Supporting Information for

A Combined Kinetic and Computational Study of the Reactions of Transient Germylenes with Oxiranes and Thiiranes in Solution.

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Figure S1. Plots of (a) k_{decay} vs. [Q] and (b) $(\Delta A_0)_0$ / $(\Delta A_{res})_Q$ vs. [Q] for $GePh_2$ in deoxygenated hexanes containing varying concentrations of CHO (●) and PrS (○) at 25 °C; the solid lines are the least squares analysis of the data to eq. 3 (a) or 4 (b). Absorbance-time profiles were recorded at 500 nm and corrected for the underlying contributions due to the formation of Ge_2Ph_4 by scaled subtraction of absorbance-time profiles recorded at 440nm, following the published procedure. S3

Figure S2. (a) Transient absorption spectra recorded 0.00-0.32 μs (○), 5.76-6.40 μs (□) and 69.60-70.24 μs (•) after the laser pulse, by laser flash photolysis of a deoxygenated hexanes solution of **2** containing 10 mM CHO. (b) Transient absorption spectra recorded 0.32-0.96 μs (○), 9.12-9.92 μs (□) and 69.92-70.72 μs (•) after the laser pulse, by laser flash photolysis of a deoxygenated hexanes solution of **2** containing 5.0 mM PrS. The insets show transient decay traces recorded at 280 nm, 350 nm and 440 nm. S4

Figure S3. (a) Plots of (a) k_{decay} vs. [Et_2S] for $GeMe_2$ (○) and $GePh_2$ (□) in deoxygenated hexanes at 25 °; the solid lines are the least squares analysis of the data to eq. 3. (b) Transient absorption spectra recorded 0.32-0.64 μs (○), 4.48-5.12 μs (□), and 101.4-103.0 μs (Δ) after the laser pulse, by laser photolysis of **1a** in deoxygenated hexanes containing 5 mM Et_2S; (c) Transient absorption spectra recorded 0.16-0.48 μs (○), 9.12-9.76 μs (□), and 69.9-70.7 μs (Δ) after the laser pulse, by laser photolysis of **2** in deoxygenated hexanes containing 4.5 mM Et_2S. The insets in (b) and (c) show transient absorbance-time profiles recorded at selected wavelengths throughout the range studied. S5

Figure S4. 500 MHz ^{1}H NMR spectra of a deoxygenated C_6D_{12} solution containing **1b** (0.040 M), CHO (0.180 M) and Si_2Me_6 (0.01 M), (a) after 15 min photolysis and b) before photolysis with 254 nm light. S6

Figure S5. Concentration vs. time plots for 254 nm irradiation of a deoxygenated solution of **1b** (0.040 M) in C_6D_{12} containing CHO (0.180 M) and Si_2Me_6 (0.01 M). The solid lines are the least squares fits of the data, the slopes of which are (in mM min^{-1}) CHO (○), -0.293 ± 0.021; **3** (□), 0. 331 ± 0. 003. The concentration of **1b** could not be quantified accurately because of spectral interferences. S7

Figure S6. 500 MHz ^{1}H NMR spectra of a deoxygenated C_6D_{12} solution containing **1a** (0.040 M), PrS (0.165 M) and Si_2Me_6 (0.01 M), (a) after 15 min photolysis and b) before photolysis with 254 nm light. * - unreactive impurity S7

Figure S7. Concentration vs. time plots for 254 nm irradiation of a deoxygenated solution of **1b** (0.045 M) in C_6D_{12} containing PrS (0.165 M) and Si_2Me_6 (0.01 M). The solid lines are the least squares fits of the data, the slopes of which are (in mM min^{-1}) S8

PrS (●), -0.63 ± 0.09; **3** (□), 0.340 ± 0.005; propene (**4**, ○), 0.103 ± 0.003. The concentration of **1b** could not be determined accurately because of spectral interferences.

Figure S8. 600 MHz ^{1}H NMR spectra of a deoxygenated solution of **1a** (0.047 M) in C_6D_{12} containing PrS (0.07 M) and Si_2Me_6 (0.012 M), a) after 15 min of photolysis and b) before photolysis. S8

Figure S9. Concentration vs. time plots for 254 nm irradiation of a deoxygenated solution of **1a** (0.047 M) in C_6D_{12} containing PrS (0.07 M) and Si_2Me_6 (0.012 M). The solid lines are the least squares fits of the data, the slopes of which are (in mM min^{-1}) PrS (●), -0.42 ± 0.39; **1a** (■), -0.58 ± 0.09; **5** (□), 0.39 ± 0.01; propene (**4**, ○), 0.108 ± 0.012. S9

Figure S10. -0.2 – 1.2 ppm region of the 600MHz ^{1}H NMR spectra of the solution of Fig. S8, (a) before photolysis, (b) after 15 min photolysis, and (c) after 15 min photolysis and spiked with $(Me_2GeS)_3$ (**6**). * - unreactive impurity. S9

Figure S11. Mass spectra of the product mixture of Fig. S8, elution times from the GC are indicated above each spectrum. S11

Figure S12. 500 MHz ^{1}H NMR spectra of a deoxygenated C_6D_{12} solution containing **2** (0.065 M), CHO (0.085 M) and Si_2Me_6 (0.005 M), (a) after 35 min photolysis and b) before photolysis with 254 nm light. * - impurity S12

Figure S13. Concentration vs. time plots for 254 nm irradiation of a deoxygenated solution of **2** (0.065 M) in C_6D_{12} containing CHO (0.085 M) and Si_2Me_6 (0.005 M). The solid lines are the least squares fits of the initial 5 points, the slopes of which are **2** (●), 0.61 ± 0.07, DMB (o), 0.34 ± 0.03 mM min^{-1}. The concentration of **2** could not be determined accurately because of spectral interferences. S12

Figure S14. 500 MHz ^{1}H NMR spectra of a deoxygenated C_6D_{12} solution containing **2** (0.058 M), PrS (0.08 M) and Si_2Me_6 (0.005 M), (a) after 36 min photolysis and b) before photolysis with 254 nm light. * - impurity S13

Figure S15. Concentration vs. time plots for 254 nm irradiation of a deoxygenated solution of **2** (0.058 M) in C_6D_{12} containing PrS (0.08 M) and Si_2Me_6 (0.005 M). The solid lines are the least squares fits of the initial 4 points, the slopes of which are PrS (■), -0.6 ± 0.2; **2** (o), 0.47 ± 0.06, DMB (□), 0.39 ± 0.01, propene (●), 0.15 ± 0.01 mM min^{-1}. The concentration of **2** could not be determined accurately because of spectral interferences. S13

Computational Studies S14

Dimethylgermylene RB3LYP/6-311+G(d,p) output S14

Oxirane RB3LYP/6-311+G(d,p) output S14

Thiirane RB3LYP/6-311+G(d,p) output S15

Dimethylgermylene-oxirane anti complex B3LYP/6-311+G(d,p) output S15

Dimethylgermylene-oxirane transition state UB3LYP/6-311+G(d,p) output S16

Dimethylgermylene-oxirane biradical UB3LYP/6-311+G(d,p) output S16
Dimethylgermanone B3LYP/6-311+G(d,p) output S17
1,1-Dimethyl-germa-2-oxetane B3LYP/6-311+G(d,p) output S17
Ethylene B3LYP/6-311+G(d,p) output S18
Dimethylgermylene-thiirane anti complex B3LYP/6-311+G(d,p) output S18
Dimethylgermylene-thiirane transition state UB3LYP/6-311+G(d,p) output S19
Dimethylgermanethione B3LYP/6-311+G(d,p) output S19

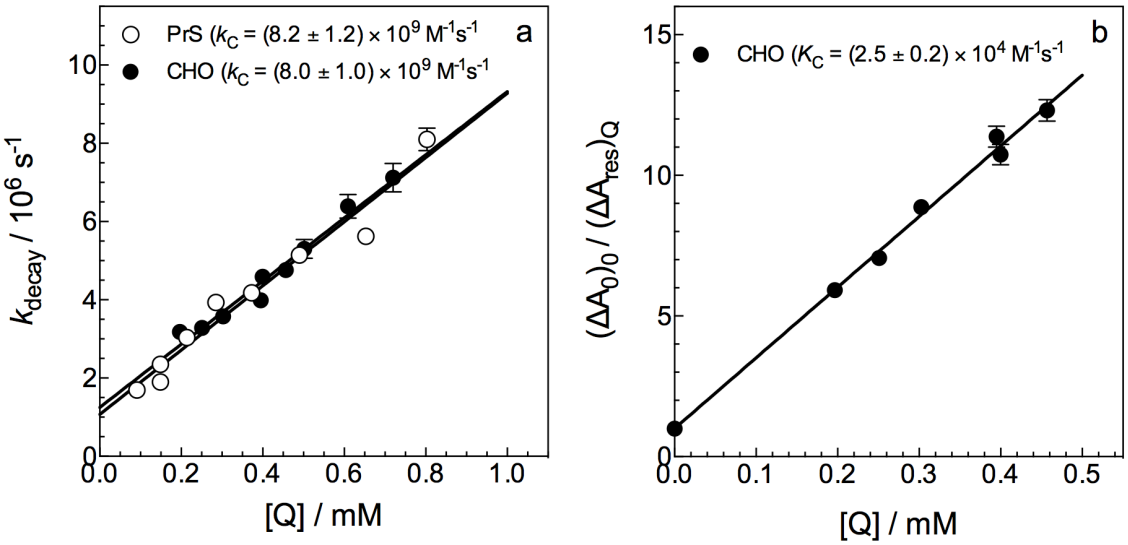


Figure S1. Plots of (a) k_{decay} vs. [Q] and (b) $(\Delta A_0)_0$ / $(\Delta A_{res})_Q$ vs. [Q] for $GePh_2$ in deoxygenated hexanes containing varying concentrations of CHO (●) and PrS (○) at 25 °C; the solid lines are the least squares analysis of the data to eq. 3 (a) or 4 (b). Absorbance-time profiles were recorded at 500 nm and corrected for the underlying contributions due to the formation of Ge_2Ph_4 by scaled subtraction of absorbance-time profiles recorded at 440nm, following the published procedure.

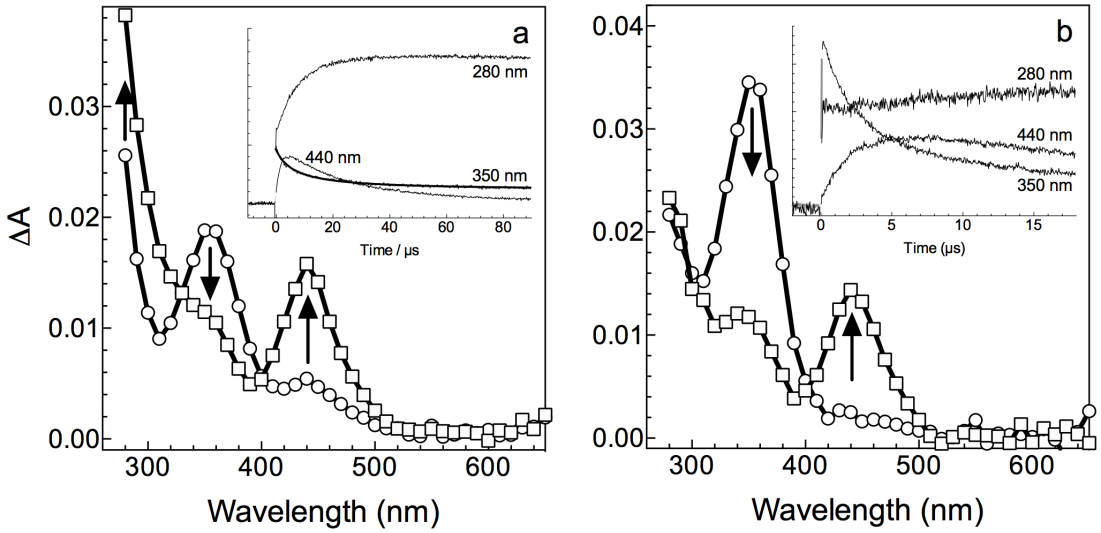


Figure S2. (a) Transient absorption spectra recorded 0.00-0.32 μs (○) and 5.76-6.40 μs (□) after the laser pulse, by laser photolysis of **2** in deoxygenated hexanes containing 0.01 M CHO; (b) Transient absorption spectra recorded 0.16-0.22 μs (○) and 6.88-7.01 μs (□) after the laser pulse, by laser photolysis of **2** in deoxygenated hexanes containing 0.005 M PrS. The insets show transient decay traces recorded at 280 nm, 350 nm and 440 nm.

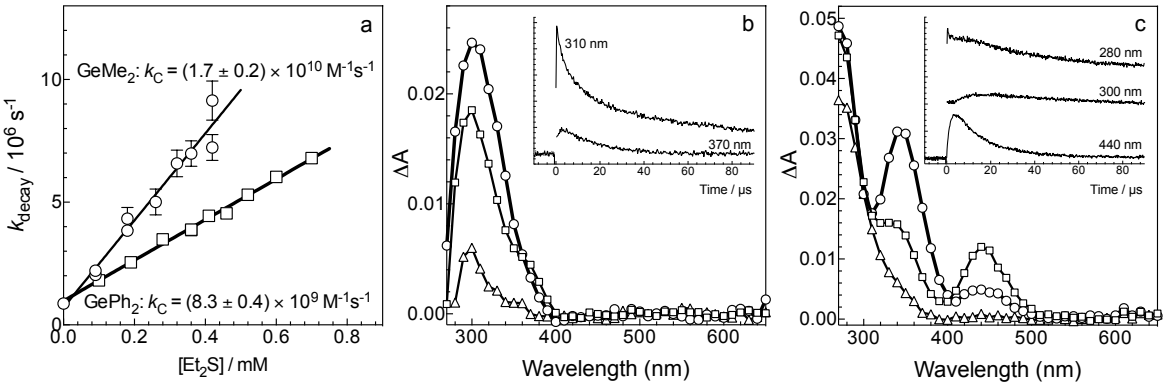


Figure S3. (a) Plots of (a) k_{decay} vs. [Et_2S] for $GeMe_2$ (○) and $GePh_2$ (□) in deoxygenated hexanes at 25 °; the solid lines are the least squares analysis of the data to eq. 3. (b) Transient absorption spectra recorded 0.32-0.64 μs (○), 4.48-5.12 μs (□), and 101.4-103.0 μs (Δ) after the laser pulse, by laser photolysis of **1a** in deoxygenated hexanes containing 5 mM Et_2S; (c) Transient absorption spectra recorded 0.16-0.48 μs (○), 9.12-9.76 μs (□), and 69.9-70.7 μs (Δ) after the laser pulse, by laser photolysis of **2** in deoxygenated hexanes containing 4.5 mM Et_2S. The insets in (b) and (c) show transient absorbance-time profiles recorded at selected wavelengths throughout the range studied.

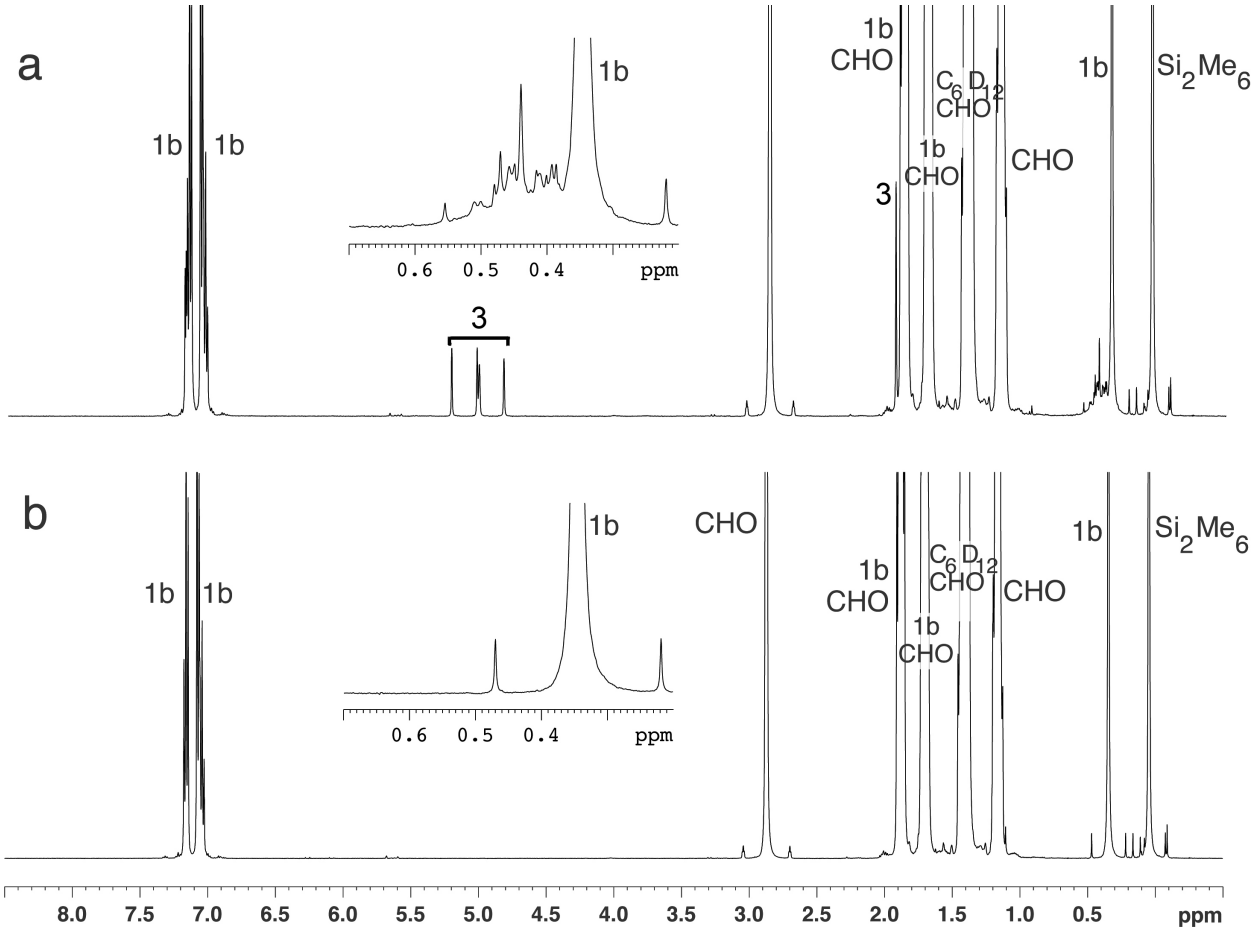


Figure S4. 500 MHz ^{1}H NMR spectra of a deoxygenated C_6D_{12} solution containing **1b** (0.040 M), CHO (0.180 M) and Si_2Me_6 (0.01 M), (a) after 15 min photolysis and b) before photolysis with 254 nm light.

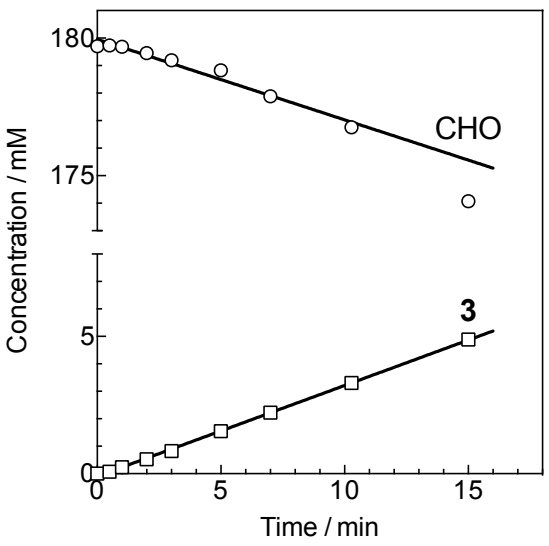


Figure S5. Concentration vs. time plots for 254 nm irradiation of a deoxygenated solution of **1b** (0.040 M) in C_6D_{12} containing CHO (0.180 M) and Si_2Me_6 (0.01 M). The solid lines are the least squares fits of the data, the slopes of which are (in mM min^{-1}) CHO (○), -0.293 ± 0.021; **3** (□), 0. 331 ± 0. 003. The concentration of **1b** could not be quantified accurately because of spectral interferences.

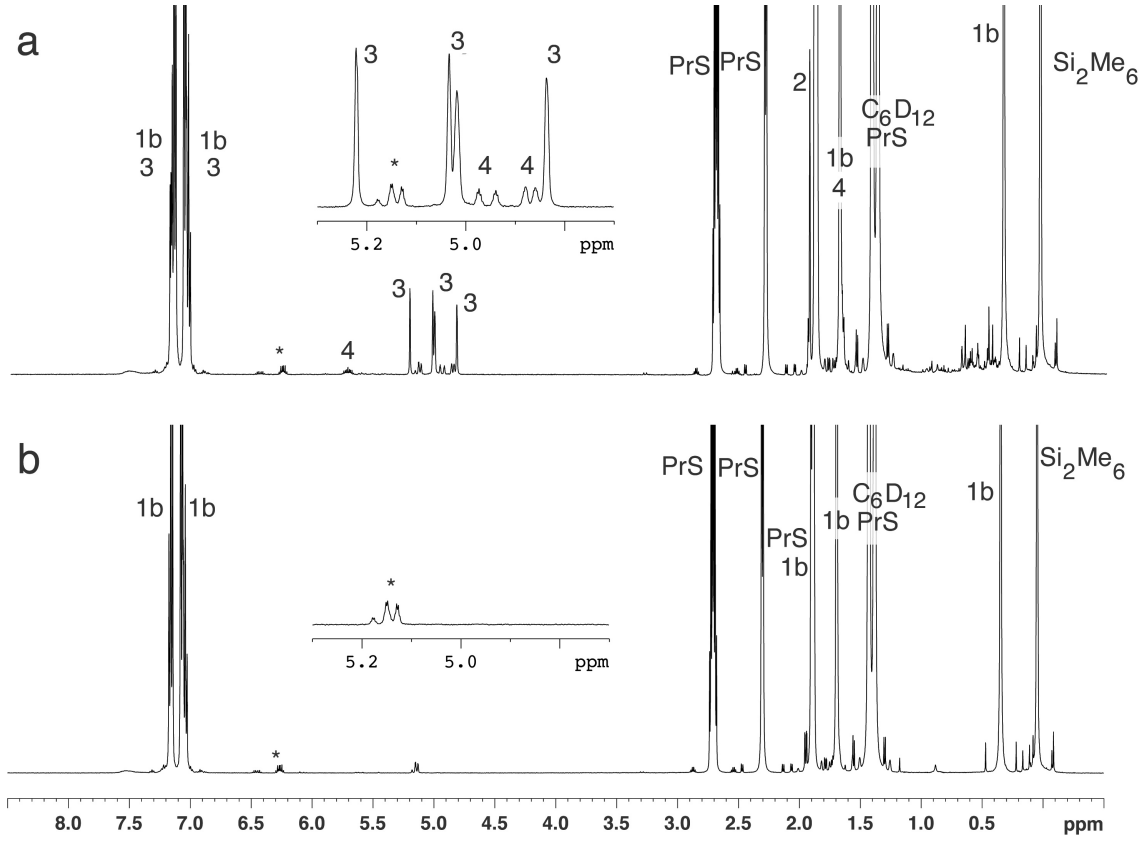


Figure S6. 500 MHz ^{1}H NMR spectra of a deoxygenated C_6D_{12} solution containing **1b** (0.045 M), PrS (0.165 M) and Si_2Me_6 (0.01 M), (a) after 15 min photolysis and b) before photolysis with 254 nm light. * - unreactive impurity

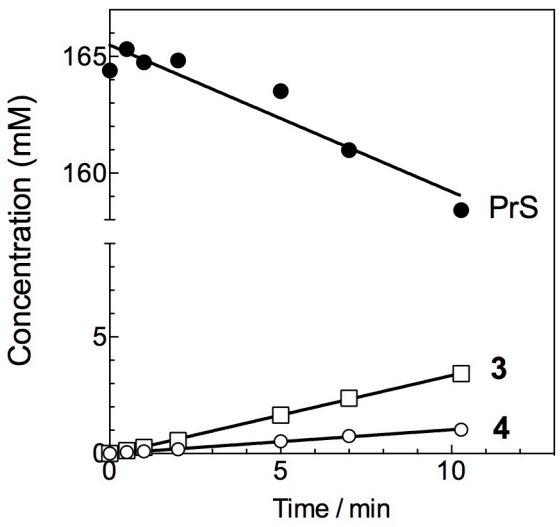


Figure S7. Concentration vs. time plots for 254 nm irradiation of a deoxygenated solution of **1b** (0.045 M) in C_6D_{12} containing PrS (0.165 M) and Si_2Me_6 (0.01 M). The solid lines are the least squares fits of the data, the slopes of which are (in mM min^{-1}) PrS (●), -0.63 ± 0.09; **3** (□), 0.340 ± 0.005; propene (**4**, ○), 0.103 ± 0.003. The concentration of **1b** could not be determined accurately because of spectral interferences.

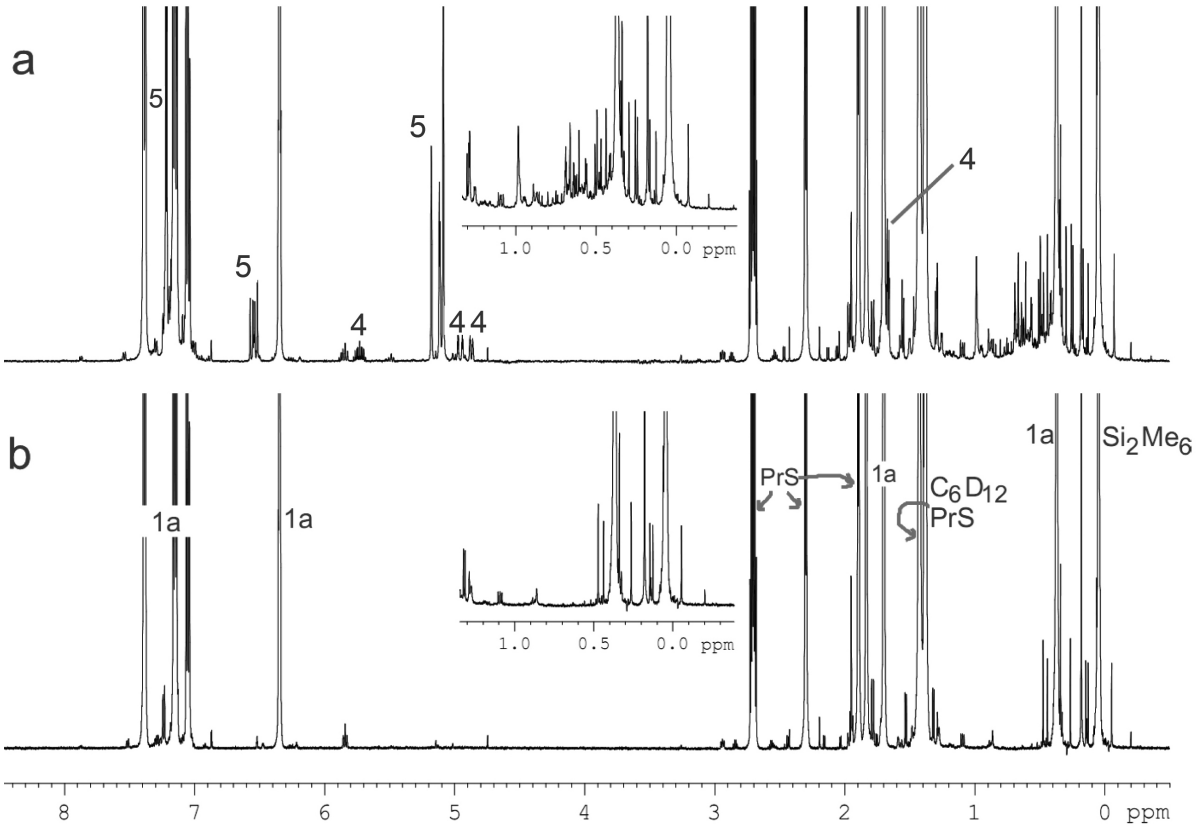
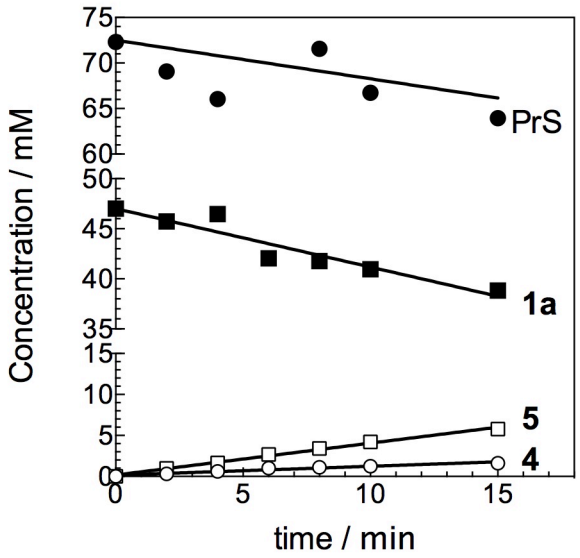


Figure S8. 600 MHz ^{1}H NMR spectra of a deoxygenated solution of **1a** (0.047 M) in C_6D_{12} containing PrS (0.07 M) and Si_2Me_6 (0.012 M), a) after 15 min of photolysis and b) before photolysis.



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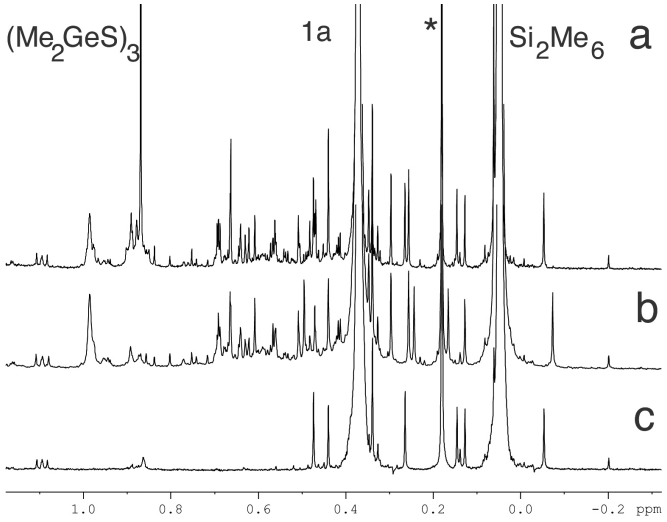
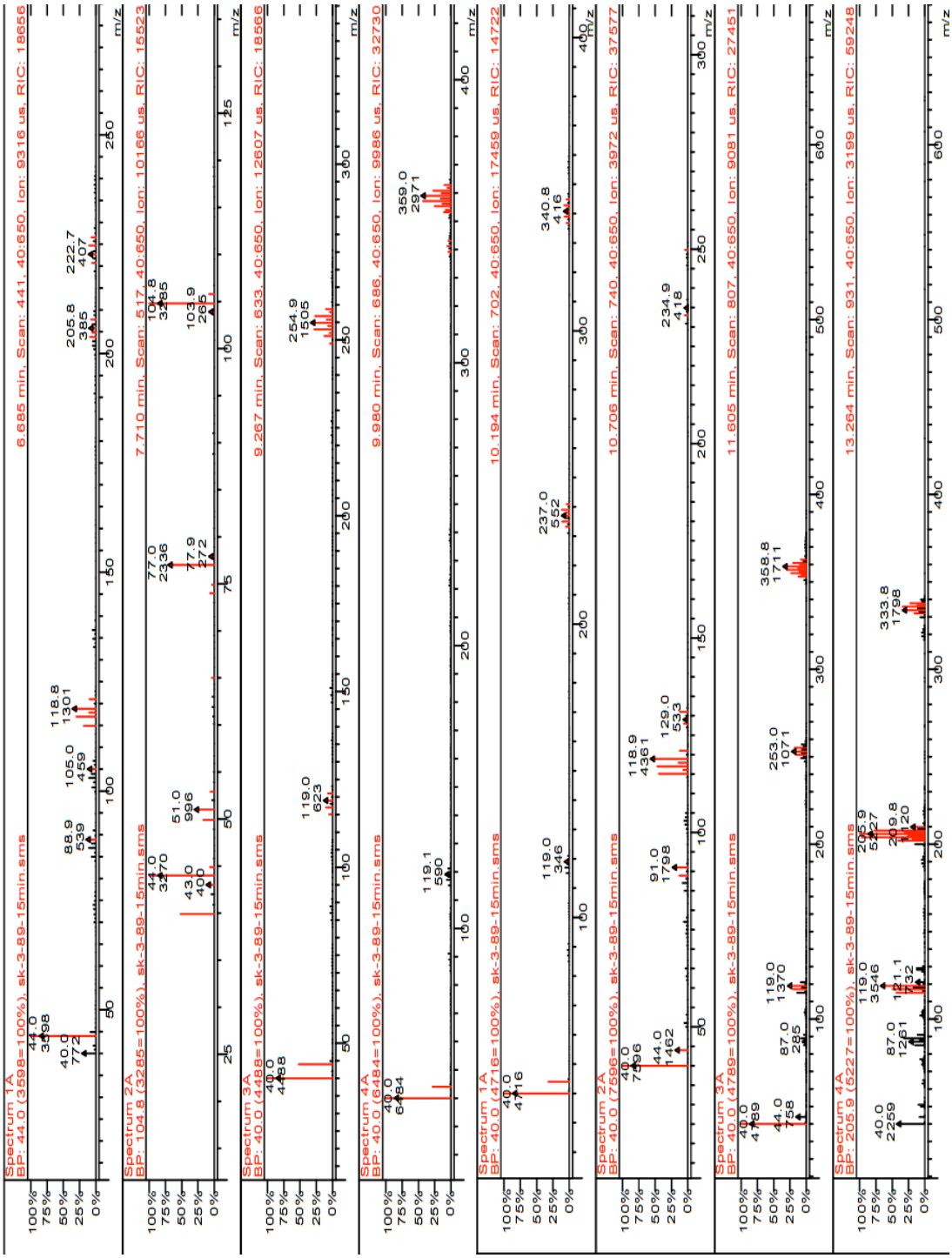


Figure S10. -0.2 – 1.2 ppm region of the 600MHz ^{1}H NMR spectra of the solution of Fig. S8, (a) before photolysis, (b) after 15 min photolysis, and (c) after 15 min photolysis and spiked with $(Me_2GeS)_3$ (**6**). * - unreactive impurity.



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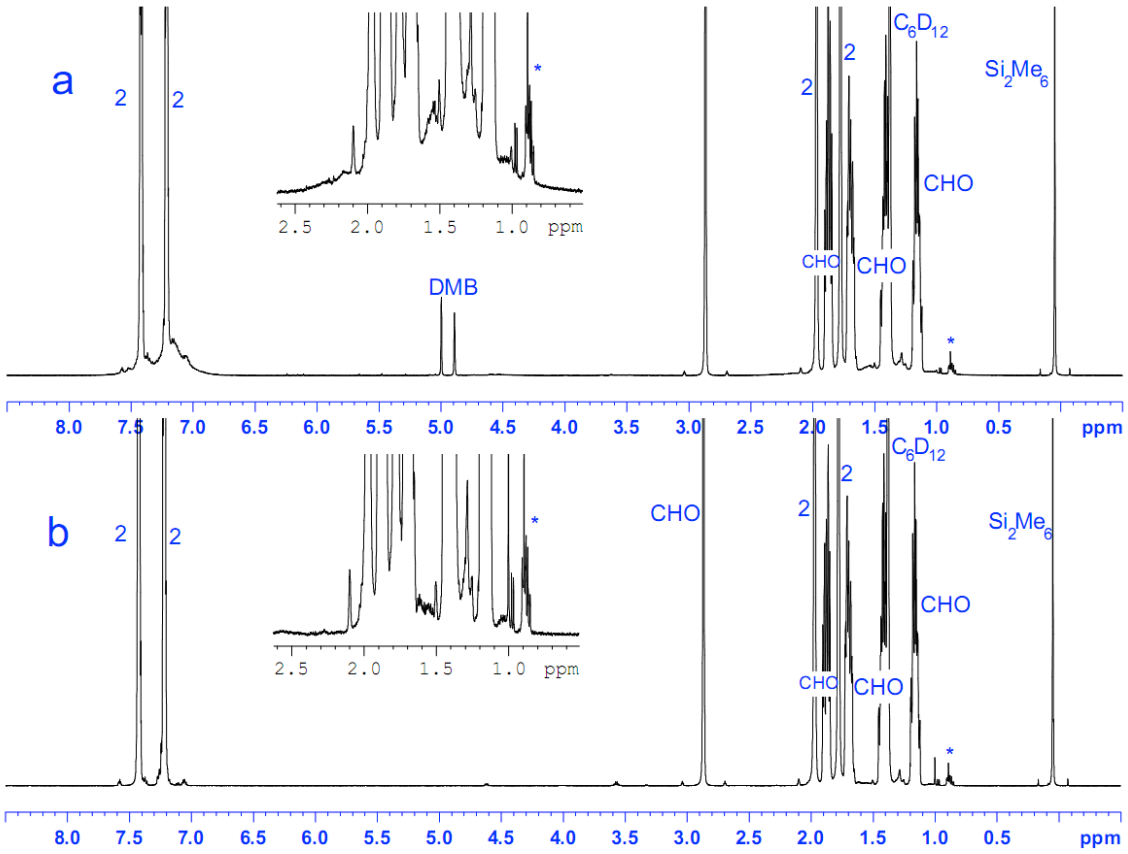

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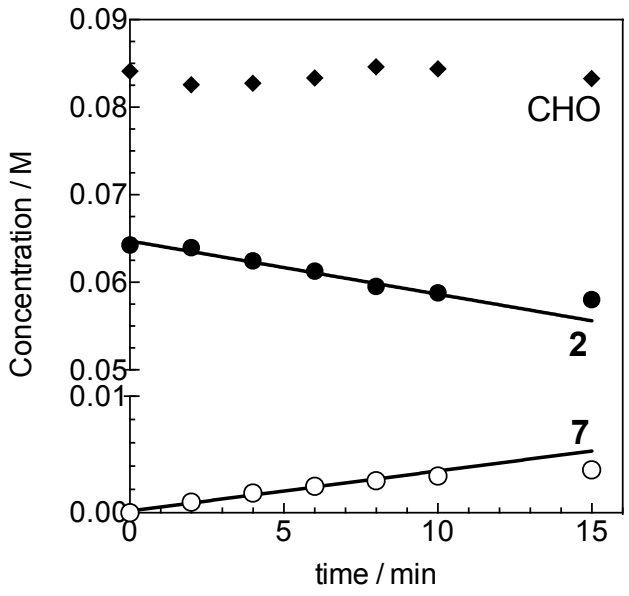
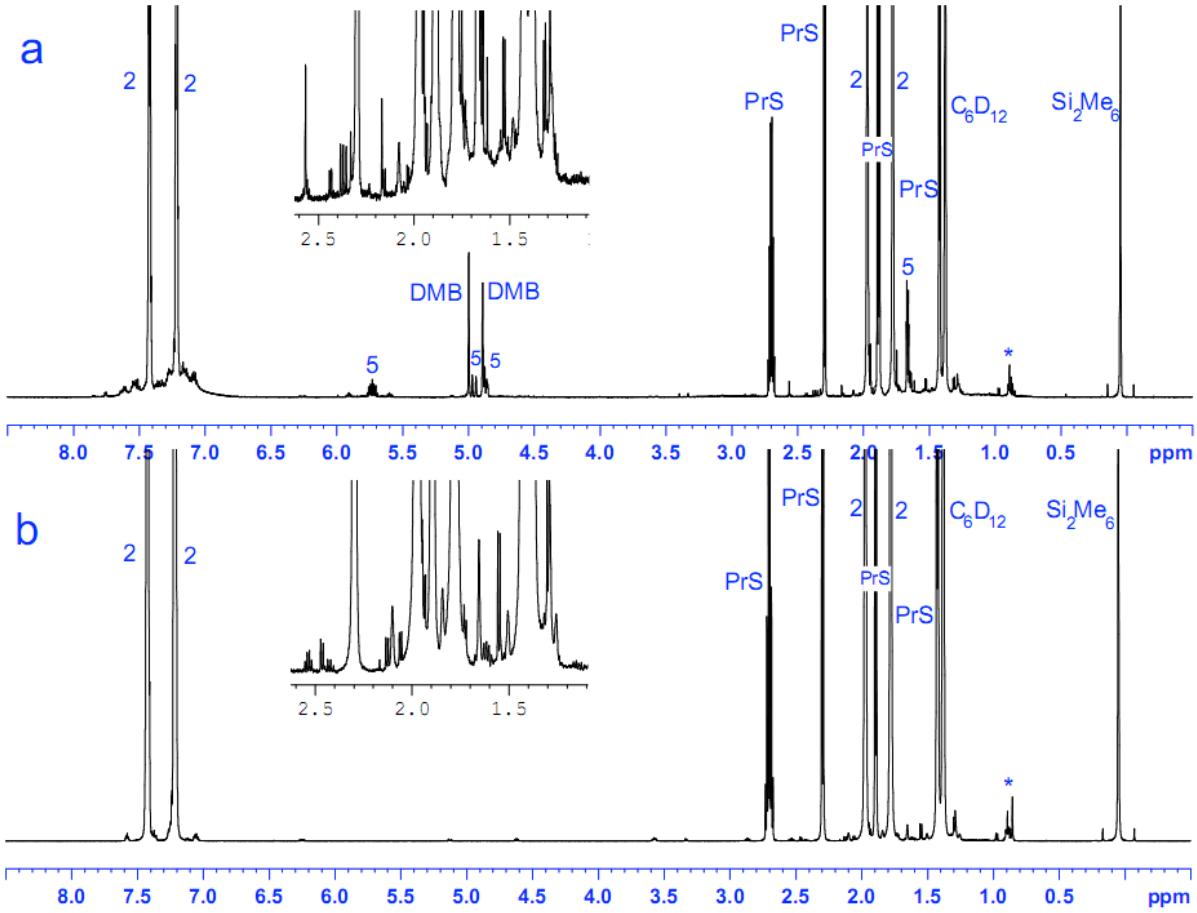


Figure S13. Concentration vs. time plots for 254 nm irradiation of a deoxygenated solution of **2** (0.065 M) in C_6D_{12} containing CHO (0.085 M) and Si_2Me_6 (0.005 M). The solid lines are the least squares fits of the initial 5 points, the slopes of which are **2** (●), 0.61 ± 0.07, DMB (o), 0.34 ± 0.03 mM min^{-1}. The concentration of **2** could not be determined accurately because of spectral interferences.



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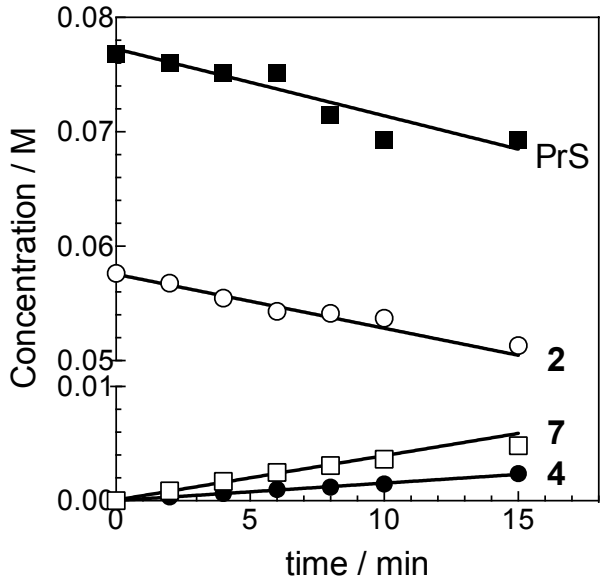

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Calculated structures and energies

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

Zero-point correction= 0.069978 (Hartree/Particle)
Thermal correction to Energy= 0.075885
Thermal correction to Enthalpy= 0.076829
Thermal correction to Gibbs Free Energy= 0.040332
Sum of electronic and zero-point Energies= -2156.764460
Sum of electronic and thermal Energies= -2156.758553
Sum of electronic and thermal Enthalpies= -2156.757608
Sum of electronic and thermal Free Energies= -2156.794105

Ge	-0.00000400	-0.51867200	0.00000000
C	-1.49619700	0.83219900	-0.00727700
H	-1.30130000	1.65872900	-0.69849800
H	-2.46474500	0.38347200	-0.23495000
H	-1.55005600	1.26340900	1.00217900
C	1.49622100	0.83217800	0.00727900
H	1.30143200	1.65864600	0.69861700
H	2.46480600	0.38344300	0.23476100
H	1.54984200	1.26354300	-1.00212100

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

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

Zero-point correction= 0.129660 (Hartree/Particle)
Thermal correction to Energy= 0.139871
Thermal correction to Enthalpy= 0.140815
Thermal correction to Gibbs Free Energy= 0.092578
Sum of electronic and zero-point Energies= -2310.555637
Sum of electronic and thermal Energies= -2310.545426
Sum of electronic and thermal Enthalpies= -2310.544482
Sum of electronic and thermal Free Energies= -2310.592718

C	-1.38091900	-1.51398900	0.65492400
C	-1.38034600	1.51443900	0.65447000
H	-0.97703300	-2.47980600	0.34060700
H	-1.14299200	-1.34577900	1.70904000
H	-2.47295600	-1.56735900	0.56067300
H	-0.97672900	2.48013500	0.33943300
H	-2.47244100	1.56765300	0.56070900
H	-1.14195600	1.34687100	1.70858600
C	2.40305400	0.73244000	-0.02050300
C	2.40308500	-0.73248100	-0.02104000
O	1.30383300	-0.00026300	0.57270800
H	3.00172700	1.27604300	0.70173600
H	2.14118800	1.25830200	-0.93326500
H	3.00177200	-1.27657800	0.70081400
H	2.14118300	-1.25765600	-0.93418800
Ge	-0.74380200	-0.00006800	-0.52946600

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

Zero-point correction= 0.127339 (Hartree/Particle)
Thermal correction to Energy= 0.137144
Thermal correction to Enthalpy= 0.138088
Thermal correction to Gibbs Free Energy= 0.091758
Sum of electronic and zero-point Energies= -2310.531368
Sum of electronic and thermal Energies= -2310.521563
Sum of electronic and thermal Enthalpies= -2310.520619
Sum of electronic and thermal Free Energies= -2310.566949

C	-1.59318300	-1.37195500	-0.68222300
H	-1.50277900	-2.35057900	-0.20775100
H	-1.09230900	-1.39621400	-1.65549300
H	-2.65502200	-1.16142300	-0.84274600
C	-0.81094900	1.63270500	-0.79810000
H	-0.26564700	2.49414300	-0.40655200
H	-1.85058800	1.93816700	-0.95253700
H	-0.39482000	1.34851400	-1.77090700
O	1.08261700	-0.52556200	0.36676600
C	2.23489500	0.31638700	0.42876300
C	2.55167400	-0.37166300	-0.81832700
H	2.00595000	1.38090700	0.35931100
H	2.85745900	0.09347600	1.29536100
H	2.17388600	0.00824900	-1.75636100
H	3.06224000	-1.32327400	-0.80252700
Ge	-0.79043500	0.06061500	0.46954400

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

Zero-point correction= 0.127038 (Hartree/Particle)
Thermal correction to Energy= 0.137740
Thermal correction to Enthalpy= 0.138684
Thermal correction to Gibbs Free Energy= 0.089667
Sum of electronic and zero-point Energies= -2310.549134
Sum of electronic and thermal Energies= -2310.538432
Sum of electronic and thermal Enthalpies= -2310.537488
Sum of electronic and thermal Free Energies= -2310.586506

C	0.74456300	1.85936200	0.38979700
H	-0.00339900	2.48164200	-0.10265400
H	0.52567200	1.80640800	1.46044800
H	1.72714000	2.31364900	0.24645300
C	1.92672100	-1.17962600	0.71016200
H	1.85712900	-2.20258300	0.33989000
H	2.96403300	-0.84440300	0.65076700

H	1.59454500	-1.15274700	1.75174200
O	-0.88759500	-0.73748600	-0.10109600
C	-2.11913700	-0.10703800	-0.49375600
C	-3.01009400	-0.04045900	0.69118400
H	-2.56791400	-0.70369300	-1.29402300
H	-1.92768800	0.89799700	-0.89883600
H	-3.80775200	-0.75798400	0.83740500
H	-2.74760500	0.60582400	1.52065800
Ge	0.75732100	0.00819800	-0.35898100

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

Zero-point correction= 0.074829 (Hartree/Particle)
Thermal correction to Energy= 0.081814
Thermal correction to Enthalpy= 0.082758
Thermal correction to Gibbs Free Energy= 0.042939
Sum of electronic and zero-point Energies= -2232.022395
Sum of electronic and thermal Energies= -2232.015411
Sum of electronic and thermal Enthalpies= -2232.014466
Sum of electronic and thermal Free Energies= -2232.054285

O	0.00000000	1.77804100	-0.00007000
C	-1.64900100	-0.94230800	0.00005700
H	-1.67688100	-1.58216500	0.88551800
H	-2.50970900	-0.27489500	-0.00047800
H	-1.67643600	-1.58307700	-0.88475500
C	1.64900100	-0.94230800	0.00005600
H	1.67688500	-1.58216000	0.88552000
H	1.67643300	-1.58308100	-0.88475200
H	2.50970900	-0.27489400	-0.00048600
Ge	0.00000000	0.12386400	-0.00002100

1,1-Dimethylgerma-2-oxetane B3LYP/6-311+G(d,p) output

Zero-point correction= 0.131248 (Hartree/Particle)
Thermal correction to Energy= 0.140339
Thermal correction to Enthalpy= 0.141283
Thermal correction to Gibbs Free Energy= 0.096933
Sum of electronic and zero-point Energies= -2310.627846
Sum of electronic and thermal Energies= -2310.618754
Sum of electronic and thermal Enthalpies= -2310.617810
Sum of electronic and thermal Free Energies= -2310.662161

C	1.42205800	-1.62443200	-0.02544900
H	0.78901100	-2.51207100	0.00963400
H	1.98918500	-1.63489400	-0.95932300

H	2.12845400	-1.65647700	0.80804900
C	1.42127600	1.62494000	-0.02662200
H	0.78726000	2.51212700	0.00189600
H	2.12314800	1.66073300	0.81055900
H	1.99343100	1.63246400	-0.95743600
O	-1.02006900	-0.00121300	-1.20613100
C	-2.08802200	-0.00019400	-0.22539900
C	-1.34569700	0.00064700	1.13779800
H	-2.71594700	-0.88737700	-0.36225500
H	-2.71549400	0.88711200	-0.36354700
H	-1.51467500	-0.88813300	1.74651100
H	-1.51466700	0.89013300	1.74548100
Ge	0.32353600	0.00001000	0.06273500

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	-0.66441900	0.00000000
C	0.00000000	0.66441900	0.00000000
H	0.92273800	-1.23519800	0.00000000
H	-0.92273800	-1.23519800	0.00000000
H	-0.92273800	1.23519800	0.00000000
H	0.92273800	1.23519800	0.00000000

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

Zero-point correction= 0.127485 (Hartree/Particle)
Thermal correction to Energy= 0.137812
Thermal correction to Enthalpy= 0.138756
Thermal correction to Gibbs Free Energy= 0.090475
Sum of electronic and zero-point Energies= -2633.558632
Sum of electronic and thermal Energies= -2633.548305
Sum of electronic and thermal Enthalpies= -2633.547361
Sum of electronic and thermal Free Energies= -2633.595642

C	1.71079900	1.52535000	0.53363800
C	1.71082200	-1.52533800	0.53363600
H	1.22262100	2.47912200	0.31687300

H	1.70506300	1.35394900	1.61375100
H	2.75725200	1.61425100	0.21718400
H	1.22265900	-2.47911700	0.31687000
H	2.75727700	-1.61422200	0.21718200
H	1.70508400	-1.35393700	1.61375000
C	-2.45802800	-0.73683100	-0.38477200
C	-2.45802400	0.73683900	-0.38475500
H	-3.29764900	-1.26124500	0.05447200
H	-1.94139300	-1.24543800	-1.19061800
H	-3.29764200	1.26124800	0.05450100
H	-1.94138700	1.24546200	-1.19059000
S	-1.31212000	-0.00001300	0.86080200
Ge	0.90839500	0.00000000	-0.54945900

Dimethylgermylene-thiirane transition state RB3LYP/6-311+G(d,p) output

Zero-point correction= 0.125536 (Hartree/Particle)
Thermal correction to Energy= 0.136012
Thermal correction to Enthalpy= 0.136956
Thermal correction to Gibbs Free Energy= 0.087871
Sum of electronic and zero-point Energies= -2633.541799
Sum of electronic and thermal Energies= -2633.531323
Sum of electronic and thermal Enthalpies= -2633.530379
Sum of electronic and thermal Free Energies= -2633.579464

C	1.40404400	1.63606700	0.72322000
C	1.57766300	-1.50258100	0.86147500
H	0.98951500	2.52105200	0.23736900
H	0.97044000	1.53064800	1.72210100
H	2.48262500	1.78024200	0.83658600
H	1.24133500	-2.46253700	0.46652600
H	2.66645800	-1.53328700	0.96386800
H	1.14481500	-1.34525200	1.85342000
C	-2.60243000	0.75160500	0.48575000
C	-2.79359500	-0.62263500	0.66702300
H	-3.25559700	1.31443300	-0.16812600
H	-2.04822100	1.32834400	1.21470200
H	-3.53031600	-1.16479400	0.09009100
H	-2.31468800	-1.15033900	1.48000200
S	-1.17007200	-0.13439200	-0.78324000
Ge	1.08939700	-0.00759300	-0.39342200

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

Zero-point correction= 0.073744 (Hartree/Particle)
Thermal correction to Energy= 0.080993
Thermal correction to Enthalpy= 0.081937
Thermal correction to Gibbs Free Energy= 0.040906

Sum of electronic and zero-point Energies= -2555.034269
Sum of electronic and thermal Energies= -2555.027020
Sum of electronic and thermal Enthalpies= -2555.026076
Sum of electronic and thermal Free Energies= -2555.067108

C	-1.27968800	1.62705700	0.00009700
H	-1.92049800	1.63789900	0.88564500
H	-0.63818100	2.50698500	-0.00038600
H	-1.92133500	1.63749400	-0.88484700
C	-1.27968800	-1.62705700	0.00009600
H	-1.92049400	-1.63790200	0.88564700
H	-1.92133900	-1.63749000	-0.88484500
H	-0.63818100	-2.50698500	-0.00039300
Ge	-0.17791600	0.00000000	-0.00000400
S	1.87560000	0.00000000	-0.00011600