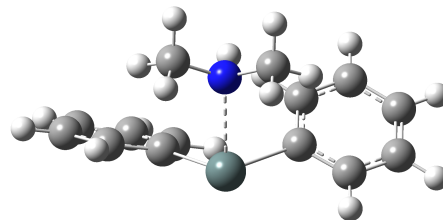


SnPh₂-Me₂NH complex (13b')

Zero-point correction= 0.277260 (Hartree/Particle)
 Thermal correction to Energy= 0.294194
 Thermal correction to Enthalpy= 0.295139
 Thermal correction to Gibbs Free Energy= 0.230042
 Sum of electronic and zero-point Energies= -812.578024
 Sum of electronic and thermal Energies= -812.561089
 Sum of electronic and thermal Enthalpies= -812.560145
 Sum of electronic and thermal Free Energies= -812.625242

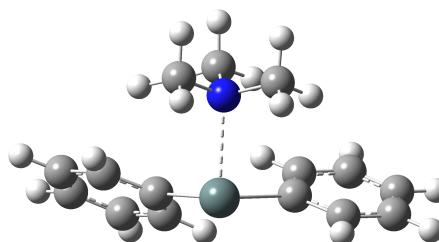
$r_{\text{Sn-N}} = 2.415$

C	-1.64474400	-0.45850500	-0.26306300
C	1.69168800	-0.46973200	-0.29316000
C	-1.63864300	-1.15672600	0.94795000
C	-2.75578600	-1.84163500	1.40518000
C	-3.91840800	-1.85326900	0.64809300
C	-3.95247200	-1.17518700	-0.56004000
C	-2.83014800	-0.48430400	-1.00006500
C	1.57553700	-1.82614700	0.01905300
C	2.97331700	0.08583300	-0.23755700
C	2.67748500	-2.58404600	0.39390200
C	3.93235100	-1.99906500	0.46838900
C	4.08022700	-0.65805600	0.14773100
H	-2.71801700	-2.37306800	2.34896200
H	-4.85546800	-1.18018900	-1.15901500
H	-2.88890000	0.05064900	-1.94374900
H	3.12377300	1.12650900	-0.51413500
H	2.55577700	-3.63540800	0.62698500
H	-0.73593600	-1.18986100	1.55252400
H	-4.79163800	-2.38990600	0.99806600
H	0.60784300	-2.31221400	-0.03697700
H	4.79250000	-2.58757400	0.76326500
H	5.05958700	-0.19558700	0.18561900
Sn	0.02376100	0.80315200	-0.99271300
C	1.11152100	2.59032300	1.54527800
H	1.99600100	1.95725300	1.50143900
H	1.22101000	3.39642000	0.81836500
H	1.03026100	3.02863200	2.54497700
N	-0.07085600	1.79841600	1.20614200
H	-0.10520300	0.98258400	1.80734900
C	-1.31584800	2.55309800	1.36464000
H	-1.32853500	3.37158100	0.64368200
H	-2.16283700	1.89823000	1.16502600
H	-1.40872600	2.96993700	2.37227300



SnPh₂-NMe₃ complex (14b')

Zero-point correction= 0.305531 (Hartree/Particle)
 Thermal correction to Energy= 0.323459
 Thermal correction to Enthalpy= 0.324403
 Thermal correction to Gibbs Free Energy= 0.257696
 Sum of electronic and zero-point Energies= -851.858731
 Sum of electronic and thermal Energies= -851.840804
 Sum of electronic and thermal Enthalpies= -851.839860
 Sum of electronic and thermal Free Energies= -851.906567



$r_{\text{Sn-N}} = 2.480$

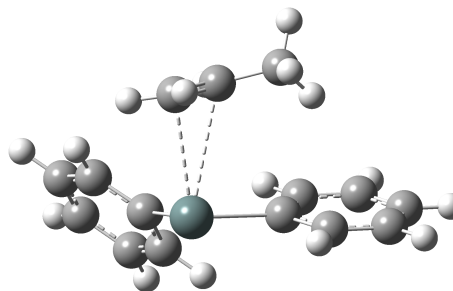
C	-1.65414200	-0.59055700	-0.27839100
C	1.70494500	-0.57286400	-0.34656500
C	-1.60129400	-1.42595800	0.84103100
C	-2.72941600	-2.07700500	1.32074200
C	-3.95064300	-1.91271600	0.68310600
C	-4.03264300	-1.09565800	-0.43317100
C	-2.89715000	-0.44560900	-0.89978600
C	1.64322200	-1.94415600	-0.08901200
C	2.95132200	0.04213000	-0.19958800
C	2.75948600	-2.65933700	0.32528100
C	3.97489000	-2.01496500	0.49736800
C	4.07075600	-0.65789400	0.22869200
H	-2.65523300	-2.71757600	2.19183800
H	-4.98088400	-0.96365600	-0.94072400
H	-2.99008300	0.19413300	-1.77328400
H	3.06812600	1.09537000	-0.44043800
H	2.67942600	-3.72342000	0.51433500
H	-0.65963100	-1.58152800	1.35600000
H	-4.83216000	-2.42148700	1.05356300
H	0.70798700	-2.47719800	-0.21941500
H	4.84552400	-2.56929900	0.82557500
H	5.02075700	-0.14834000	0.33948300
Sn	0.00554300	0.61198900	-1.11197900
C	0.93713900	3.08284700	0.75294900
H	1.94183200	2.66443400	0.71396300
H	0.73630100	3.60479900	-0.18251000
H	0.88766100	3.79982000	1.58193700
C	-1.38948300	2.56274200	1.01974200
H	-1.62162600	3.09553200	0.09701800
H	-2.11000900	1.75613600	1.14714300
H	-1.47255900	3.25957600	1.86282500
N	-0.03669000	2.00527500	0.93868000
C	0.27365000	1.25856100	2.16010600
H	-0.47499400	0.48369700	2.30984700
H	1.25172800	0.78911500	2.06481900
H	0.27368900	1.92615600	3.03116600

SnPh₂-propene complex (15b')

Zero-point correction= 0.263105 (Hartree/Particle)
 Thermal correction to Energy= 0.280109
 Thermal correction to Enthalpy= 0.281053
 Thermal correction to Gibbs Free Energy= 0.215318
 Sum of electronic and zero-point Energies= -795.307797
 Sum of electronic and thermal Energies= -795.290793
 Sum of electronic and thermal Enthalpies= -795.289849
 Sum of electronic and thermal Free Energies= -795.355584

$r_{\text{Sn-C1}} = 2.842$, $r_{\text{Sn-C2}} = 3.096$

C	1.47881900	0.49602900	-0.38297900
C	-1.81952600	0.23202800	-0.21150800
C	1.37603000	1.41661700	0.66342300
C	2.46017200	2.18362300	1.06258900
C	3.68179700	2.05062000	0.41613800
C	3.80939500	1.14873000	-0.62773600
C	2.71778300	0.38145500	-1.01587300
C	-1.87431000	1.62811100	-0.21701900
C	-2.96385200	-0.44804300	0.21181600
C	-3.00744500	2.31301900	0.20126800
C	-4.11868600	1.61259200	0.64403700
C	-4.09583900	0.22595500	0.64711900
H	2.35443200	2.88597800	1.88095800
H	4.75875000	1.03949300	-1.13817600
H	2.84612900	-0.32731600	-1.82909500
H	-2.99018000	-1.53412400	0.19548800
H	-3.02124400	3.39632700	0.18315200
H	0.43515500	1.53234400	1.19001200
H	4.52986100	2.64846900	0.72659800
H	-1.01860300	2.20307700	-0.55481200
H	-5.00166400	2.14399100	0.97699200
H	-4.96430000	-0.33038100	0.97916200
Sn	-0.10960400	-0.87825500	-1.04290100
C	-0.13092100	-2.63291500	1.19324100
H	-1.21223000	-2.57915700	1.16967600
H	0.33072400	-3.51118800	0.75648000
C	0.59117800	-1.72116700	1.85207300
H	0.07342200	-0.87959700	2.30397300
C	2.06583300	-1.78494200	2.05407300
H	2.54252800	-0.85529100	1.73810500
H	2.28436300	-1.91482300	3.11746500
H	2.51050200	-2.61533200	1.50512100

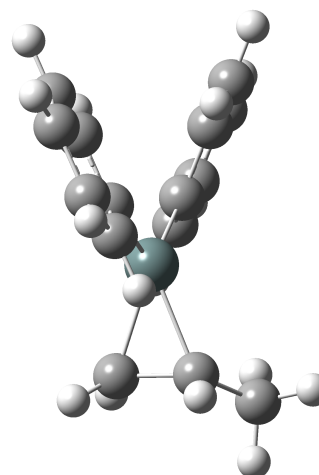


2-methyl-1,1-diphenylstannirane (19b)

Zero-point correction= 0.262939 (Hartree/Particle)
 Thermal correction to Energy= 0.279103
 Thermal correction to Enthalpy= 0.280047
 Thermal correction to Gibbs Free Energy= 0.215802
 Sum of electronic and zero-point Energies= -795.279286
 Sum of electronic and thermal Energies= -795.263123
 Sum of electronic and thermal Enthalpies= -795.262179
 Sum of electronic and thermal Free Energies= -795.326424

$r_{\text{Sn-C2}} = 2.135$, $r_{\text{Sn-C3}} = 2.132$

C	-1.65450400	-0.63982700	-0.01269700
C	-2.84993600	-0.31378200	-0.65056300
C	-1.58599200	-1.83058200	0.70928000
C	-3.95138600	-1.15261600	-0.56337100
H	-2.92722900	0.59995400	-1.22903500
C	-2.68411000	-2.67447900	0.79017000
H	-0.67021600	-2.10952900	1.21925500
C	-3.86941700	-2.33527500	0.15578500
H	-4.87393600	-0.88398100	-1.06303900
H	-2.61430900	-3.59692600	1.35334800
H	-4.72761700	-2.99230900	0.22053400
C	1.90946700	-0.30197400	-0.04644200
C	3.04724700	0.37724200	0.38477400
C	2.03299700	-1.63456000	-0.43562500
C	4.27993500	-0.25738000	0.41852100
H	2.97850900	1.41170000	0.70238400
C	3.26464400	-2.27231400	-0.39582500
H	1.16473600	-2.18739800	-0.77771200
C	4.39025900	-1.58398400	0.02953900
H	5.15575900	0.28458500	0.75342900
H	3.34462700	-3.30828400	-0.70127300
H	5.35202100	-2.08049100	0.05895400
Sn	0.02005400	0.65809400	-0.11309600
C	-0.23814100	2.51385100	-1.13085600
H	-1.19017500	2.70820600	-1.61782400
H	0.59850600	2.92558000	-1.68568400
C	-0.22456000	2.71763700	0.39326000
H	0.66827100	3.22079400	0.75575400
C	-1.49490800	3.22491900	1.03328100
H	-1.44315700	3.17385700	2.12161500
H	-1.68296400	4.26667300	0.74885800
H	-2.36508400	2.64160400	0.71988800

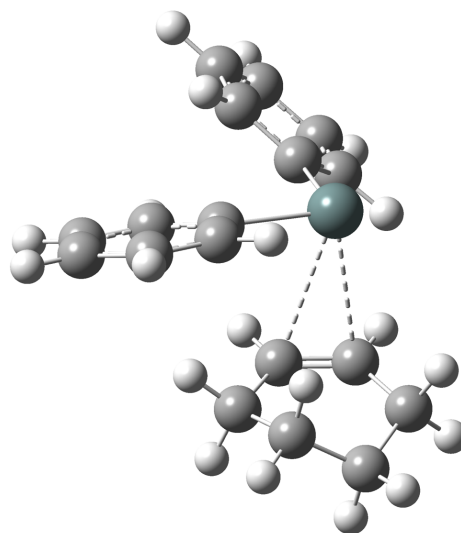


SnPh₂-cyclohexene complex (16b)

Zero-point correction= 0.330252 (Hartree/Particle)
 Thermal correction to Energy= 0.348935
 Thermal correction to Enthalpy= 0.349879
 Thermal correction to Gibbs Free Energy= 0.279892
 Sum of electronic and zero-point Energies= -911.991367
 Sum of electronic and thermal Energies= -911.972684
 Sum of electronic and thermal Enthalpies= -911.971740
 Sum of electronic and thermal Free Energies= -912.041727

$r_{\text{Sn-C1}} = 2.935$, $r_{\text{Sn-C2}} = 3.043$

C	1.74438200	-3.18223200	-0.00283000
C	0.64926300	-2.38435200	0.64984300
C	0.87016500	-1.31025400	1.41852700
C	2.23973500	-0.75728600	1.67348300
C	3.25987500	-1.28921300	0.67333700
C	3.12872000	-2.80087100	0.51935600
H	0.03091500	-0.83534600	1.91684900
H	-0.36295900	-2.76518400	0.55784200
H	1.69432600	-3.04080400	-1.08729200
H	1.55223000	-4.24470300	0.16699500
H	2.53188500	-1.02895500	2.69495100
H	2.20581600	0.33317400	1.64693300
H	4.26868800	-1.01944400	0.98937100
H	3.09296900	-0.80578600	-0.29488400
H	3.28969900	-3.27160100	1.49433300
H	3.89770300	-3.19012900	-0.14992800
Sn	-0.25329400	-0.31796300	-1.22954200
C	0.74579100	1.44980000	-0.38366600
C	0.37235500	2.11142700	0.78907000
C	1.90159300	1.89292300	-1.02908300
C	1.11853400	3.16516100	1.29494400
H	-0.51046800	1.79156700	1.33150600
C	2.65676500	2.94753300	-0.53166600
H	2.23297600	1.40340900	-1.94085500
C	2.26541900	3.58503200	0.63461500
H	0.80887100	3.65820100	2.20882100
H	3.55025100	3.26934500	-1.05311300
H	2.85110000	4.40601900	1.02959200
C	-2.17143400	-0.10202400	-0.17212600
C	-2.90144700	-1.22982000	0.21013100
C	-2.77347300	1.14323900	0.02588500
C	-4.15475500	-1.12514500	0.79643100
H	-2.49666900	-2.22388600	0.04290200
C	-4.03425500	1.25907900	0.59590700
H	-2.25452900	2.04960400	-0.26812900
C	-4.72463600	0.12393500	0.99156900
H	-4.69152400	-2.01866700	1.09220300
H	-4.47692100	2.23842700	0.73379400
H	-5.70525200	0.21132100	1.44286200

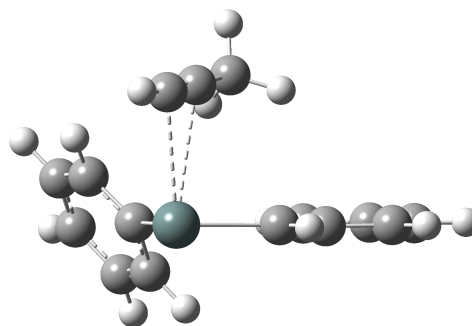


SnPh₂-propyne complex (17b')

Zero-point correction= 0.238578
 (Hartree/Particle)
 Thermal correction to Energy= 0.255512
 Thermal correction to Enthalpy= 0.256457
 Thermal correction to Gibbs Free Energy= 0.191063
 Sum of electronic and zero-point Energies= -794.077406
 Sum of electronic and thermal Energies= -794.060472
 Sum of electronic and thermal Enthalpies= -794.059528
 Sum of electronic and thermal Free Energies= -794.124922

$r_{\text{Sn-C1}} = 2.779$, $r_{\text{Sn-C2}} = 2.975$

C	1.65344700	0.24984200	-0.29608000
C	-1.65471100	0.16625900	-0.38729400
C	1.47621100	1.49552900	0.31021200
C	2.55698700	2.29756900	0.64892200
C	3.85002000	1.86803200	0.38696900
C	4.05374100	0.63673800	-0.21611100
C	2.96511000	-0.15621600	-0.55343600
C	-1.72981500	1.46724600	-0.88945900
C	-2.75518500	-0.30657200	0.33064900
C	-2.84402400	2.26767600	-0.67227500
C	-3.91414200	1.78197700	0.06260400
C	-3.86731900	0.48971200	0.56498400
H	2.39060000	3.26053100	1.11741400
H	5.06020100	0.29486900	-0.42587700
H	3.15028800	-1.11577100	-1.02808100
H	-2.74903900	-1.31721100	0.72793500
H	-2.87405100	3.27322000	-1.07480000
H	0.47578900	1.85122100	0.53029000
H	4.69510000	2.49236400	0.65003700
H	-0.90357500	1.87913400	-1.46120200
H	-4.78231200	2.40482000	0.23915900
H	-4.70256400	0.09903900	1.13418900
Sn	0.04956300	-1.13871100	-0.88317900
C	-0.06680700	-0.26903700	2.78262000
H	-0.85338100	0.37074500	2.37824300
H	-0.26506200	-0.44984800	3.83992600
H	0.88859600	0.24567600	2.67863200
C	-0.02032300	-2.58755400	1.48723300
H	-0.00537800	-3.58222700	1.10847400
C	-0.03708300	-1.52970500	2.06456500

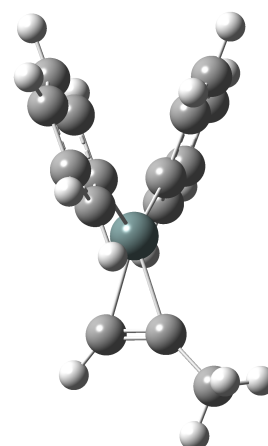


2-methyl-1,1-diphenylstannirene (20b)

Zero-point correction= 0.239492 (Hartree/Particle)
 Thermal correction to Energy= 0.255513
 Thermal correction to Enthalpy= 0.256457
 Thermal correction to Gibbs Free Energy= 0.192556
 Sum of electronic and zero-point Energies= -794.060034
 Sum of electronic and thermal Energies= -794.044013
 Sum of electronic and thermal Enthalpies= -794.043069
 Sum of electronic and thermal Free Energies= -794.106969

$r_{\text{Sn-C2}} = 2.102$, $r_{\text{Sn-C3}} = 2.092$

C	-0.01727200	2.53285700	-1.09751000
C	0.06871500	2.73068400	0.21524700
H	-0.05117700	3.22410200	-1.93621500
C	0.13768200	3.92809700	1.09415400
H	1.04601700	3.91096600	1.69969900
H	0.12494400	4.85098900	0.50640000
H	-0.70645000	3.94270900	1.78651400
C	-1.79194400	-0.46055700	0.01331900
C	-2.96513500	-0.00505700	-0.58407300
C	-1.82483700	-1.65278200	0.73408600
C	-4.14464900	-0.72454900	-0.46328600
H	-2.96277700	0.92015100	-1.14977500
C	-3.00390300	-2.37478800	0.85342600
H	-0.92809700	-2.02795600	1.21538000
C	-4.16502500	-1.91120800	0.25454700
H	-5.04965900	-0.35872300	-0.93243400
H	-3.01527900	-3.29925000	1.41751600
H	-5.08557700	-2.47372600	0.34739800
C	1.77138000	-0.51781300	-0.07579200
C	2.99132600	0.06332600	0.26324900
C	1.73460700	-1.87973300	-0.36735900
C	4.14860400	-0.69925900	0.30876100
H	3.04446100	1.12198700	0.49228300
C	2.89173100	-2.64449400	-0.31949400
H	0.79992000	-2.35658400	-0.64195400
C	4.09971400	-2.05495700	0.01912200
H	5.09065800	-0.23445500	0.57229600
H	2.84901800	-3.70181900	-0.55009300
H	5.00303600	-2.65085900	0.05629400
Sn	0.00510000	0.66307700	-0.15947400

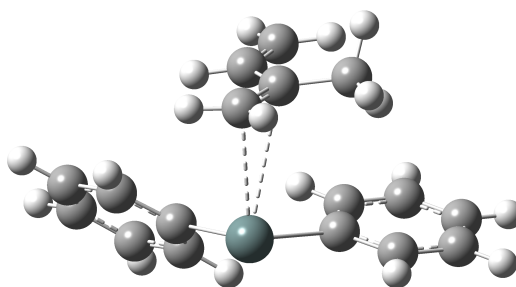


SnPh₂-isoprene complex (18b)

Zero-point correction= 0.297196
 (Hartree/Particle)
 Thermal correction to Energy= 0.316027
 Thermal correction to Enthalpy= 0.316971
 Thermal correction to Gibbs Free Energy= 0.247885
 Sum of electronic and zero-point Energies= -872.680131
 Sum of electronic and thermal Energies= -872.661300
 Sum of electronic and thermal Enthalpies= -872.660356
 Sum of electronic and thermal Free Energies= -872.729442

$r_{\text{Sn-C1}} = 2.796$, $r_{\text{Sn-C2}} = 3.177$

C	1.50947300	0.64624800	-0.51354300
C	-1.81964700	0.38360900	-0.43442200
C	1.40225600	1.37049900	0.67604600
C	2.50371700	1.99180200	1.24670600
C	3.74653200	1.90500300	0.63520600
C	3.87913100	1.19673700	-0.54890500
C	2.77043600	0.57736400	-1.11072200
C	-1.88820200	1.73425400	-0.08718600
C	-2.95596100	-0.39339400	-0.19721200
C	-3.02552100	2.27792800	0.49586600
C	-4.12691800	1.47608400	0.75087100
C	-4.09173100	0.13466300	0.39909000
H	2.39321100	2.54306600	2.17327100
H	4.84539700	1.12493500	-1.03365500
H	2.90082400	0.02096400	-2.03483300
H	-2.96817800	-1.44126000	-0.48523400
H	-3.04996500	3.33011300	0.75361600
H	0.44864000	1.43379700	1.18554100
H	4.60759600	2.38854500	1.08010700
H	-1.04153500	2.38618600	-0.27330900
H	-5.01256800	1.89580800	1.21168700
H	-4.95362500	-0.49663800	0.57993700
Sn	-0.09783300	-0.50032800	-1.47977000
C	-0.06949400	-2.73295100	0.20311400
H	-1.14822300	-2.81653100	0.13853300
H	0.51231100	-3.34142200	-0.47709800
C	0.51251100	-2.06176700	1.21854500
C	1.99907900	-2.06504900	1.40011100
H	2.39116100	-1.04850900	1.46172100
H	2.25776200	-2.58029700	2.32836300
H	2.49347100	-2.57186900	0.57301800
C	-0.32314400	-1.35748000	2.19217200
H	-1.39226400	-1.39363600	2.01250200
C	0.13665700	-0.68748100	3.24335700
H	1.19517000	-0.60163500	3.45551900
H	-0.54259400	-0.19165900	3.92423500

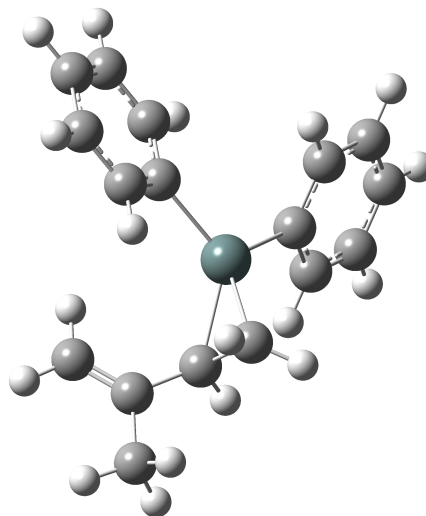


2-methylethenyl-1,1-diphenylstannirane (21b)

Zero-point correction= 0.296290 (Hartree/Particle)
 Thermal correction to Energy= 0.314630
 Thermal correction to Enthalpy= 0.315574
 Thermal correction to Gibbs Free Energy= 0.246161
 Sum of electronic and zero-point Energies= -872.646448
 Sum of electronic and thermal Energies= -872.628109
 Sum of electronic and thermal Enthalpies= -872.627165
 Sum of electronic and thermal Free Energies= -872.696578

$r_{\text{Sn-C2}} = 2.130$, $r_{\text{Sn-C3}} = 2.129$

C	1.07194900	1.44813900	-0.06227400
C	2.40368100	1.51356700	-0.46708100
C	0.48147300	2.58208200	0.49148100
C	3.12803200	2.68664700	-0.32087300
H	2.88857600	0.64228100	-0.89218100
C	1.20551900	3.75730300	0.63508300
H	-0.55151800	2.55621200	0.82145700
C	2.52959600	3.81098900	0.22881200
H	4.16311400	2.72277500	-0.63738900
H	0.73396000	4.63085900	1.06800300
H	3.09561200	4.72714000	0.34152100
C	-2.14020000	-0.11519500	-0.02010800
C	-2.88582700	-1.06766900	0.67179600
C	-2.79936400	0.99373000	-0.54911000
C	-4.25671200	-0.91998800	0.82466700
H	-2.39752500	-1.93462800	1.10234200
C	-4.16921200	1.14608100	-0.39106000
H	-2.24691800	1.75055900	-1.09526600
C	-4.90001300	0.18802500	0.29466800
H	-4.82245800	-1.67011100	1.36328100
H	-4.66645100	2.01316300	-0.80795000
H	-5.96947400	0.30521000	0.41672700
Sn	-0.04477200	-0.34142300	-0.26676600
C	0.73965400	-1.91220400	-1.47163800
H	1.69142100	-1.71373800	-1.95721300
H	0.08579300	-2.53054200	-2.07747900
C	0.84002800	-2.25507300	0.03573500
H	0.14023900	-3.03922100	0.32304800
C	2.20994400	-2.49589900	0.57882300
C	2.83658900	-1.65975700	1.39888600
H	3.83798700	-1.86740000	1.75803700
H	2.36692000	-0.74648900	1.74376900
C	2.85107600	-3.77457000	0.10921300
H	2.25922400	-4.63575600	0.43211700
H	2.88893900	-3.80896200	-0.98248600
H	3.86389300	-3.88743400	0.49585500

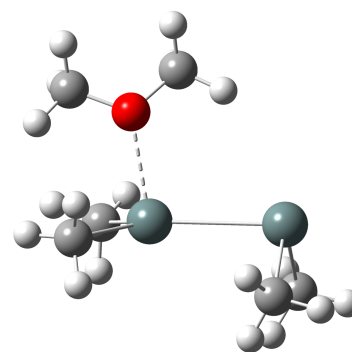


Me₂O-Sn₂Me₄ complex (22a)

Zero-point correction= 0.225061 (Hartree/Particle)
 Thermal correction to Energy= 0.244214
 Thermal correction to Enthalpy= 0.245159
 Thermal correction to Gibbs Free Energy= 0.173576
 Sum of electronic and zero-point Energies= -743.223969
 Sum of electronic and thermal Energies= -743.204816
 Sum of electronic and thermal Enthalpies= -743.203871
 Sum of electronic and thermal Free Energies= -743.275454

$r_{\text{Sn-O}} = 2.377$, $r_{\text{Sn-Sn}} = 2.932$

Sn	0.77868200	-0.64646600	0.09856400
C	1.85734100	-1.83962500	-1.35918000
C	1.94596000	-0.97909900	1.89999300
H	1.57693300	-1.87887200	2.39760800
H	3.00298300	-1.12682500	1.67319100
H	2.01054300	-1.26294500	-2.27307600
H	2.82066700	-2.18501400	-0.98142000
H	1.25562300	-2.71230700	-1.61994800
H	1.83725500	-0.14835400	2.59849200
Sn	-1.86808100	0.59583400	-0.11986200
C	-2.56757400	-1.01147900	-1.48462700
C	-2.51865200	-0.38596800	1.76712900
H	-2.45813600	-1.47439100	1.72529800
H	-3.56389000	-0.11366900	1.93365700
H	-2.02751800	-0.99647300	-2.43325800
H	-3.62223500	-0.82427200	-1.70148800
H	-2.48642500	-2.00710200	-1.04615500
H	-1.94504600	-0.03203800	2.62610000
O	2.15862600	1.21481200	-0.43198800
C	1.73969500	2.51064200	-0.01559100
H	0.65582600	2.54957300	-0.11182700
H	2.02952000	2.68725200	1.02445000
H	2.19751700	3.26499200	-0.65938200
C	3.56718900	1.05039000	-0.38788600
H	3.79358300	0.05218200	-0.75494800
H	4.04493600	1.79266700	-1.03175900
H	3.93507700	1.15952700	0.63625500

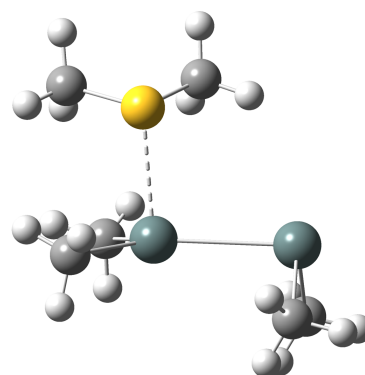


Me₂S-Sn₂Me₄ complex (22b)

Zero-point correction= 0.220673 (Hartree/Particle)
 Thermal correction to Energy= 0.240381
 Thermal correction to Enthalpy= 0.241325
 Thermal correction to Gibbs Free Energy= 0.168474
 Sum of electronic and zero-point Energies= -1066.223553
 Sum of electronic and thermal Energies= -1066.203845
 Sum of electronic and thermal Enthalpies= -1066.202901
 Sum of electronic and thermal Free Energies= -1066.275752

$r_{\text{Sn-S}} = 2.723$, $r_{\text{Sn-Sn}} = 2.947$

Sn	0.60289600	-0.82883000	0.10341100
C	1.66439700	-2.24791700	-1.15812800
C	1.69730900	-1.03178100	1.97857300
H	1.16853000	-1.75304300	2.60519600
H	2.71362400	-1.39657800	1.82363900
H	1.52440600	-2.01723600	-2.21423900
H	2.73100200	-2.26670900	-0.92834700
H	1.26156700	-3.24614200	-0.97549000
H	1.72900500	-0.08966500	2.52898000
Sn	-1.93149800	0.65302600	-0.14768500
C	-2.88336500	-0.90272700	-1.40735000
C	-2.63465300	-0.14903100	1.80301700
H	-2.70095800	-1.23791400	1.81353600
H	-3.63564900	0.25116900	1.98349200
H	-2.39516100	-0.98758800	-2.37988500
H	-3.91937100	-0.60089300	-1.58149200
H	-2.89324100	-1.88275000	-0.92865500
H	-1.99673000	0.17463400	2.62812300
C	1.70030100	2.53181400	0.32622100
H	0.65849900	2.75030000	0.09133400
H	1.77959700	2.22214900	1.36764700
H	2.31881100	3.40795600	0.14025000
C	3.84193200	0.82222800	-0.12211300
H	4.20813500	-0.05073800	-0.65946300
H	4.50806600	1.66386800	-0.30481000
H	3.79244000	0.60008100	0.94244000
S	2.20387600	1.19461100	-0.76624100

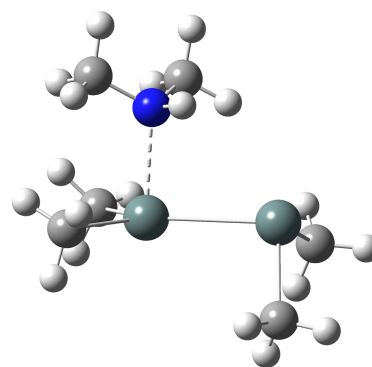


Me₂NH-Sn₂Me₄ complex (22c)

Zero-point correction= 0.240562 (Hartree/Particle)
 Thermal correction to Energy= 0.258636
 Thermal correction to Enthalpy= 0.259580
 Thermal correction to Gibbs Free Energy= 0.192643
 Sum of electronic and zero-point Energies= -723.351520
 Sum of electronic and thermal Energies= -723.333446
 Sum of electronic and thermal Enthalpies= -723.332502
 Sum of electronic and thermal Free Energies= -723.399439

$r_{\text{Sn-N}} = 2.364$, $r_{\text{Sn-Sn}} = 2.931$

Sn	0.85245200	-0.66367700	0.27006900
C	2.00500700	-2.00017400	-0.99901700
C	2.17397400	-0.49792400	1.99092500
H	2.20494700	-1.46323300	2.50022100
H	3.19275300	-0.25108300	1.68383100
H	1.74518500	-1.87187100	-2.05091200
H	3.07818800	-1.85040000	-0.87075700
H	1.77166000	-3.03127600	-0.72619400
H	1.82195100	0.24725000	2.70420800
Sn	-1.80394600	0.38630200	-0.38801200
C	-2.87055000	-1.54441400	-0.48157500
C	-2.35001600	0.88251800	1.70224500
H	-2.34728800	0.00302400	2.34732200
H	-3.36057100	1.29888600	1.69990600
H	-2.48309400	-2.18100500	-1.27865000
H	-3.92111100	-1.33791400	-0.70021800
H	-2.82092200	-2.08706500	0.46299700
H	-1.68462300	1.63458600	2.13217600
C	1.62786700	2.41615700	0.24504200
H	0.59677600	2.48992400	0.59157500
H	2.27762700	2.23000200	1.09966600
H	1.91457800	3.36251400	-0.22104400
N	1.74288100	1.29920800	-0.70021100
H	1.06363900	1.45228100	-1.44242600
C	3.08539900	1.18886900	-1.27334500
H	3.78942700	0.92043900	-0.48525600
H	3.09844200	0.40666700	-2.02964000
H	3.40687500	2.13241800	-1.72382400



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