

Supporting Information for

Silanones and Silanethiones from the Reactions of Transient Silylenes with Oxiranes and Thiiranes in Solution. The Direct Detection of Diphenylsilanethione.

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Calculated Structures and Energies

Silylene B3LYP/6-311+G(d,p) output	S21
Dimethylsilylene RB3LYP/6-311+G(d,p) output	S21
Oxirane B3LYP/6-311+G(d,p) output	S22
Thiirane B3LYP/6-311+G(d,p) output	S22
Silylene-oxirane anti-complex B3LYP/6-311+G(d,p) output	S23
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Silanone B3LYP/6-311+G(d,p) output	S25
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Silanethione B3LYP/6-311+G(d,p) output	S30
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Experimental Procedures, Materials, and Supplementary Data

Preparation and Purification of Compounds

^1H and ^{13}C NMR spectra were recorded on Bruker AV200, AV500 or AV600 spectrometers in deuterated chloroform or cyclohexane- d_{12} and were referenced to the residual solvent proton and ^{13}C signals, respectively, while ^{29}Si spectra were recorded on either the AV500 or AV600 using the HMBC pulse sequence and were referenced to an external solution of tetramethylsilane. GC/MS analyses were carried out on a Varian Saturn 2200 GC/MS/MS system equipped with a VF-5 ms capillary column (30 m \times 0.25 mm; 0.25 mm; Varian, Inc.). High-resolution electron impact mass spectra and exact masses were determined on a Micromass ToFSpec 2E mass spectrometer using electron impact ionization (25 eV).

All commercially available materials were obtained from Sigma-Aldrich, Inc. unless otherwise noted, and purified before use as described below. Tetrahydrofuran (THF, Caledon Reagent) was refluxed over calcium hydride for two hours, distilled into a flask containing sodium and refluxed for several days, and finally distilled under nitrogen. Hexanes (EMD OmniSolv) were dried by passage through activated alumina under nitrogen using a Solv-Tek solvent purification system (Solv-Tek, Inc).

Dodecamethylcyclotrisiloxane (**1**) was dried under high vacuum before use. 1,1,3,3-Tetramethyl-2,2-diphenyl-1,2,3-trisilacyclohexane (**2**) and 2,2-diphenyl-1,1,1,3,3,3-hexamethyltrisilane (**3**) were synthesized according to literature procedures.¹⁻² They were purified by column chromatography on silica gel with hexanes as eluant, followed by recrystallization from methanol (m.p. = 50.4-50.8 °C (**2**), m.p. \approx 16 °C (**3**)). The purities of **1-3** were determined by GC/MS analysis and ^1H NMR spectroscopy and were >97% in each case. Hexamethylcyclotrisiloxane (D_3) and octamethylcyclotetrasiloxane (D_4) were recrystallized from hexanes and dried under mild vacuum prior to use. Propylene sulfide (PrS) and

tetrahydrothiophene (THT) were purified by bulb to bulb distillation from anhydrous sodium sulfate.³ Cyclohexene oxide (CycO) and propylene oxide (PrO) were purified by distillation from calcium hydride. Dichlorodiphenylsilane (Gelest, Inc.), 30% lithium dispersion in mineral oil, and elemental sulfur (Cerac) were used as received from the suppliers.

1,1,3,3-Tetraphenylcyclodisilthiane (**12**) was prepared via a reported procedure⁴ and purified by column chromatography on silica gel; the column was packed using dichloromethane as eluant and gradually changed to ethyl acetate ($R_f = 0.7$ in ethyl acetate), the solvent was removed under vacuum to afford the compound as a white powder, which exhibited ^1H and ^{29}Si NMR spectra and melting point (m.p. 163-165 °C) in agreement with reported data.⁴⁻⁵

1,1,3,3,5,5-Hexaphenylcyclotrisilthiane was prepared by a modification of the reported procedures.⁵⁻⁶ Li_2S was prepared by treating lithium (0.94 g of a 30% dispersion in mineral oil; 60 mmol) with elemental sulfur (0.768 g, 30 mmol) in dry THF (10 mL) under N_2 . Refluxing for 12 h yielded a black solution with a yellow layer on top. Dichlorodiphenylsilane (6.1 mL, 29 mmol) was added in THF (5 mL) through an addition funnel over 30 min at 3-5 °C, which resulted in the formation of a tan-colored suspension. The solvent was removed under vacuum and replaced with dry benzene, after which the lithium salts were removed by gravity filtration. The solvent was again removed under vacuum to afford a sticky brown solid, which was re-dissolved in a 6:1 (v:v) mixture of hexanes and benzene to afford a yellow solution containing a brown solid suspension. Filtration followed by dropwise addition of additional hexanes resulted in the formation of light yellow crystals of the desired compound (2.0 g, 9.7 mmol, 32%, m.p. = 182-183 °C; lit.⁶ 183-184 °C).

Laser Flash Photolysis Experiments

Laser flash photolysis experiments were carried out using a Lambda Physik Compex 120 excimer laser filled with a $\text{F}_2/\text{Kr}/\text{Ne}$ mixture (excitation wavelength - 248 nm, 25 ns, 90-120

mJ/pulse) and a Luzchem Research mLFP-111 laser flash photolysis system, modified as described previously.⁷ The solutions were prepared in deoxygenated anhydrous hexanes such that the absorbance at the excitation wavelength (248 nm) was between 0.5 and 0.7 ($[1] \approx 5 \times 10^{-4}$ M, $[2] \approx 8 \times 10^{-5}$ M). The solutions were flowed rapidly through a 7×7 mm Suprasil flow cell connected to a calibrated 100 mL or 250 mL reservoir, which contain a glass frit to allow bubbling of argon gas through the solution for 40 min prior to and throughout the experiment. The glassware, sample cell, and transfer lines were dried in a vacuum oven (65-85 °C) before use. Solution temperatures were measured with a Teflon-coated copper/constantan thermocouple inserted into the thermostatted sample compartment in close proximity to the sample cell. Substrates were added directly to the reservoir by microliter syringe as aliquots of standard solutions. Transient absorbance-time profiles at each concentration of scavenger are the signal-averaged result of 7-40 laser shots. Decay rate constants were calculated by non-linear least squares analysis of the transient absorbance-time profiles using the Prism 5.0 software package (GraphPad Software, Inc.) and the appropriate user-defined fitting equations, after importing the raw data from the Luzchem mLFP software. Rate constants were calculated by linear least-squares analysis of decay rate-concentration data (generally 4-7 points) that spanned as large a range in transient decay rate as possible. Errors are quoted as twice the standard error obtained from the least-squares analyses, and reflect the precision associated with a given experiment.

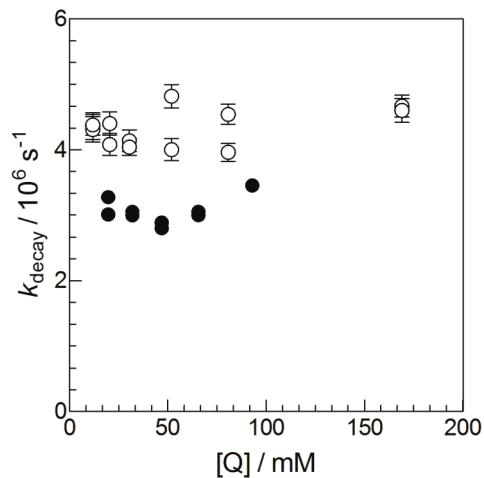


Figure S1. Plots of the first order rate coefficients for decay (k_{decay}) of the SiMe₂-CHO complex (O) and the SiMe₂-PrO complex (●) vs. CHO or PrO concentration (monitored at 310 nm).

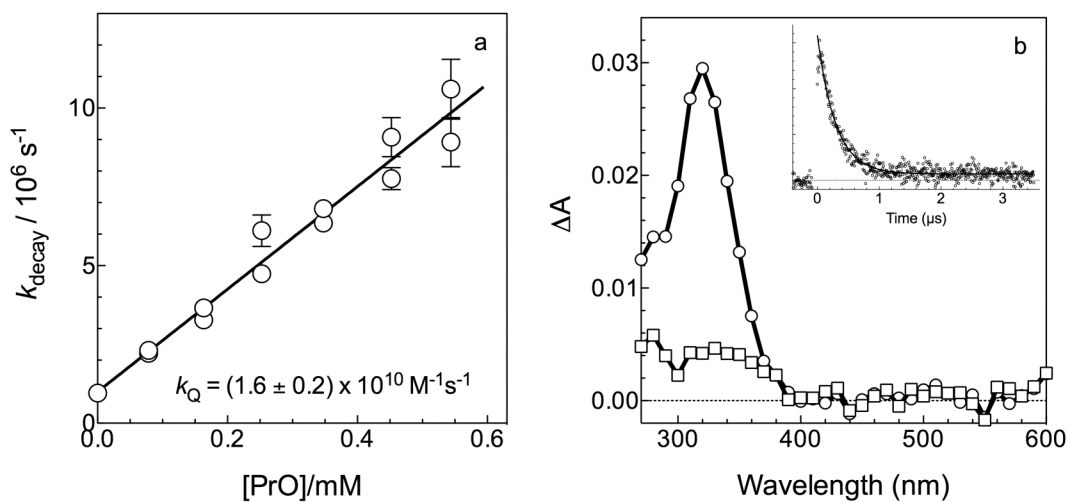


Figure S2. (a) Plot of the first order rate coefficients for decay (k_{decay}) of SiMe₂ (monitored at 470 nm) vs. [PrO]. (b) Transient absorption spectra from laser flash photolysis of a hexanes solution of **1** containing 10 mM PrO, recorded 83-109 ns (O) and 0.69-0.74 μs (□) after the laser pulse; the inset shows a transient absorbance-time profile recorded at 310 nm.

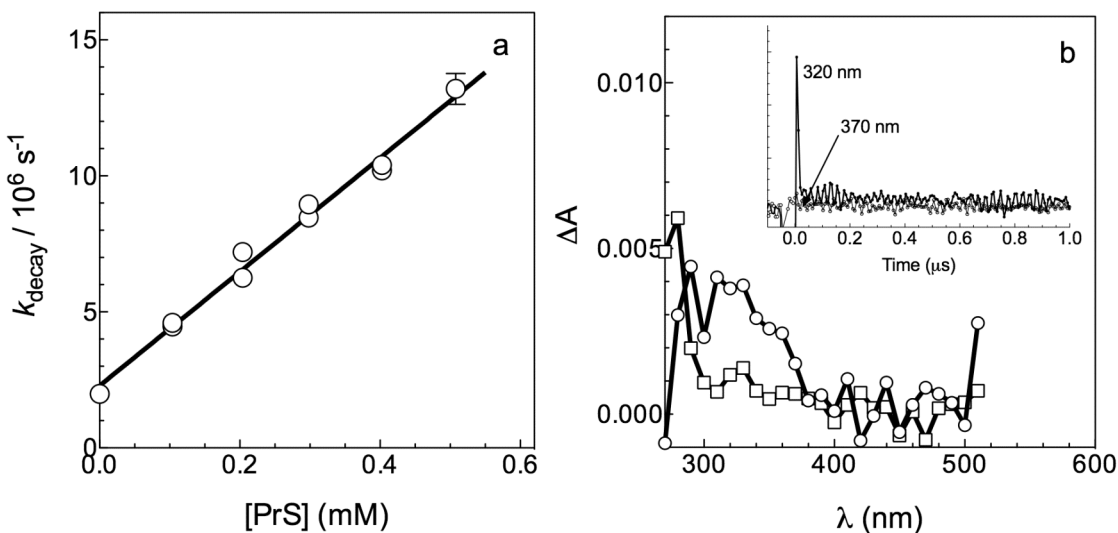


Figure S3. (a) Plot of the first order rate coefficients for decay (k_{decay}) of SiMe_2 vs. $[\text{PrS}]$. (b) Transient absorption spectra recorded 19-32 ns (O) and 1.65-1.70 μs (□) after the laser pulse, by laser flash photolysis of deoxygenated hexanes solution of **1** containing 5.0 mM PrS.

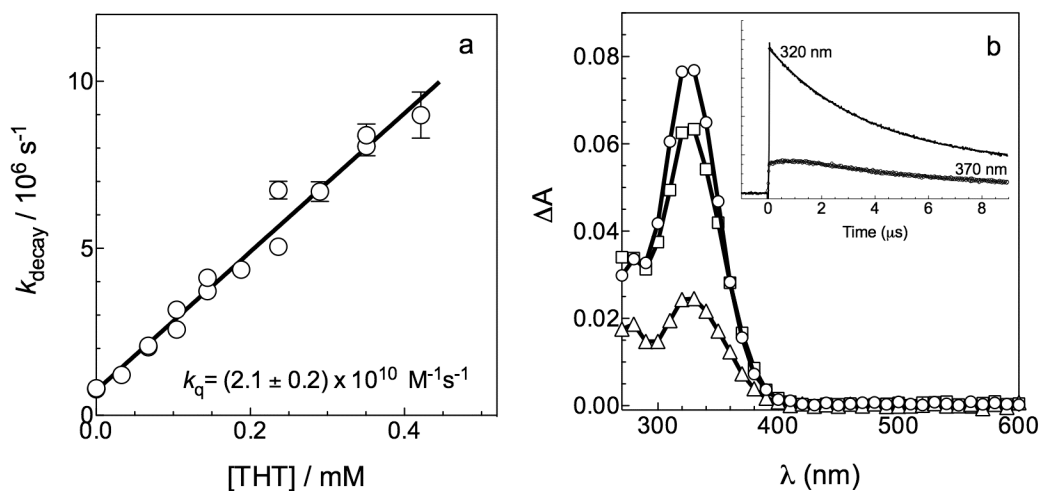


Figure S4. (a) Plot of the first order rate coefficients for decay (k_{decay}) of SiMe_2 vs. $[\text{THT}]$. (b) Transient absorption spectra recorded 48-80 ns (O), 0.88-0.91 μs (□), and 6.96-6.99 μs (Δ) after the laser pulse, by laser flash photolysis of deoxygenated hexanes solution of **1** containing 5.3 mM THT. The insets show transient decay/growth profiles recorded at 320 and 370 nm.

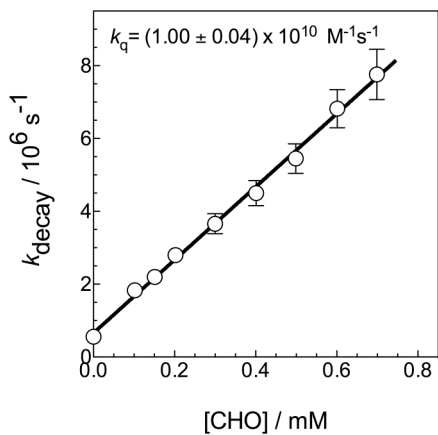


Figure S5. Plot of the first order rate coefficients for decay (k_{decay}) of SiPh₂ (monitored at 530 nm) vs. [CHO].

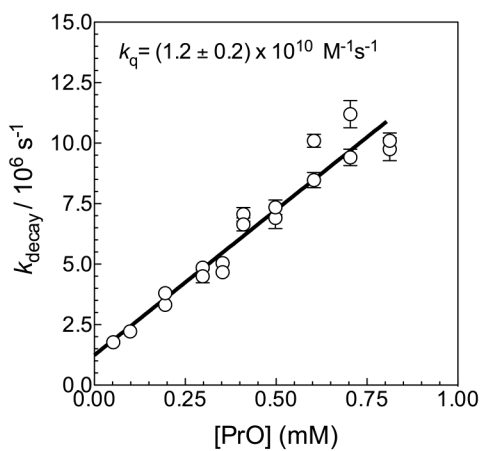


Figure S6. Plot of the first order rate coefficients for decay (k_{decay}) of SiPh₂ vs. [PrO].

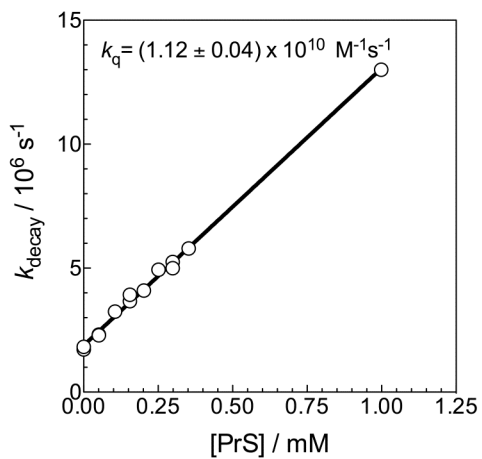


Figure S7. Plot of the first order rate coefficients for decay (k_{decay}) of SiPh₂ vs. [PrS].

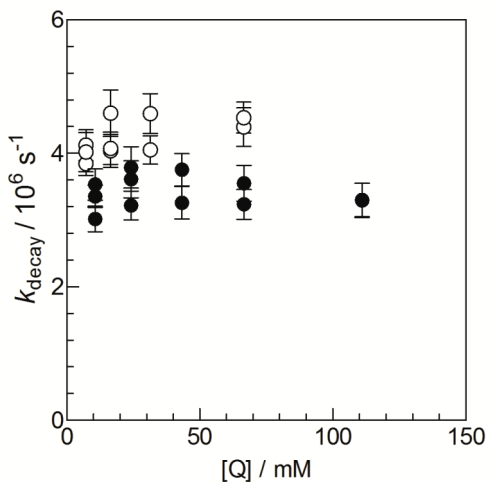


Figure S8. Plots of the first order rate coefficients for decay (k_{decay}) of the SiPh₂-CHO complex vs. [CHO] (○) and of the SiPh₂-PrO complex (●) vs. [PrO] (monitored at 370 nm).

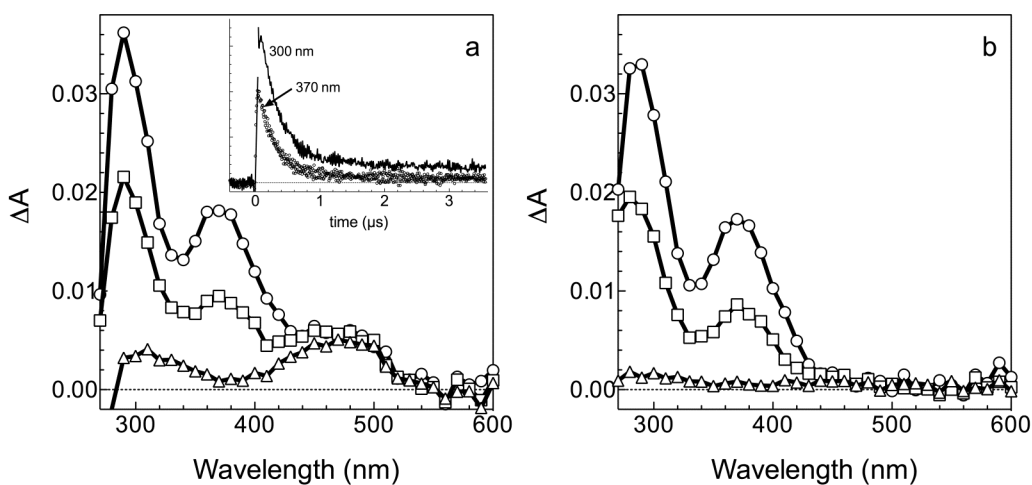


Figure S9. (a) Transient absorption spectra recorded 65-77 ns (○), 0.27-0.29 μs (□), and 3.50-3.57 μs (Δ) after the laser pulse, by laser flash photolysis of deoxygenated hexanes solution of **2** containing 11.0 mM PrO; the inset shows transient decay/growth profiles recorded at 300 and 370 nm. (b) Transient difference spectra, calculated by subtraction of the 3.50-3.57 μs spectrum in (a) from spectra recorded 65-77 ns (○), 0.27-0.29 μs (□), and 1.17-1.23 μs (Δ) after the laser pulse.

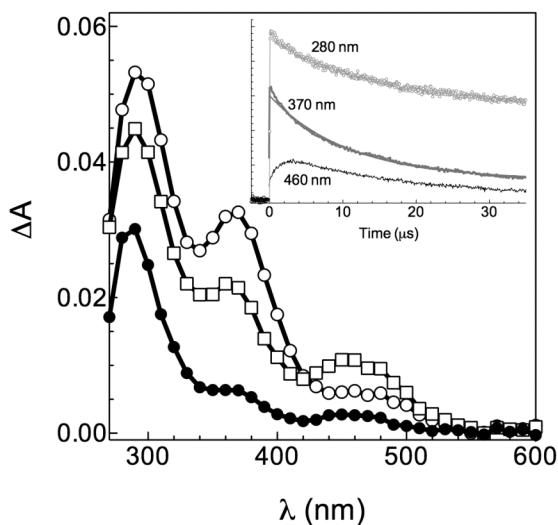


Figure S10. Transient absorption spectra recorded 0.06-0.19 μs (\square), and 4.16-4.42 μs (\square), and 34.2-34.4 μs (\bullet) after the laser pulse, by laser flash photolysis of deoxygenated hexanes solution of **2** containing 5.3 mM THT. The insets show transient decay/growth profiles recorded at 280, 370, and 460 nm.

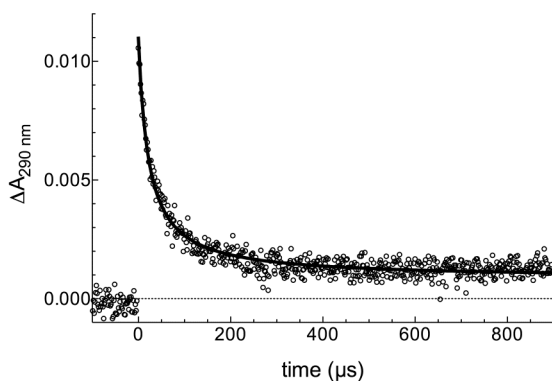


Figure S11. Transient absorbance vs. time profile recorded at 290 nm, with a deoxygenated hexanes solution of **2** containing 4.7 mM PrS.

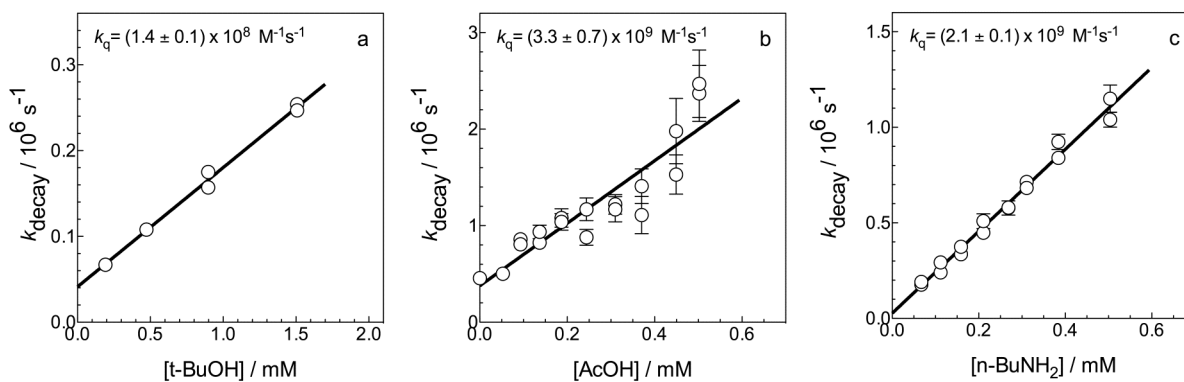


Figure S12. Plots of the first order rate coefficients for decay (k_{decay}) of the 290 nm absorption vs. (a) [t-BuOH] (b) [AcOH], and (c) [n-BuNH₂] from laser photolysis of a deoxygenated solution of **2** containing 20 mM PrS.

Steady State Photolysis Experiments

In a typical steady-state photolysis experiment, a solution of non-volatile reagents in cyclohexane- d_{12} (1 mL) was placed in a quartz NMR tube, sealed with a rubber septum and degassed with dry argon for 5 min. Volatile reagents were then added as the neat liquids using a glass syringe. The solution was then photolyzed in a Rayonet photochemical reactor (Southern New England Ultraviolet Co.) equipped with two RPP-2537 lamps and a merry-go-round apparatus, monitoring the course of the photolysis at selected time intervals by ^1H NMR spectroscopy and GC/MS. The products were identified based on the following spectroscopic data.

Propene (**6**), ^1H NMR δ (C_6D_{12}) = 5.73 (ddd, J = 20.4, 12.09, 7.80 Hz, 1H), 4.87 (ddt, J = 1.67, 4.32, 12.09 Hz, 1H), 4.96 (dp, J = 20.4, 2.24 Hz, 1H), 1.67 (dt, J = 7.80, 1.92 Hz, 3H).

7, ^1H NMR⁸ δ (C_6D_{12}) = 0.39 (s, 18H), expected singlet at $\delta \approx 0.1$ not resolvable from other components of mixture; ^{29}Si NMR δ 3.0, expected singlet in the δ -10 - +5 range not resolvable from other components of mixture.

12, ^1H NMR δ (CDCl_3)⁵ = 7.79 (dd, J = 1.4, 8.0 Hz, 4H), 7.48 (tt, J = 1.4, 7.4 Hz, 4H), 7.43 (t, J = 8.1 Hz, 2H); ^1H NMR δ (C_6D_{12}) = 7.63 (dd, J = 1.5, 7.8 Hz, 4H), 7.29 (m, 2H), 7.25 (m, 4H); ^{13}C NMR δ (CDCl_3)⁵ = 136.0168, 134.6930, 131.0171, 128.3330; ^{29}Si NMR δ (CDCl_3)⁵ = -3.7; ^{29}Si NMR δ (C_6D_{12}) = -4.1.

14, ^1H NMR δ (C_6D_{12})⁹ = 5.36 (s, 1H), 3.52 (s, 3H), ^{29}Si NMR δ (C_6D_{12}) = -9.3

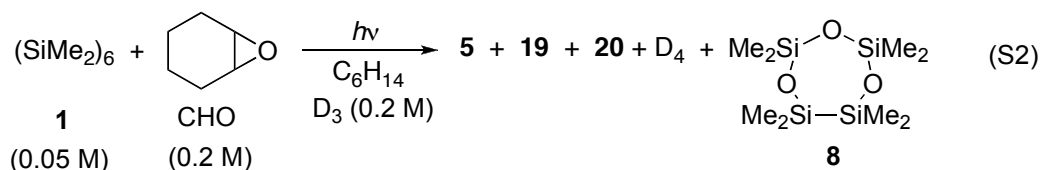
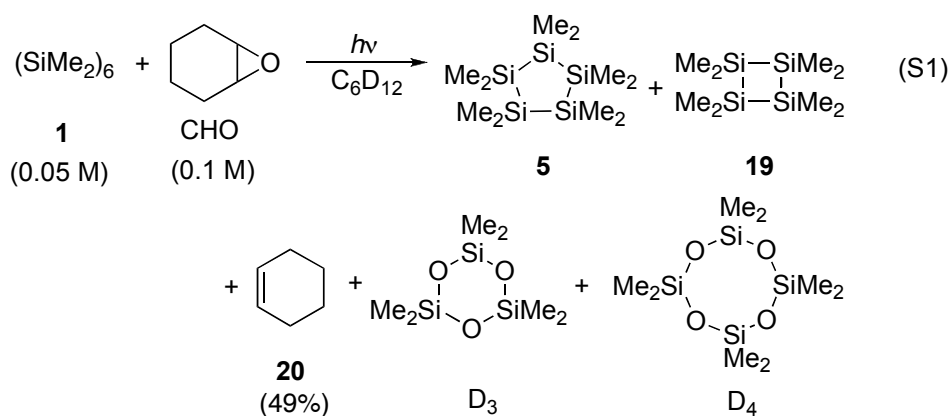
15, ^1H NMR δ (C_6D_{12}) = 7.25 (m, 6H), 7.63 (dd, J = 1.5, 8.0 Hz, 4H), 3.59 (s, 3H); ^{13}C NMR δ (C_6D_{12}) = 134.8, 135, 131, 128.5, 50; ^{29}Si δ (C_6D_{12}) = -4.7; HRMS m/z (I) = 246.0527 (15, M^+), 213.0500 (100), 183.0495 (60), 181.0434 (8), 136.9829 (3), 105.0132 (2), 77.0351 (1).

Cyclohexene (**20**), ^1H NMR δ (C_6D_{12}) = 5.59 (s, 2H), 1.96 (m, 4H), 1.60 (m, 4H)

Photolysis of **1** in the presence of CHO

Photolysis of **1** in the presence of CHO afforded pentamethylcyclopentasilane (**5**), octamethylcyclotetrasilane (**19**), and cyclohexene (**20**) as the major products, along with small amounts of D_3 , 1,1,3,3,5,5,7,7-octamethylcyclotetrasiloxane (D_4), and numerous other minor products that were not identified (eq. S1). The two oligosiloxanes were present in an

approximate ratio of D₃:D₄ ~ 4.3:1 (by GC/MS; uncalibrated) after 15 minutes photolysis time, which decreased to *ca.* 3:1 upon doubling the irradiation time. Concentration vs. time plots constructed for CHO and **17** from the NMR integrals (Figure S13, S14) indicated that the alkene was formed in 49% yield relative to consumed CHO during the early stages of the photolysis (0-2% conversion of CHO), but decreased upon continued irradiation. Photolysis of **1** in hexanes containing added D₃ (0.2 M) in addition to CHO (0.2 M) resulted in a considerably cleaner product mixture, which consisted mainly of **5**, **19**, **20**, **7**, D₄, and compound **8** (eq. S2). GC/MS analysis of the photolysate indicated compound **8** and D₄ to be present in a ratio of **8**:D₄ ≈ 1:2.2 after 15 minutes of photolysis.



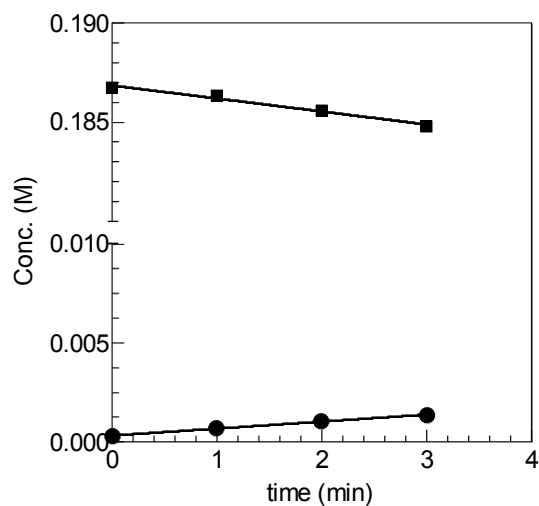


Figure S13. Concentration vs. time plots for 254 nm irradiation of a deoxygenated solution of **1** (0.05 M) in C_6D_{12} containing CHO (0.2 M). The solid lines are the least squares fits of the data, the slopes of which are CHO (■), -0.00065 ± 0.00006 ; **19** (●), 0.00035 ± 0.00001 .

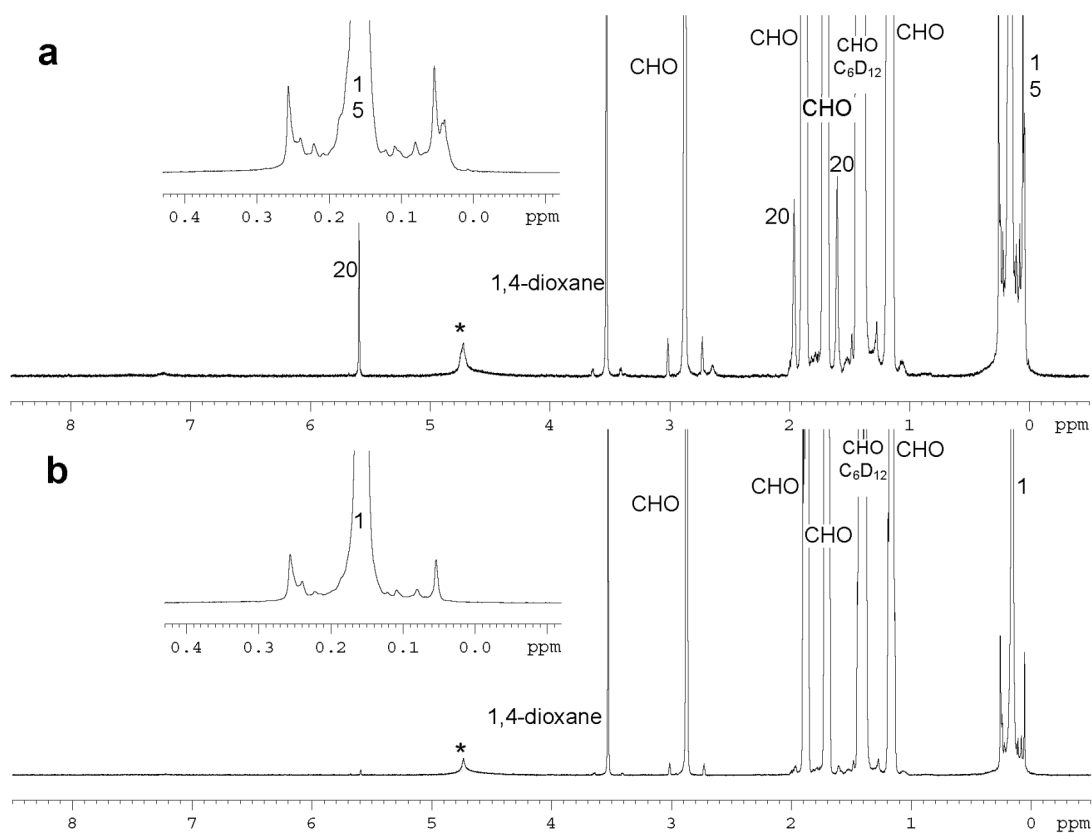


Figure S14. 600 MHz 1H NMR spectra of the solution of Fig. S13 a) after 8 min of photolysis and b) before photolysis. * - unreactive impurity.

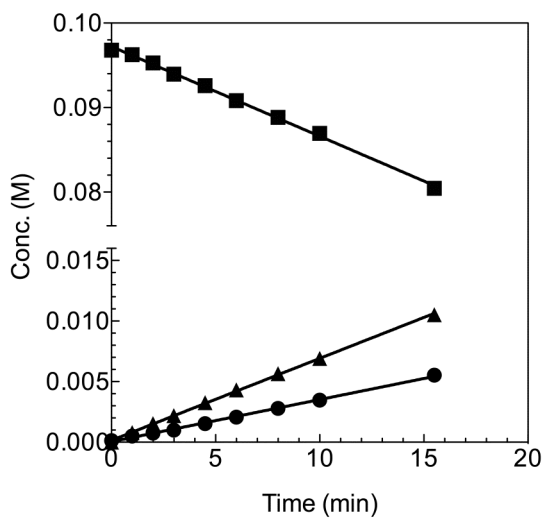


Figure S15. Concentration vs. time plots for 254 nm irradiation of a deoxygenated solution of **1** (0.05 M) in C_6D_{12} containing D_3 (0.2 M) and PrS (0.10 M). The solid lines are the least squares fits of the data, the slopes of which are PrS (■), -0.00106 ± 0.00002 ; **7** (●), 0.000348 ± 0.000006 ; **6** (▲), 0.000676 ± 0.000007 .

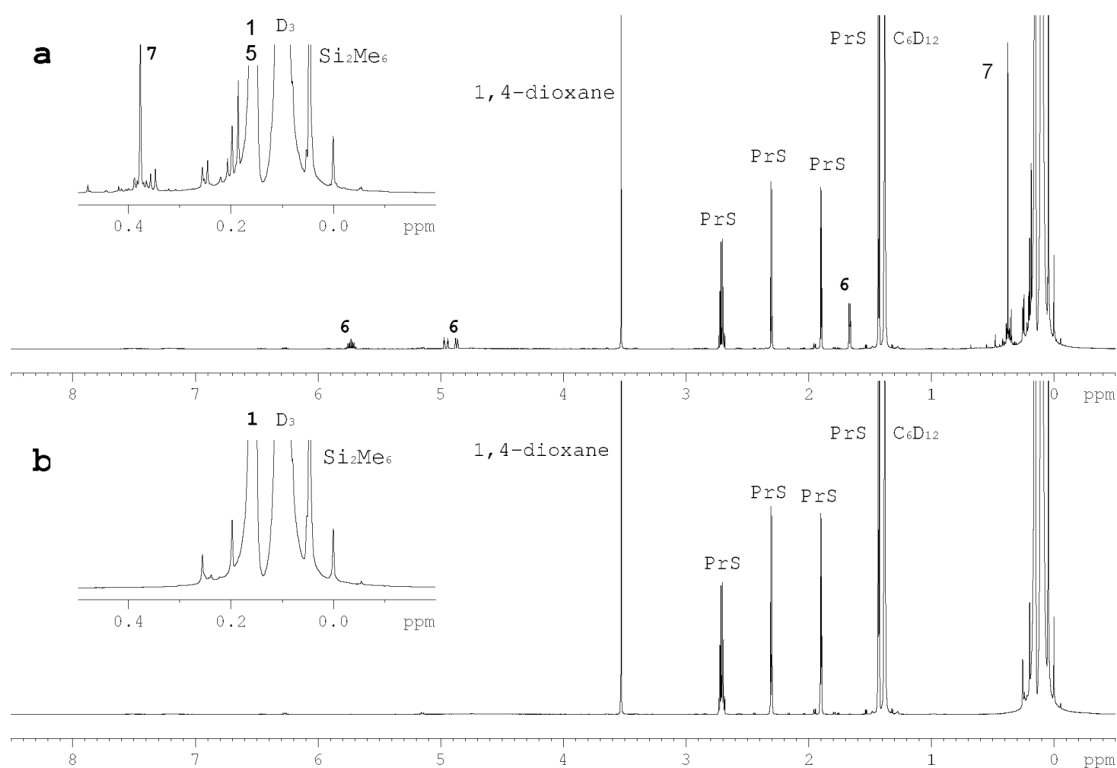


Figure S16. 600 MHz 1H NMR spectra of the solution of Fig. S15, a) after 15.5 min of photolysis and b) before photolysis.

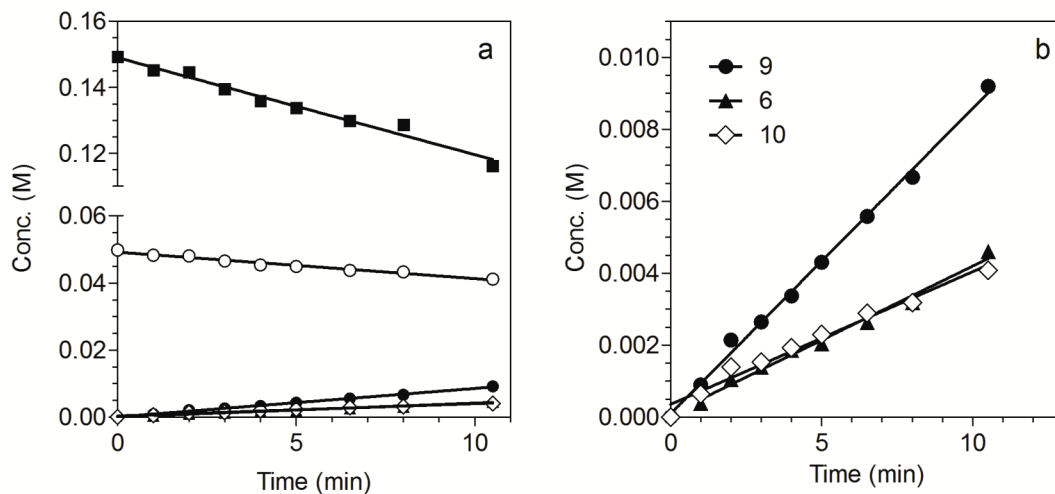


Figure S17. Concentration vs. time plots for 254 nm irradiation of deoxygenated solutions of **2** (0.05 M) in C₆D₁₂ containing D₃ (0.2 M) and PrO (0.15 M). The solid lines are the least squared fit of the data, and are characterized by the following slopes: PrO (■), -0.0029 ± 0.0002 ; **2** (○), -0.00079 ± 0.00005 ; **9** (●), 0.00085 ± 0.00002 ; **6** (▲), 0.00041 ± 0.00002 ; **10** (◇), 0.00037 ± 0.00002 .

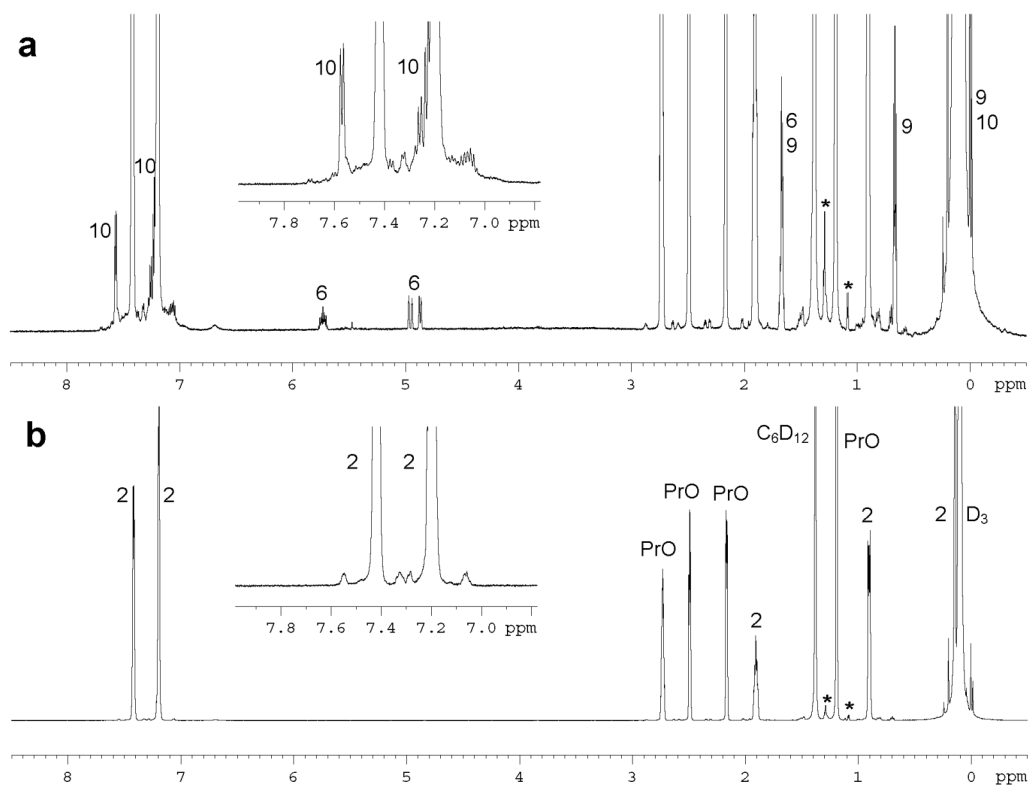


Figure S18. 600 MHz ¹H NMR spectra of a solution of 0.05 M **2**, 0.15 M PrO, 0.2 M D₃ in C₆D₁₂, after a) 8 min of photolysis; b) 0 min of photolysis. * - unreactive impurity.

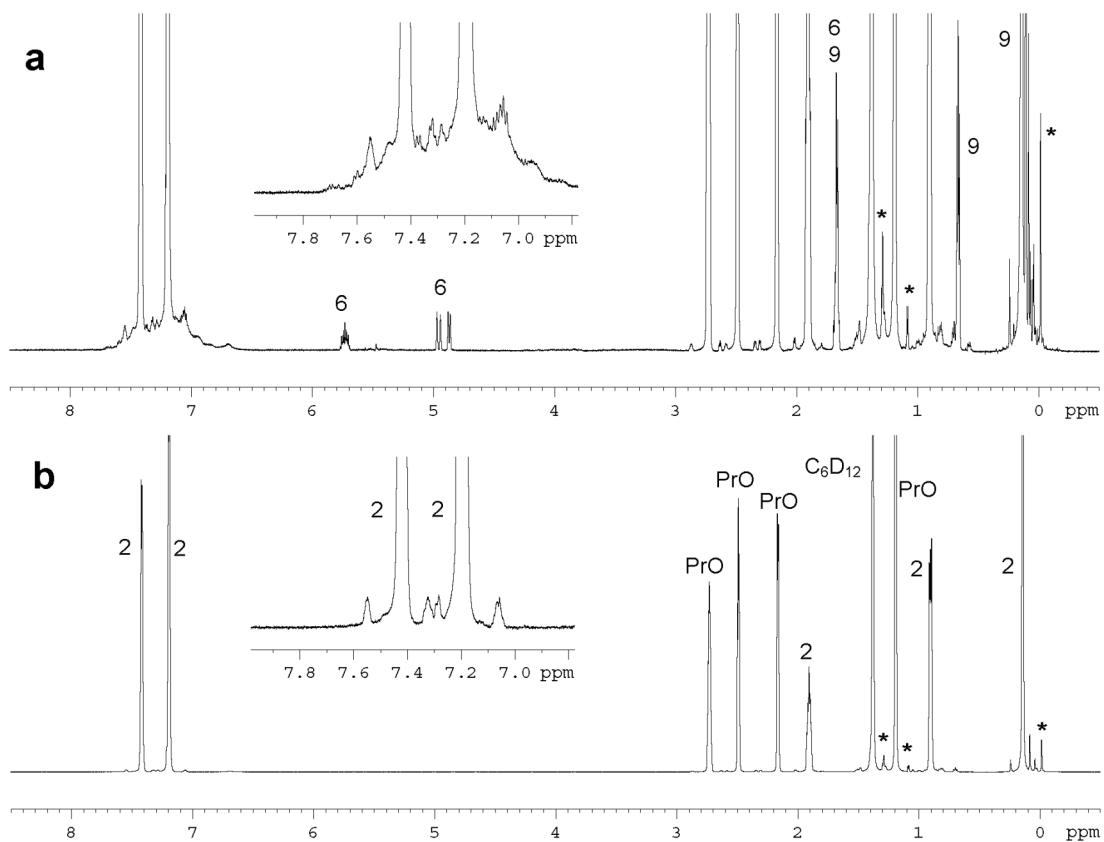


Figure S19. 600 MHz ¹H NMR spectra of a deoxygenated solution of **2** (0.05 M) and PrO (0.15 M) in C₆D₁₂, after (a) 8 min of and (b) before photolysis with 254 nm light. * - unreactive impurity.

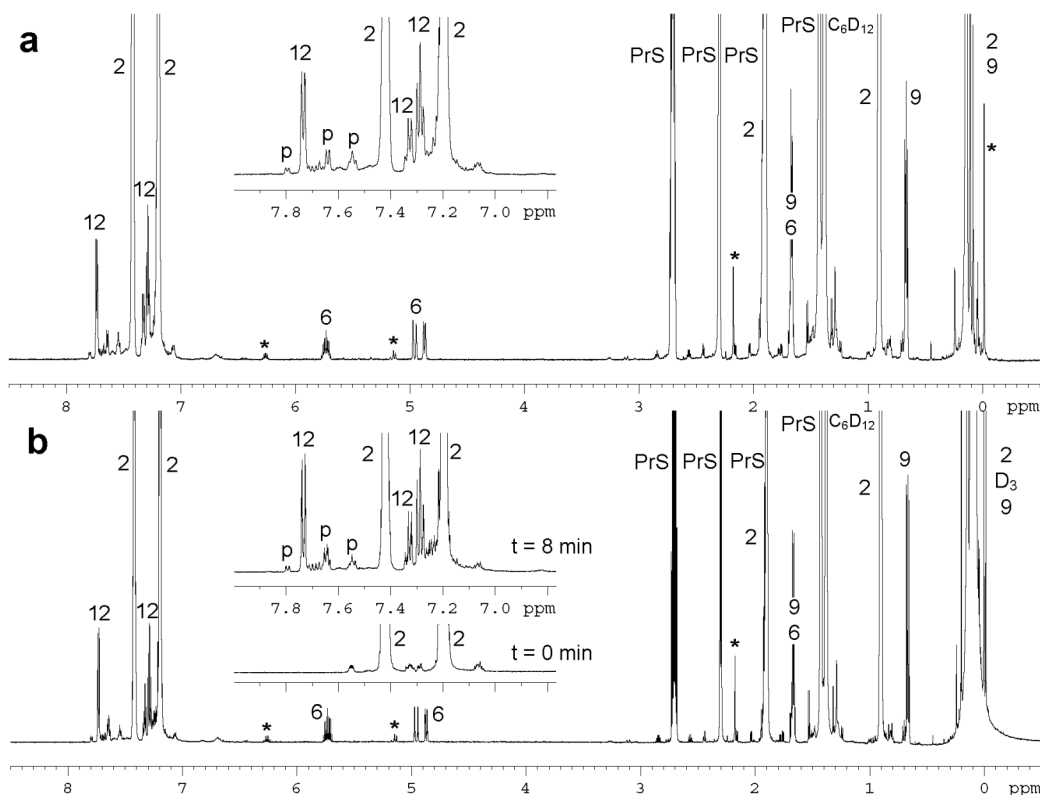


Figure S20. (a) 600 MHz ^1H NMR spectra of a solution of **2** (0.05 M) and PrS (0.2 M) in C_6D_{12} , after 8 min of photolysis; (b) 600 MHz ^1H NMR spectra of a solution of 0.05 M **2**, 0.2 M PrS and 0.2 M D_3 in C_6D_{12} , after 8 min of photolysis, the inset shows the phenyl region at the beginning of photolysis for comparison. * - unreactive impurity in the sample, p – unidentified product

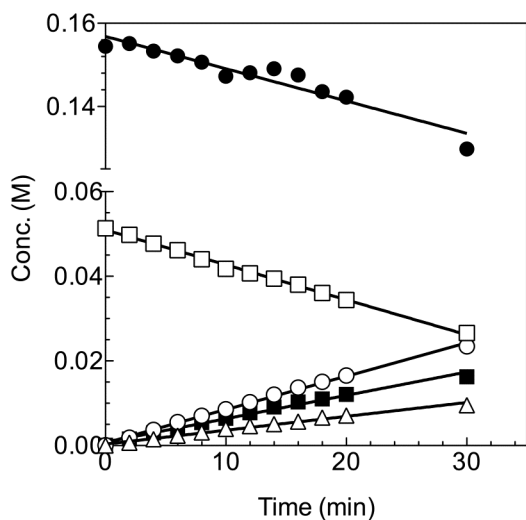


Figure S21. Concentration vs. time plots from steady state photolysis of **2** (0.05 M) in deoxygenated C_6D_{12} containing PrS (0.165 M) and D_3 (0.2 M) as determined by ^1H NMR spectroscopy. The solid lines are the least squares fits of the data, and are characterized by the following slopes: PrS (●), -0.00077 ± 0.00007 ; **2** (□), -0.00083 ± 0.00002 ; **9** (○), 0.00079 ± 0.00001 ; **6** (■), 0.00055 ± 0.00002 ; **12** (Δ), 0.00033 ± 0.00001 .

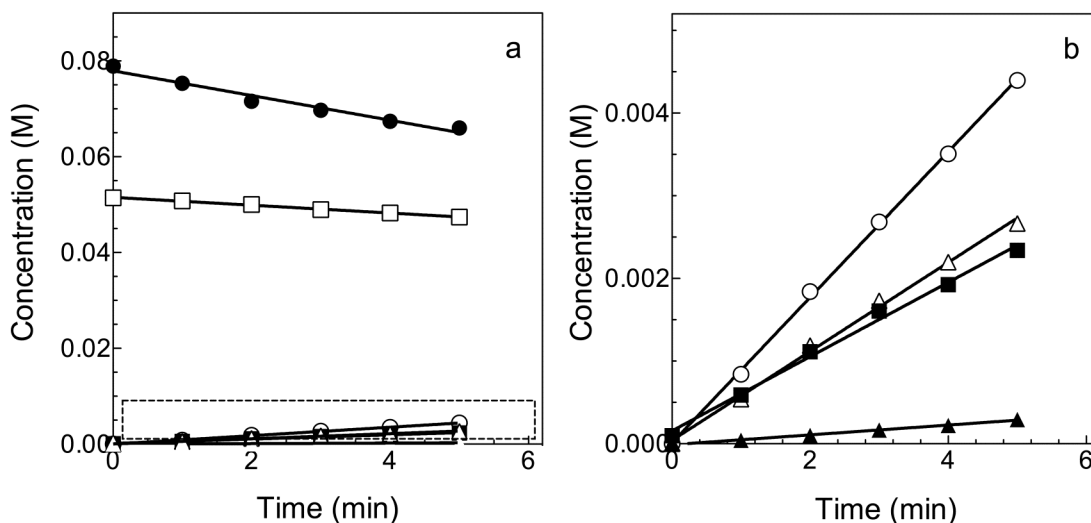


Figure S22. Concentration vs. time plots for 254 nm irradiation of deoxygenated solutions of **2** (0.05 M) in C_6D_{12} containing PrS (0.08 M) and MeOH (0.005 M). The solid lines are the least squared fit of the data, and are characterized by the following slopes: PrS (\bullet), -0.0026 ± 0.0002 ; **2** (\square), -0.00082 ± 0.00002 ; **9** (\circ), 0.00088 ± 0.00001 ; **6** (\blacksquare), 0.00045 ± 0.00002 ; **15** (\triangle), 0.00054 ± 0.00002 ; **14** (\blacktriangle), 0.000059 ± 0.000002 . Figure (b) shows a blow-up of the plots for the products.

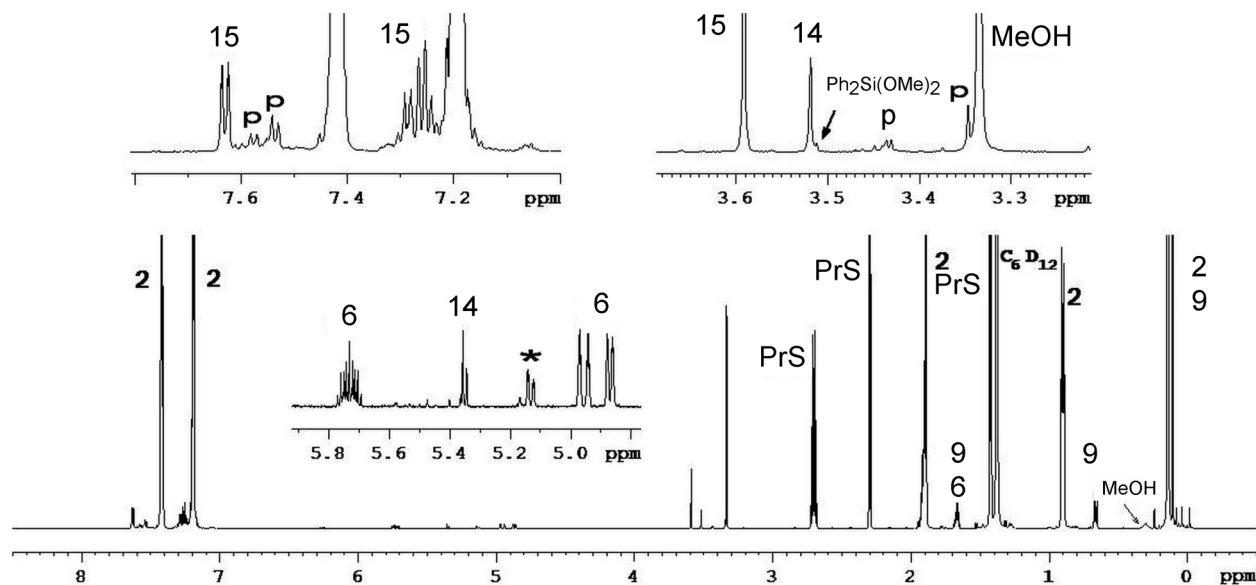


Figure S23. 600 MHz 1H NMR spectrum of a solution of **2** (0.05M), PrS (0.08 M) and MeOH (0.005 M) in C_6D_{12} after 5 min of photolysis followed by 4 hrs standing at room temperature in the dark. * - unreactive impurity; p – unidentified product

Computational Studies

All calculations were carried out using the Gaussian 09 suite of programs.¹⁰

Table S1. Calculated (B3LYP/6-311G(d)//B3LYP/6-311G(d)) Zero-point Corrected Electronic Energies (ΔE_0), Standard Enthalpies (ΔH_{298}) and Free Energies (ΔG_{298}) of stationary points on the potential energy surfaces for the reactions of SiH₂ and SiMe₂ with oxirane, in kcal mol⁻¹ relative to the energies of the isolated reactants.

	SiH ₂ + oxirane			SiMe ₂ + oxirane		
	ΔE_0	ΔH_{298}	ΔG_{298}	ΔE_0	ΔH_{298}	ΔG_{298}
<i>anti</i> -Complex	-15.7	-16.5	-6.4	-10.8	-10.9	+0.3
<i>gauche</i> -Complex	-16.1	-17.0	-6.5	-9.3	-9.5	+1.9
Transition State	-6.6	-7.6	+3.3	-3.1	-3.5	+8.7
Biradical	-26.2	-26.4	-17.8	-26.8	-26.5	-16.5
R ₂ Si=X + C ₂ H ₄	-57.3	-57.3	-58.4	-64.9	-64.4	-65.5

Table S2. Calculated (B3LYP/6-311G(d)//B3LYP/6-311G(d)) Zero-point Corrected Electronic Energies (ΔE_0), Standard Enthalpies (ΔH_{298}) and Free Energies (ΔG_{298}) of Reaction of SiMe₂ and SiPh₂ with Oxirane and Thiirane, in kcal mol⁻¹.

	ΔE_0	ΔH_{298}	ΔG_{298}
SiMe ₂ + oxirane	-64.9	-64.4	-65.5
SiPh ₂ + oxirane	-62.4	-61.8	-62.2
SiMe ₂ + thiirane	-52.1	-51.5	-52.4
SiPh ₂ + thiirane	-50.0	-49.4	-49.5

Calculated structures and energies

Silylene B3LYP/6-311+G(d,p) output

Zero-point correction= 0.011646 (Hartree/Particle)
 Thermal correction to Energy= 0.014513
 Thermal correction to Enthalpy= 0.015457
 Thermal correction to Gibbs Free Energy= -0.008094
 Sum of electronic and zero-point Energies= -290.628784
 Sum of electronic and thermal Energies= -290.625917
 Sum of electronic and thermal Enthalpies= -290.624973
 Sum of electronic and thermal Free Energies= -290.648524

Si	0.00000000	0.00000000	0.13325700
H	0.00000000	1.09320700	-0.93279800
H	0.00000000	-1.09320700	-0.93279800

Dimethylsilylene B3LYP/6-311+G(d,p) output

Zero-point correction= 0.070637 (Hartree/Particle)
 Thermal correction to Energy= 0.076267
 Thermal correction to Enthalpy= 0.077211
 Thermal correction to Gibbs Free Energy= 0.042651
 Sum of electronic and zero-point Energies= -369.252596
 Sum of electronic and thermal Energies= -369.246966
 Sum of electronic and thermal Enthalpies= -369.246021
 Sum of electronic and thermal Free Energies= -369.280581

C	-1.44581200	-0.49828700	-0.01008600
Si	0.00000000	0.75569100	0.00000000
C	1.44581200	-0.49828700	0.01008600
H	-2.40503500	-0.04820500	-0.27615600
H	-1.26718600	-1.37225200	-0.64745100
H	-1.54259500	-0.87965900	1.01913000
H	2.40503500	-0.04820500	0.27615500
H	1.26718700	-1.37225100	0.64745200
H	1.54259500	-0.87966000	-1.01913000

Oxirane B3LYP/6-311+G(d,p) output

Zero-point correction= 0.057135 (Hartree/Particle)
 Thermal correction to Energy= 0.060296
 Thermal correction to Enthalpy= 0.061240
 Thermal correction to Gibbs Free Energy= 0.033047
 Sum of electronic and zero-point Energies= -153.778906
 Sum of electronic and thermal Energies= -153.775745
 Sum of electronic and thermal Enthalpies= -153.774801
 Sum of electronic and thermal Free Energies= -153.802993

C	-0.73333300	-0.37353200	0.00001000
C	0.73375600	-0.37311300	0.00001500
O	-0.00042400	0.85531300	-0.00002800
H	-1.27036200	-0.59118300	-0.91954300
H	-1.27036800	-0.59112200	0.91957400
H	1.27079500	-0.59019600	-0.91964800
H	1.27078800	-0.59013500	0.91969500

Thiirane B3LYP/6-311+G(d,p) output

Zero-point correction= 0.054814 (Hartree/Particle)
 Thermal correction to Energy= 0.058198
 Thermal correction to Enthalpy= 0.059142
 Thermal correction to Gibbs Free Energy= 0.029521
 Sum of electronic and zero-point Energies= -476.778846
 Sum of electronic and thermal Energies= -476.775462
 Sum of electronic and thermal Enthalpies= -476.774518
 Sum of electronic and thermal Free Energies= -476.804139

C	0.73986000	-0.80636400	0.00000000
C	-0.73984200	-0.80629100	0.00000000
H	1.25429400	-1.07931400	0.91415300
H	1.25429400	-1.07931400	-0.91415300
H	-1.25434800	-1.07931600	0.91410300
H	-1.25434800	-1.07931600	-0.91410300
S	0.00000000	0.87457400	0.00000000

Silylene-oxirane anti-complex B3LYP/6-311+G(d,p) output

Zero-point correction= 0.073712 (Hartree/Particle)
 Thermal correction to Energy= 0.079553
 Thermal correction to Enthalpy= 0.080498
 Thermal correction to Gibbs Free Energy= 0.044550
 Sum of electronic and zero-point Energies= -444.429173
 Sum of electronic and thermal Energies= -444.423332
 Sum of electronic and thermal Enthalpies= -444.422388
 Sum of electronic and thermal Free Energies= -444.458335

Si	1.57993900	-0.00022400	-0.19883300
C	-1.39894500	-0.73230500	-0.17205200
C	-1.39808600	0.73264700	-0.17173600
O	-0.37061200	-0.00032300	0.54983500
H	-2.06624000	-1.27907200	0.48309500
H	-1.02411800	-1.25420100	-1.04688200
H	-2.06503200	1.28004200	0.48329600
H	-1.02305200	1.25458400	-1.04648600
H	1.90399300	-1.11425100	0.78864000
H	1.90239100	1.11656800	0.78605200

Silylene-oxirane gauche complex B3LYP/6-311+G(d,p) output

Zero-point correction= 0.073901 (Hartree/Particle)
 Thermal correction to Energy= 0.079547
 Thermal correction to Enthalpy= 0.080491
 Thermal correction to Gibbs Free Energy= 0.045335
 Sum of electronic and zero-point Energies= -444.429969
 Sum of electronic and thermal Energies= -444.424323
 Sum of electronic and thermal Enthalpies= -444.423379
 Sum of electronic and thermal Free Energies= -444.458535

Si	1.62852100	-0.10533100	-0.00193100
C	-1.38717700	0.72996200	0.19346900
C	-1.38425200	-0.73669100	0.14886800
O	-0.36118800	0.01642000	-0.55544400
H	-2.06245400	1.29050000	-0.44281300
H	-1.00314000	1.22972700	1.07480600
H	-2.05825000	-1.26326400	-0.51653400
H	-1.00964900	-1.28606700	1.00541400
H	1.15151500	0.00059000	1.45844300
H	1.70076100	1.41216600	-0.16275300

Silylene-oxirane transition state UB3LYP/6-311+G(d,p) output

Zero-point correction= 0.071718 (Hartree/Particle)
 Thermal correction to Energy= 0.077114
 Thermal correction to Enthalpy= 0.078058
 Thermal correction to Gibbs Free Energy= 0.043556
 Sum of electronic and zero-point Energies= -444.415663
 Sum of electronic and thermal Energies= -444.410267
 Sum of electronic and thermal Enthalpies= -444.409322
 Sum of electronic and thermal Free Energies= -444.443824

Si	1.56984300	-0.02908300	0.02053200
C	-1.73822500	0.63601800	0.17003800
C	-1.21540000	-0.72069000	0.13352000
O	-0.14350900	-0.02828800	-0.53632900
H	-2.34006100	1.01600400	-0.64246200
H	-1.44940300	1.29989100	0.97119300
H	-1.70030800	-1.43336800	-0.53032800
H	-0.90829600	-1.17078700	1.07693600
H	1.36528700	0.01185100	1.52627100
H	1.92481200	1.41790500	-0.21977500

Silylene-oxirane singlet biradical UB3LYP/6-311+G(d,p) output

Zero-point correction= 0.070402 (Hartree/Particle)
 Thermal correction to Energy= 0.077118
 Thermal correction to Enthalpy= 0.078062
 Thermal correction to Gibbs Free Energy= 0.039708
 Sum of electronic and zero-point Energies= -444.448655
 Sum of electronic and thermal Energies= -444.441939
 Sum of electronic and thermal Enthalpies= -444.440995
 Sum of electronic and thermal Free Energies= -444.479349

Si	1.59910300	0.03841000	0.10291300
C	-2.15378100	0.48964400	-0.01021300
C	-1.10078400	-0.52018900	0.24178800
O	0.07289000	-0.20423200	-0.52725100
H	-3.16003800	0.20142300	-0.28425300
H	-1.90897000	1.54248400	0.05334800
H	-1.43455100	-1.51987800	-0.05055100
H	-0.83988700	-0.56517600	1.31328400
H	1.51691200	0.90630200	1.32243800
H	2.38336000	0.71423000	-0.96648600

Silanone B3LYP/6-311+G(d,p) output

Zero-point correction= 0.018396 (Hartree/Particle)
 Thermal correction to Energy= 0.021512
 Thermal correction to Enthalpy= 0.022456
 Thermal correction to Gibbs Free Energy= -0.004893
 Sum of electronic and zero-point Energies= -365.934759
 Sum of electronic and thermal Energies= -365.931643
 Sum of electronic and thermal Enthalpies= -365.930699
 Sum of electronic and thermal Free Energies= -365.958048

Si	-0.44100600	0.00000000	-0.00011000
O	1.08931100	0.00000000	0.00015000
H	-1.27019900	-1.22918000	0.00015900
H	-1.27019900	1.22918000	0.00017300

Ethylene b3lyp/6-311+G(d,p) output

Zero-point correction= 0.050784 (Hartree/Particle)
 Thermal correction to Energy= 0.053826
 Thermal correction to Enthalpy= 0.054770
 Thermal correction to Gibbs Free Energy= 0.028605
 Sum of electronic and zero-point Energies= -78.564729
 Sum of electronic and thermal Energies= -78.561686
 Sum of electronic and thermal Enthalpies= -78.560742
 Sum of electronic and thermal Free Energies= -78.586908

C	0.00000000	-0.66440000	0.00000000
C	0.00000000	0.66440000	0.00000000
H	0.92270000	-1.23520000	0.00000000
H	-0.92270000	-1.23520000	0.00000000
H	-0.92270000	1.23520000	0.00000000
H	0.92270000	1.23520000	0.00000000

Dimethylsilylene-oxirane anti complex B3LYP/6-311+G(d,p) output

Zero-point correction= 0.131108 (Hartree/Particle)
 Thermal correction to Energy= 0.140608
 Thermal correction to Enthalpy= 0.141552
 Thermal correction to Gibbs Free Energy= 0.096597
 Sum of electronic and zero-point Energies= -523.045275
 Sum of electronic and thermal Energies= -523.035775
 Sum of electronic and thermal Enthalpies= -523.034831
 Sum of electronic and thermal Free Energies= -523.079786

C	-1.57231700	-1.46673800	0.33097800
Si	-0.86956800	0.00000000	-0.70276400
C	-1.57231400	1.46673900	0.33097500
H	-1.12847700	-2.42827300	0.05464300
H	-1.47438800	-1.33009800	1.41373600
H	-2.64511900	-1.54400400	0.10665700
H	-1.12847200	2.42827300	0.05464400
H	-2.64511200	1.54400400	0.10662600
H	-1.47441700	1.33011100	1.41373800
C	2.08563000	0.73206900	-0.04291500
C	2.08563700	-0.73205900	-0.04292900
O	0.93728800	-0.00001300	0.46593800
H	2.61813800	1.27792300	0.72675600
H	1.88775000	1.25300700	-0.97448400
H	2.61815800	-1.27792000	0.72672900
H	1.88777400	-1.25298100	-0.97451000

Dimethylsilylene-oxirane complex (gauche) RB3LYP/6-311+G(d,p) output

Zero-point correction= 0.130992 (Hartree/Particle)
 Thermal correction to Energy= 0.140464
 Thermal correction to Enthalpy= 0.141408
 Thermal correction to Gibbs Free Energy= 0.096500
 Sum of electronic and zero-point Energies= -523.042752
 Sum of electronic and thermal Energies= -523.033281
 Sum of electronic and thermal Enthalpies= -523.032337
 Sum of electronic and thermal Free Energies= -523.077244

C	1.00634700	1.58680200	0.45881600
Si	1.02250000	0.08165500	-0.76370000
C	1.80630600	-1.22724700	0.41373500
H	0.32715800	2.38915500	0.14996100
H	0.82043900	1.34545400	1.51303300
H	2.01557700	2.01972700	0.41051200
H	1.72424400	-2.24137900	0.01236800
H	2.87936100	-1.00281500	0.48895700

H	1.40311000	-1.21827000	1.43352300
C	-2.16918300	0.14414600	-0.51407700
C	-1.83507800	-0.17567600	0.87824600
O	-0.96086500	-0.58738800	-0.21214800
H	-2.90927200	-0.44361000	-1.04544500
H	-1.99945200	1.15020800	-0.88290800
H	-2.32067800	-1.00775700	1.37518100
H	-1.41892700	0.59707100	1.51348500

Dimethylsilylene-oxirane transition state UB3LYP/6-311+G(d,p) output

Zero-point correction=	0.129267 (Hartree/Particle)
Thermal correction to Energy=	0.138291
Thermal correction to Enthalpy=	0.139235
Thermal correction to Gibbs Free Energy=	0.095811
Sum of electronic and zero-point Energies=	-523.033348
Sum of electronic and thermal Energies=	-523.024324
Sum of electronic and thermal Enthalpies=	-523.023380
Sum of electronic and thermal Free Energies=	-523.066804

C	1.02221600	1.60498100	0.50253400
Si	0.93385300	0.08578000	-0.67573000
H	0.41570900	2.45155400	0.16653300
H	0.73921100	1.35465600	1.53430400
H	2.05924600	1.95973300	0.53323200
C	1.80987400	-1.25448700	0.36966800
H	1.70976300	-2.24626800	-0.07916100
H	2.88150600	-1.03293700	0.43482800
H	1.41621100	-1.29530700	1.39399000
O	-0.80363300	-0.49705800	-0.41991600
C	-2.00842800	0.27984300	-0.43668500
C	-2.03058800	-0.37633500	0.86412600
H	-2.70249200	-0.05981900	-1.20230100
H	-1.83815600	1.35474700	-0.46420500
H	-2.48857200	-1.34682100	0.98119200
H	-1.59574700	0.11198600	1.72327200

Dimethylsilylene-oxirane biradical UB3LYP/6-311+G(d,p) output

Zero-point correction= 0.128194 (Hartree/Particle)
 Thermal correction to Energy= 0.138344
 Thermal correction to Enthalpy= 0.139288
 Thermal correction to Gibbs Free Energy= 0.092604
 Sum of electronic and zero-point Energies= -523.072807
 Sum of electronic and thermal Energies= -523.062658
 Sum of electronic and thermal Enthalpies= -523.061713
 Sum of electronic and thermal Free Energies= -523.108397

C	0.94776600	1.80182300	0.08651900
Si	0.90412600	-0.01807100	-0.44299900
H	0.14049800	2.38118400	-0.36822300
H	0.85796000	1.88409600	1.17640300
H	1.89447500	2.26074500	-0.21274300
C	2.21000200	-1.02704600	0.46292400
H	2.18280100	-2.07343400	0.15169500
H	3.21205000	-0.63610000	0.26627400
H	2.03037600	-0.98868500	1.54352700
O	-0.56081000	-0.72958700	-0.03608500
C	-1.84803400	-0.30947100	-0.49976300
C	-2.70969500	0.09514000	0.63514600
H	-2.29898100	-1.14319800	-1.04829600
H	-1.73300800	0.51572600	-1.22772100
H	-3.75553300	-0.18148300	0.67171600
H	-2.30214900	0.70815700	1.42907800

Dimethylsilanone B3LYP/6-311+G(d,p) output

Zero-point correction= 0.076047 (Hartree/Particle)
 Thermal correction to Energy= 0.081781
 Thermal correction to Enthalpy= 0.082725
 Thermal correction to Gibbs Free Energy= 0.047000
 Sum of electronic and zero-point Energies= -444.569382
 Sum of electronic and thermal Energies= -444.563648
 Sum of electronic and thermal Enthalpies= -444.562704
 Sum of electronic and thermal Free Energies= -444.598429

Si	0.00000000	0.19270700	-0.00003600
O	0.00000400	1.72757300	0.00002300
C	-1.55515600	-0.84421800	0.00000300
H	-1.58798700	-1.49414400	0.88058900
H	-2.43855800	-0.20461400	-0.00059100
H	-1.58745700	-1.49514900	-0.87985300
C	1.55515300	-0.84422300	0.00000300
H	1.58798700	-1.49414400	0.88059200

H	1.58744800	-1.49515900	-0.87985000
H	2.43855600	-0.20462100	-0.00059900

Silylene-thiirane anti-complex B3LYP/6-311+G(d,p) output

Zero-point correction=	0.071039 (Hartree/Particle)
Thermal correction to Energy=	0.077149
Thermal correction to Enthalpy=	0.078093
Thermal correction to Gibbs Free Energy=	0.041191
Sum of electronic and zero-point Energies=	-767.437222
Sum of electronic and thermal Energies=	-767.431112
Sum of electronic and thermal Enthalpies=	-767.430168
Sum of electronic and thermal Free Energies=	-767.467070

Si	1.77872200	-0.37638100	0.00042200
C	-1.46242700	-0.48244700	0.73631600
C	-1.46214800	-0.48360800	-0.73574800
H	-2.30628600	-0.05185400	1.26085400
H	-0.92680800	-1.27222400	1.24978700
H	-2.30577200	-0.05394600	-1.26140400
H	-0.92625300	-1.27418500	-1.24771000
S	-0.33422800	0.78718400	-0.00051000
H	2.22861200	0.55957900	-1.11702900
H	2.22949400	0.56334800	1.11433200

Silylene-thiirane gauche complex B3LYP/6-311+G(d,p) output

Zero-point correction=	0.070832 (Hartree/Particle)
Thermal correction to Energy=	0.076968
Thermal correction to Enthalpy=	0.077912
Thermal correction to Gibbs Free Energy=	0.040987
Sum of electronic and zero-point Energies=	-767.435303
Sum of electronic and thermal Energies=	-767.429168
Sum of electronic and thermal Enthalpies=	-767.428224
Sum of electronic and thermal Free Energies=	-767.465148

Si	1.87892100	0.22138000	-0.06055600
C	-1.42006300	0.64458900	-0.63270800
C	-1.54545700	0.27380800	0.79463900
H	-2.21537200	0.36842300	-1.31432000
H	-0.87682400	1.54740800	-0.88575400
H	-2.42779000	-0.26776400	1.11626400
H	-1.07196700	0.90515500	1.53560800
S	-0.33132000	-0.75461600	-0.15302900
H	1.26628900	1.44450700	0.62924000
H	2.11500900	-0.53358700	1.24361900

Silylene-thiirane transition state UB3LYP/6-311+G(d,p) output

Zero-point correction= 0.069103 (Hartree/Particle)
 Thermal correction to Energy= 0.075344
 Thermal correction to Enthalpy= 0.076288
 Thermal correction to Gibbs Free Energy= 0.038518
 Sum of electronic and zero-point Energies= -767.425129
 Sum of electronic and thermal Energies= -767.418888
 Sum of electronic and thermal Enthalpies= -767.417943
 Sum of electronic and thermal Free Energies= -767.455714

Si	1.89813500	0.18767300	0.00021200
C	-1.77480200	0.39423500	-0.70106800
C	-1.77541700	0.39264900	0.70174300
H	-2.38594000	-0.30593000	-1.25508200
H	-1.36920000	1.23094900	-1.25285600
H	-2.38681600	-0.30893300	1.25366700
H	-1.37005200	1.22796600	1.25581400
S	-0.09274500	-0.71658300	-0.00071800
H	1.86147500	1.13780700	-1.16860400
H	1.86188100	1.13474400	1.17152300

Silanethione B3LYP/6-311+G(d,p) output

Zero-point correction= 0.016930 (Hartree/Particle)
 Thermal correction to Energy= 0.020200
 Thermal correction to Enthalpy= 0.021144
 Thermal correction to Gibbs Free Energy= -0.007598
 Sum of electronic and zero-point Energies= -688.919753
 Sum of electronic and thermal Energies= -688.916482
 Sum of electronic and thermal Enthalpies= -688.915538
 Sum of electronic and thermal Free Energies= -688.944280

Si	-0.92516700	0.00000000	-0.00002800
S	1.03066500	0.00000000	0.00002200
H	-1.76915500	1.21915900	0.00002000
H	-1.76915600	-1.21915800	0.00002300

Dimethylsilylene-thiirane anti complex B3LYP/6-311+G(d,p) output

Zero-point correction= 0.128620 (Hartree/Particle)
 Thermal correction to Energy= 0.138426
 Thermal correction to Enthalpy= 0.139370
 Thermal correction to Gibbs Free Energy= 0.093163
 Sum of electronic and zero-point Energies= -846.047237
 Sum of electronic and thermal Energies= -846.037431
 Sum of electronic and thermal Enthalpies= -846.036487
 Sum of electronic and thermal Free Energies= -846.082694

C	1.91732300	1.47432300	0.20834700
Si	1.07589100	0.00000300	-0.72473600
C	1.91734900	-1.47430900	0.20833600
H	1.41907400	2.42945200	0.01525300
H	2.02035000	1.34517600	1.29152600
H	2.93252500	1.56606200	-0.20078600
H	1.41912200	-2.42944600	0.01522500
H	2.93256100	-1.56602500	-0.20077500
H	2.02035100	-1.34516900	1.29151900
C	-2.18435800	-0.73628700	-0.38883600
C	-2.18434300	0.73630700	-0.38881000
H	-2.98693300	-1.26264700	0.11255400
H	-1.71994700	-1.24157300	-1.22835400
H	-2.98690700	1.26266800	0.11259800
H	-1.71992800	1.24161200	-1.22831400
S	-0.94928500	-0.00002200	0.77072700

Dimethylsilylene-thiirane gauche complex B3LYP/6-311+G(d,p) output

Zero-point correction= 0.128531 (Hartree/Particle)
 Thermal correction to Energy= 0.138315
 Thermal correction to Enthalpy= 0.139259
 Thermal correction to Gibbs Free Energy= 0.093311
 Sum of electronic and zero-point Energies= -846.044008
 Sum of electronic and thermal Energies= -846.034224
 Sum of electronic and thermal Enthalpies= -846.033279
 Sum of electronic and thermal Free Energies= -846.079228

C	1.13720300	1.71794400	0.28422800
Si	1.28259400	0.07750000	-0.74254000
C	2.24092800	-0.99998400	0.55154000
H	0.40389100	2.42158300	-0.12383600
H	0.94847500	1.58329800	1.35586700
H	2.11104200	2.21798200	0.19463800
H	2.20190800	-2.06734000	0.31270300
H	3.29702200	-0.70782000	0.47778400

H	1.93981200	-0.86173100	1.59579700
C	-2.18210200	0.35871100	-0.58243800
C	-1.99433200	0.31602700	0.88445300
H	-3.08108800	-0.07239200	-1.00599400
H	-1.76221000	1.19205700	-1.13523000
H	-2.75461900	-0.15305900	1.49760700
H	-1.43385800	1.11399500	1.35528500
S	-0.93980400	-0.88173500	-0.05973500

Dimethylsilylene-thiirane transition state UB3LYP/6-311+G(d,p) output

Zero-point correction=	0.127074 (Hartree/Particle)
Thermal correction to Energy=	0.136680
Thermal correction to Enthalpy=	0.137624
Thermal correction to Gibbs Free Energy=	0.092199
Sum of electronic and zero-point Energies=	-846.038803
Sum of electronic and thermal Energies=	-846.029197
Sum of electronic and thermal Enthalpies=	-846.028253
Sum of electronic and thermal Free Energies=	-846.073679

C	1.45690700	1.65255500	0.39529400
Si	1.31380600	-0.00069100	-0.56946200
C	1.93808900	-1.31662200	0.68008500
H	0.97728600	2.47747000	-0.13828200
H	1.05132000	1.60347300	1.41323000
H	2.51891400	1.90727000	0.48750300
H	1.70993800	-2.33022300	0.34090000
H	3.02830200	-1.23895200	0.76038200
H	1.52233700	-1.18264500	1.68512900
C	-2.04336100	0.79502500	0.27451400
C	-2.31687200	-0.48154500	0.84985700
H	-2.77720900	1.24576500	-0.38298300
H	-1.43771300	1.50427800	0.82705900
H	-3.15387500	-1.07544300	0.51012000
H	-1.79098600	-0.81343600	1.73356800
S	-0.89063600	-0.37402300	-0.77891600

Dimethylsilanethione B3LYP/6-311+G(d,p) output

Zero-point correction= 0.074759 (Hartree/Particle)
 Thermal correction to Energy= 0.081586
 Thermal correction to Enthalpy= 0.082531
 Thermal correction to Gibbs Free Energy= 0.043093
 Sum of electronic and zero-point Energies= -767.551495
 Sum of electronic and thermal Energies= -767.544668
 Sum of electronic and thermal Enthalpies= -767.543724
 Sum of electronic and thermal Free Energies= -767.583161

Si	-0.22764200	0.00000000	-0.00000400
C	-1.29162500	1.54281800	0.00000000
H	-1.94226600	1.55936300	0.88090800
H	-0.67483200	2.44185600	-0.00005900
H	-1.94236700	1.55930800	-0.88083300
C	-1.29162700	-1.54281600	0.00000100
H	-1.94229100	-1.55934800	0.88089300
H	-1.94234800	-1.55931800	-0.88084900
H	-0.67483600	-2.44185600	-0.00003300
S	1.73784000	-0.00000100	0.00000100

Dimethylsilanethione B3LYP/6-311G(d) output

Zero-point correction= 0.075276 (Hartree/Particle)
 Thermal correction to Energy= 0.082074
 Thermal correction to Enthalpy= 0.083018
 Thermal correction to Gibbs Free Energy= 0.043633
 Sum of electronic and zero-point Energies= -767.540221
 Sum of electronic and thermal Energies= -767.533423
 Sum of electronic and thermal Enthalpies= -767.532479
 Sum of electronic and thermal Free Energies= -767.571864

Si	-0.22622500	0.00000000	-0.00000300
C	-1.29317400	1.54176400	0.00000300
H	-1.94548200	1.56260700	0.87938800
H	-0.68137900	2.44402300	-0.00005400
H	-1.94557800	1.56255500	-0.87931200
C	-1.29317400	-1.54176400	0.00000300
H	-1.94550300	-1.56259400	0.87937300
H	-1.94555700	-1.56256800	-0.87932800
H	-0.68138000	-2.44402300	-0.00002700
S	1.73938200	0.00000000	-0.00000200

Silylene-oxirane singlet biradical UMP2/6-31G(d,p) output

Zero-point correction= 0.073490 (Hartree/Particle)
 Thermal correction to Energy= 0.079958
 Thermal correction to Enthalpy= 0.080902
 Thermal correction to Gibbs Free Energy= 0.043536
 Sum of electronic and zero-point Energies= -443.390295
 Sum of electronic and thermal Energies= -443.383827
 Sum of electronic and thermal Enthalpies= -443.382883
 Sum of electronic and thermal Free Energies= -443.420249

Si	-1.63148700	0.06690600	-0.01886000
C	2.30231400	-0.23972900	0.11885100
C	1.03343600	0.49340800	-0.11114900
O	-0.04578000	-0.44677500	-0.16325900
H	3.24543200	0.24553100	-0.07473100
H	2.28611800	-1.13956800	0.71089700
H	1.08216500	1.05914700	-1.04742500
H	0.85468300	1.22452300	0.69228300
H	-1.82027100	0.87991200	1.20878300
H	-2.45556100	-1.15409900	0.03409500

Silylene-oxirane singlet biradical UQCISD/6-31G(d,p) output

E(CORR)= -443.53519787 (Hartree/Particle)

Si	-1.63379200	0.06385600	-0.01925900
C	2.30392000	-0.24252000	0.12277700
C	1.03441300	0.49555700	-0.10781500
O	-0.04665600	-0.43598700	-0.16745700
H	3.25066700	0.23204300	-0.08528300
H	2.28613200	-1.15608900	0.69555000
H	1.08756600	1.06513200	-1.04169200
H	0.85529800	1.22473200	0.69743900
H	-1.81930000	0.87779900	1.21014900
H	-2.44401900	-1.16791600	0.04334700

Diphenylsilylene B3LYP/6-311G(d) output

Zero-point correction= 0.180779 (Hartree/Particle)
Thermal correction to Energy= 0.191804
Thermal correction to Enthalpy= 0.192748
Thermal correction to Gibbs Free Energy= 0.142291
Sum of electronic and zero-point Energies= -752.683478
Sum of electronic and thermal Energies= -752.672453
Sum of electronic and thermal Enthalpies= -752.671509
Sum of electronic and thermal Free Energies= -752.721966

Si	0.00000000	1.68729700	-0.00000100
C	-1.48989600	0.50351800	0.03057800
C	-1.52155400	-0.77307100	0.62941500
C	-2.70254800	1.00341600	-0.48730000
C	-2.69800600	-1.51383500	0.69355300
H	-0.61619600	-1.18666300	1.06162500
C	-3.87466800	0.25329300	-0.45633900
H	-2.72534000	2.00028700	-0.92210800
C	-3.87369400	-1.00688800	0.13949600
H	-2.70038500	-2.48927700	1.17081100
H	-4.79054400	0.65462200	-0.87929600
H	-4.78939200	-1.58864400	0.18244000
C	1.48989600	0.50351800	-0.03057900
C	1.52155500	-0.77307100	-0.62941500
C	2.70254800	1.00341600	0.48729900
C	2.69800700	-1.51383600	-0.69355200
H	0.61619700	-1.18666300	-1.06162400
C	3.87466800	0.25329300	0.45633900
H	2.72534000	2.00028800	0.92210700
C	3.87369400	-1.00688900	-0.13949500
H	2.70038500	-2.48927800	-1.17081000
H	4.79054400	0.65462200	0.87929700
H	4.78939200	-1.58864400	-0.18243900

Diphenylsilanone B3LYP/6-311G(d) output

Zero-point correction=	0.185610 (Hartree/Particle)
Thermal correction to Energy=	0.197623
Thermal correction to Enthalpy=	0.198568
Thermal correction to Gibbs Free Energy=	0.145585
Sum of electronic and zero-point Energies=	-827.993344
Sum of electronic and thermal Energies=	-827.981330
Sum of electronic and thermal Enthalpies=	-827.980386
Sum of electronic and thermal Free Energies=	-828.033369

Si	-0.00000500	1.19224800	-0.00011100
O	-0.00000700	2.72704600	-0.00000800
C	1.58050400	0.21660700	-0.02132900
C	1.68172800	-1.10230600	-0.49688700
C	2.75301800	0.87039300	0.39948100
C	2.91248300	-1.75239000	-0.53484000
H	0.80020400	-1.62161300	-0.85820500
C	3.98013100	0.21590900	0.37136800
H	2.69551800	1.89891700	0.74066600
C	4.06033700	-1.09625400	-0.09395300
H	2.97681900	-2.76831800	-0.91120200
H	4.87553600	0.73036700	0.70497600
H	5.01891400	-1.60480000	-0.12024900
C	-1.58050800	0.21660300	0.02126400
C	-1.68169100	-1.10230200	0.49685400
C	-2.75305800	0.87037900	-0.39946300
C	-2.91243900	-1.75239600	0.53489700
H	-0.80013700	-1.62160200	0.85811200
C	-3.98016300	0.21588400	-0.37126000
H	-2.69558500	1.89889600	-0.74067200
C	-4.06032700	-1.09627300	0.09408300
H	-2.97674100	-2.76832100	0.91127400
H	-4.87559500	0.73033200	-0.70481400
H	-5.01889900	-1.60482600	0.12045200

Diphenylsilanethione B3LYP/6-311G(d) output

Zero-point correction= 0.184068 (Hartree/Particle)
Thermal correction to Energy= 0.196399
Thermal correction to Enthalpy= 0.197343
Thermal correction to Gibbs Free Energy= 0.143306
Sum of electronic and zero-point Energies= -1150.978599
Sum of electronic and thermal Energies= -1150.966269
Sum of electronic and thermal Enthalpies= -1150.965324
Sum of electronic and thermal Free Energies= -1151.019361

Si	0.00000100	1.00761000	-0.00000700
S	0.00000200	2.97905200	-0.00002100
C	1.56225600	-0.00652000	-0.02156300
C	1.61356200	-1.30110000	-0.57049800
C	2.75567200	0.56101800	0.46115600
C	2.81312800	-2.00561300	-0.62563400
H	0.71641000	-1.75843900	-0.97419500
C	3.95043400	-0.14950000	0.41844500
H	2.74407600	1.56785000	0.86558500
C	3.98080100	-1.43353100	-0.12472200
H	2.83681700	-2.99941900	-1.06116400
H	4.86034300	0.30032600	0.80237400
H	4.91507900	-1.98464200	-0.16351900
C	-1.56225600	-0.00651700	0.02156200
C	-1.61356900	-1.30107900	0.57054100
C	-2.75566500	0.56100500	-0.46119000
C	-2.81313600	-2.00558900	0.62568800
H	-0.71642200	-1.75840600	0.97426300
C	-3.95042900	-0.14951000	-0.41846700
H	-2.74406400	1.56782300	-0.86565200
C	-3.98080400	-1.43352200	0.12474400
H	-2.83683200	-2.99937900	1.06125200
H	-4.86033400	0.30030400	-0.80242200
H	-4.91508300	-1.98463200	0.16354900

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