

Electronic Supplementary Information

An *ab initio* and DFT study of some homolytic substitution reactions of methoxycarbonyl radicals at silicon, germanium and tin.

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Tables, S1, S2, S3, S4, Figure S1 and Gaussian Archive entries for the optimized transition structures **8** - **11** and higher-level calculated single-point energies (37 pages).

Table S1. Important calculated geometric features of the transition state **8** (X = Si) and **9** (X=Si) involved in the reaction of methoxycarbonyl radical with dimethylsilane (Scheme 3, X = Si).

Method	8			9		
	r_1	r_2	θ	r_1	r_2	θ
UHF/6-311G(d,p)	2.137 Å	2.110 Å	164.4°	2.156 Å	2.122 Å	74.4°
UHF/DZP	2.135 Å	2.113 Å	168.4°	2.119 Å	2.154 Å	87.0°
MP2/6-311G(d,p)	2.012 Å	2.085 Å	158.2°	2.007 Å	2.128 Å	76.2°
MP2/DZP	2.045 Å	2.119 Å	171.0°	1.974 Å	2.112 Å	79.4°
MP2/cc-pVDZ	2.062 Å	2.121 Å	168.4°	2.025 Å	2.135 Å	76.6°
MP2/aug-cc-pVDZ	2.043 Å	2.102 Å	160.8°	2.021 Å	2.145 Å	76.7°
BHandHLYP/6-311G(d,p)	2.061 Å	2.102 Å	165.9°	2.015 Å	2.086 Å	80.1°
BHandHLYP/6-311++G(d,p)	2.064 Å	2.113 Å	165.2	2.013 Å	2.066 Å	80.7°
BHandHLYP/DZP	2.054 Å	2.112 Å	169.5°	2.016 Å	2.092 Å	78.9°
BHandHLYP/cc-pVDZ	2.073 Å	2.119 Å	167.8°	2.022 Å	2.093 Å	80.3°
BHandHLYP/cc-pVTZ	2.061 Å	2.109 Å	165.5°	2.018 Å	2.074 Å	79.7°
BHandHLYP/aug-cc-pVDZ	2.081 Å	2.103 Å	166.3°	2.021 Å	2.078 Å	81.2°
B3LYP/6-311G(d,p)	2.047 Å	2.199 Å	168.3°	2.066 Å	2.013 Å	82.5°
B3LYP/cc-pVDZ	2.054 Å	2.214 Å	170.2°	2.079 Å	2.020 Å	82.3°
B3LYP/aug-cc-pVDZ	2.064 Å	2.182 Å	168.6°	2.002 Å	2.103 Å	82.6°
M05-2X/6-311G(d,p)	2.044 Å	2.116 Å	169.3°	2.000 Å	2.102 Å	79.3°
M05-2X/DZP	2.043 Å	2.116 Å	169.3°	1.990 Å	2.101 Å	80.0°
M05-2X/aug-cc-pVDZ	2.063 Å	2.114 Å	168.8°	2.001 Å	2.101 Å	80.5°
M06-2X/6-311G(d,p)	2.035 Å	2.135 Å	169.6°	1.997 Å	2.110 Å	79.0°
M06-2X/DZP	2.044 Å	2.134 Å	170.5°	2.000 Å	2.098 Å	79.3°
M06-2X/aug-cc-pVDZ	2.050 Å	2.132 Å	169.9°	1.999 Å	2.110 Å	80.1°

Table S2. Calculated energy barriers^a for the forward ($\Delta E_1^\ddagger$) and reverse ($\Delta E_2^\ddagger$) homolytic substitution reactions of methoxycarbonyl radical with dimethylsilane and imaginary frequencies (ν)^b of transition states **8** (X=Si) and **9** (X=Si).

Method	8					9				
	$\Delta E_1^\ddagger$	$\Delta E_1^\ddagger +$ ZPE	$\Delta E_2^\ddagger$	$\Delta E_2^\ddagger +$ ZPE	ν	$\Delta E_1^\ddagger$	$\Delta E_1^\ddagger +$ ZPE	$\Delta E_2^\ddagger$	$\Delta E_2^\ddagger +$ ZPE	ν
UHF/6-311G(d,p)	181.5	179.3	169.8	179.7	2429i	179.2	179.6	167.5	180.0	788i
UHF/DZP	179.8	177.8	166.2	176.5	2167i7	181.6	181.6	167.0	180.3	763i
MP2/6-311G(d,p)	116.1	112.6	85.1	93.7	1033i	113.0	112.1	82.0	93.2	681i
MP2/DZP	113.8	110.8	80.0	88.2	1239i	112.4	110.7	78.6	88.1	669i
MP2/cc-pVDZ	114.2	111.7	80.9	89.7	1317i	110.9	109.8	77.6	87.8	670i
MP2/aug-cc-pVDZ	96.9	93.6	75.3	82.5	1129i	92.3	91.0	70.8	80.0	671i
BHandHLYP/6-311G(d,p)	114.6	113.7	77.9	87.8	790i	113.3	111.8	87.0	96.5	422i
BHandHLYP/DZP	115.0	114.2	86.7	97.0	861i	115.9	113.0	86.7	95.9	405i
BHandHLYP/6-311++G(d,p)	111.0	109.8	83.1	92.7	894i	119.7	118.3	91.8	101.2	467i
BHandHLYP/cc-pVDZ	100.8	100.0	72.9	83.1	777i	121.5	120.3	93.5	103.5	450i
BHandHLYP/cc-pVTZ	110.4	109.2	89.2	99.0	856i	118.1	117.3	97.1	107.1	456i
BHandHLYP/aug-cc-pVDZ	100.1	99.0	78.1	86.8	796i	120.3	118.9	98.2	106.8	453i
B3LYP/6-311G(d,p)	79.2	78.6	45.6	55.7	417i	90.7	89.6	57.1	66.7	274i
B3LYP/cc-pVDZ	80.1	79.9	45.0	55.7	425i	92.3	91.5	57.2	67.4	275i
B3LYP/aug-cc-pVDZ	79.9	79.4	51.1	60.2	434i	91.7	90.8	62.9	71.8	269i
M05-2X/6-311G(d,p)	71.3	70.5	54.6	64.3	606i	71.4	69.6	54.7	63.3	324i
M05-2X/DZP	69.3	68.8	49.6	51.6	606i	70.6	69.8	50.9	55.6	306i
M05-2X/aug-cc-pVDZ	67.7	65.6	58.1	62.0	631i	67.3	64.2	57.7	64.6	324i
M06-2X/6-311G(d,p)	70.9	69.0	53.0	63.3	522i	73.5	70.8	55.7	65.2	296i
M06-2X/DZP	72.8	70.9	52.5	63.2	559i	77.8	74.7	57.5	67.0	296i
M06-2X/aug-cc-pVDZ	68.2	66.2	55.8	64.8	536i	70.8	67.9	58.3	66.9	303i
ROMP2/6-311G(d,p)//MP2/6-311G(d,p)	121.0		88.3			116.7		83.9		
ROMP2/DZP//MP2/DZP	121.9		86.4			116.4		80.8		
ROMP2/cc-pVDZ//MP2/cc-pVDZ	123.3		87.9			115.3		80.0		
ROMP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ	105.2		82.3			96.0		73.1		
ROMP2/6-311G(d,p)//BHandHLYP/6-311G(d,p)	125.9		93.0			108.7		75.9		
ROMP2/DZP//BHandHLYP/DZP	122.5		86.2			106.7		71.2		
ROMP2/cc-pVDZ//BHandHLYP/cc-pVDZ	124.6		89.4			104.8		69.5		
ROMP2/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ	106.9		83.8			84.4		61.3		
ROMP2/6-311G(d,p)//B3LYP/6-311G(d,p)	116.2		83.1			120.9		87.7		
QCISD/6-311G(d,p)//MP2/6-311G(d,p)	104.0		74.2			113.9		84.1		
QCISD/DZP//MP2/DZP	104.3		70.6			115.5		81.7		
QCISD/cc-pVDZ//MP2/cc-pVDZ	104.5		73.1			111.4		80.0		
QCISD/aug-cc-pVDZ//MP2/aug-cc-pVDZ	88.6		67.6			83.9		62.9		
QCISD/6-311G(d,p)//BHandHLYP/6-311G(d,p)	107.6		78.4			110.5		81.3		
QCISD/DZP//BHandHLYP/DZP	104.8		71.7			112.1		79.0		
QCISD/cc-pVDZ//BHandHLYP/cc-pVDZ	104.0		73.2			116.3		85.5		
QCISD/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ	89.9		68.1			88.5		65.7		
QCISD/6-311G(d,p)//B3LYP/6-311G(d,p)	102.6		73.5			122.7		92.8		
CCSD(T)/6-311G(d,p)//MP2/6-311G(d,p)	93.7		63.9			103.6		73.9		
CCSD(T)/DZP//MP2/DZP	95.6		62.9			102.8		70.1		
CCSD(T)/cc-pVDZ//MP2/cc-pVDZ	94.6		63.3			101.4		70.1		
CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ	77.0		56.8			72.7		52.5		
CCSD(T)/6-311G(d,p)//BHandHLYP/6-311G(d,p)	96.4		67.0			103.5		74.1		
CCSD(T)/DZP//BHandHLYP/DZP	93.9		61.7			103.3		71.0		
CCSD(T)/cc-pVDZ//BHandHLYP/cc-pVDZ	93.5		62.6			101.6		70.8		
CCSD(T)/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ	77.5		57.7			87.4		67.6		
CCSD(T)/6-311G(d,p)//B3LYP/6-311G(d,p)	95.1		65.3			104.1		74.3		
CCSD(T)/6-311G(d,p)//M06-2X/6-311G(d,p)	96.7		67.0			103.9		74.2		
CCSD(T)/6-311++G(d,p)//M06-2X/6-311G(d,p)	93.4		69.0			99.6		75.2		

CCSD(T)/cc-pVTZ//M06-2X/6-311G(d,p)	85.2	57.7	90.1	62.6
CCSD(T)/aug-cc-pVTZ//M06-2X/6-311G(d,p)	80.1	56.2	84.7	58.8
G3(MP2)-RAD	79.1	67.8	86.0	74.7

^a Energies in kJ mol⁻¹. ^b Frequencies in cm⁻¹.

Table S3. Important calculated geometric features of the transition states **8** (X=Ge, Sn) and **9** (X=Ge, Sn) involved in the reaction of methoxycarbonyl radical with dimethylgermane and dimethylstannane.

X	Method	8			9		
		r ₁	r ₂	θ	r ₁	r ₂	θ
Ge	UHF/6-311G(d,p)	2.268 Å	2.227 Å	170.4°	2.292 Å	2.244 Å	72.3°
	UHF/DZP	2.268 Å	2.227 Å	170.3°	2.294 Å	2.245 Å	72.2°
	MP2/6-311G(d,p)	2.154 Å	2.199 Å	173.4°	2.102 Å	2.182 Å	76.4°
	MP2/DZP	2.159 Å	2.200 Å	173.0°	2.105 Å	2.185 Å	75.4°
	MP2/cc-pVDZ	2.145 Å	2.202 Å	174.3°	2.089 Å	2.188 Å	77.0°
	MP2/aug-cc-pVDZ	2.142 Å	2.183 Å	173.2°	2.079 Å	2.176 Å	77.6°
	BHandHLYP/6-311G(d,p)	2.180 Å	2.196 Å	171.8°	2.144 Å	2.138 Å	78.4°
	BHandHLYP/6-311++G(d,p)	2.180 Å	2.173 Å	171.4°	2.139 Å	2.137 Å	78.0°
	BHandHLYP/DZP	2.183 Å	2.201 Å	171.5°	2.146 Å	2.142 Å	77.0°
	BHandHLYP/cc-pVDZ	2.180 Å	2.203 Å	172.6°	2.142 Å	2.141 Å	78.5°
	BHandHLYP/cc-pVTZ	2.175 Å	2.178 Å	171.4°	2.139 Å	2.141 Å	78.7°
	BHandHLYP/aug-cc-pVDZ	2.190 Å	2.191 Å	171.4°	2.146 Å	2.134 Å	79.0°
	B3LYP/6-311G(d,p)	2.167 Å	2.261 Å	173.1°	2.122 Å	2.145 Å	81.9°
	B3LYP/cc-pVDZ	2.164 Å	2.274 Å	174.0°	2.120 Å	2.156 Å	81.7°
	B3LYP/aug-cc-pVDZ	2.178 Å	2.250 Å	172.8°	2.128 Å	2.133 Å	82.8°
	BHandHLYP/SDB- aug-cc-pVTZ	2.190 Å	2.185 Å	171.4°	2.157 Å	2.152 Å	76.8°
	BHandHLYP/SDB- aug-cc-pVQZ	2.191 Å	2.186 Å	171.2°	2.155 Å	2.149 Å	77.0°
Sn	UHF/DZP	2.452 Å	2.395 Å	175.2°	2.481 Å	2.434 Å	68.8°
	MP2/DZP	2.342 Å	2.327 Å	172.5°	2.332 Å	2.383 Å	69.4°
	BHandHLYP/DZP	2.361 Å	2.354 Å	177.3°	2.362 Å	2.370 Å	71.3°
	BHandHLYP/SDB- aug-cc-pVTZ	2.380 Å	2.361 Å	177.3°	2.379 Å	2.374 Å	71.2°
	BHandHLYP/SDB- aug-cc-pVTZ	2.378 Å	2.358 Å	176.4°	2.377 Å	2.370 Å	71.3°

Table S4. Calculated energy barriers^a for the forward ($\Delta E_1^\ddagger$) and reverse ($\Delta E_2^\ddagger$) homolytic substitution reactions of methoxycarbonyl radical with dimethylgermane and dimethylstannane and imaginary frequencies (ν)^b of transition states **8** and **9** (X=Ge, Sn).

X	Method	8					9				
		$\Delta E_1^\ddagger$	$\Delta E_1^\ddagger + \text{ZPE}$	$\Delta E_2^\ddagger$	$\Delta E_2^\ddagger + \text{ZPE}$	ν	$\Delta E_1^\ddagger$	$\Delta E_1^\ddagger + \text{ZPE}$	$\Delta E_2^\ddagger$	$\Delta E_2^\ddagger + \text{ZPE}$	ν
Ge	UHF/6-311G(d,p)	166.8	164.2	159.7	169.7	185i	168.4	167.5	161.3	172.9	647i
	UHF/DZP	168.9	166.2	158.4	168.2	2034i	168.3	167.5	157.8	169.5	650i
	MP2/6-311G(d,p)	106.3	104.1	80.4	90.5	1138i	108.1	106.3	82.1	92.7	520i
	MP2/DZP	110.1	107.4	80.6	88.7	1218i	109.0	108.7	80.6	90.0	534i
	MP2/cc-pVDZ	102.8	101.0	75.1	84.8	1085i	106.1	104.2	78.4	88.1	523i
	BHandHLYP/6-311G(d,p)	106.7	105.6	94.7	104.3	796i	121.6	120.1	109.6	118.9	383i
	BHandHLYP/DZP	108.9	107.4	77.9	87.9	681i	120.7	120.6	99.8	108.6	354i
	BHandHLYP/6-311G++(d,p)	106.7	105.6	94.7	104.3	796i	121.6	120.1	109.6	118.9	382i
	BHandHLYP/cc-pVDZ	108.4	107.6	85.9	96.4	775i	111.5	109.7	89.0	98.4	322i
	BHandHLYP/cc-pVTZ	107.0	105.8	91.9	101.9	801i	120.6	119.2	105.5	115.2	399i
	BHandHLYP/aug-cc-pVDZ	108.0	107.1	91.1	100.1	655i	122.6	121.4	105.8	114.5	323i
	BHandHLYP/SBD-aug-cc-pVTZ	109.0	107.5	100.4	110.2	839i	122.8	121.5	114.2	123.2	424i
	BHandHLYP/SBD-aug-cc-pVQZ	105.7	104.1	99.8	109.6	840i	120.0	118.4	114.1	123.9	421i
	B3LYP/6-311G(d,p)	78.8	78.3	52.1	62.0	373	96.1	94.3	69.4	78.0	152i
	B3LYP/cc-pVDZ	76.4	76.0	47.3	57.8	364i	93.6	91.8	64.6	73.6	158i
	B3LYP/aug-cc-pVDZ	76.6	76.0	53.5	62.3	373i	93.7	91.6	70.6	77.9	137i
	ROMP2/6-311G(d,p)//MP2 ^c	116.7		89.0			110.7		83.0		
	ROMP2/DZP//MP2/DZP	120.8		89.6			111.0		81.8		
	ROMP2/6-311G(d,p)//BHandHLYP ^c	118.6		90.7			91.2		63.3		
	ROMP2/DZP//BHandHLYP/DZP	123.5		92.3			97.6		66.4		
	ROMP2/SBD-aug-cc-pVTZ ^d	108.5		89.9			80.7				
	QCISD/6-311G(d,p)//MP2/6-311G(d,p)	99.7		74.3			97.4		72.0		
	QCISD/DZP//MP2/DZP	101.2		72.4			110.6		82.0		
	QCISD/6-311G(d,p)//BHandHLYP ^c	99.2		74.3			111.1		86.2		
	QCISD/DZP//BHandHLYP/DZP	100.9		73.7			111.5		83.3		
	CCSD(T)/6-311G(d,p)//MP2 ^c	88.2		62.9			88.2		62.9		
	CCSD(T)/DZP//MP2/DZP	90.3		61.6			98.5		70.8		
	CCSD(T)/6-311G(d,p)//BHandHLYP ^c	87.3		62.2			99.0		74.0		
	CCSD(T)/DZP//BHandHLYP/DZP	89.2		60.9			99.2		70.8		
	CCSD(T)/aug-cc-pVDZ ^e	75.7		61.1			89.3		70.1		
	CCSD(T)/SBD-aug-cc-PVT ^d	73.4		57.7			85.6		69.9		
Sn	UHF/DZP	148.8	145.1	139.4	148.0	327i	129.1	128.1	119.7	131.0	581i
	MP2/DZP	98.1	95.5	70.4	79.7	511i	85.9	85.3	58.1	69.5	543i
	BHandHLYP/DZP	79.2	77.3	56.2	65.6	672i	81.6	81.0	58.6	69.4	350i
	BHandHLYP/SBD-aug-cc-pVTZ	74.2	72.5	60.7	70.2	665i	78.0	77.3	64.5	75.0	354i
	BHandHLYP/SBD-aug-cc-pVQZ	71.3	69.2	61.1	70.4	668i	74.6	73.8	64.4	74.9	352i
	ROMP2/DZP//MP2/DZP	110.2		80.6			90.4		60.9		
	ROMP2/DZP/BHandHLYP/DZP	113.7		82.5			81.9		53.2		
	ROMP2/SBD-aug-cc-pVTZ ^d	100.8		81.8			76.5		57.5		
	QCISD/DZP//MP2/DZP	85.7		58.3			82.3		54.9		
	QCISD/DZP//BHandHLYP/DZP	83.5		56.7			82.0		55.2		
	QCISD/SBD-aug-cc-pVTZ ^d	70.3		53.9			70.2		53.8		
	CCSD(T)/DZP//MP2/DZP	73.8		46.8			72.7		45.7		
	CCSD(T)/DZP//BHandHLYP/DZP	71.8		45.2			71.9		45.2		
	CCSD(T)/SBD-aug-cc-PVT ^d	66.1		40.0			68.3		42.2		

^a Energies in kJ mol⁻¹. ^b Frequencies in cm⁻¹. ^c 6-311G(d,p). ^d BHandHLYP/ SBD-aug-cc-PVTZ ^e BHandHLYP/ aug-cc-pVDZ

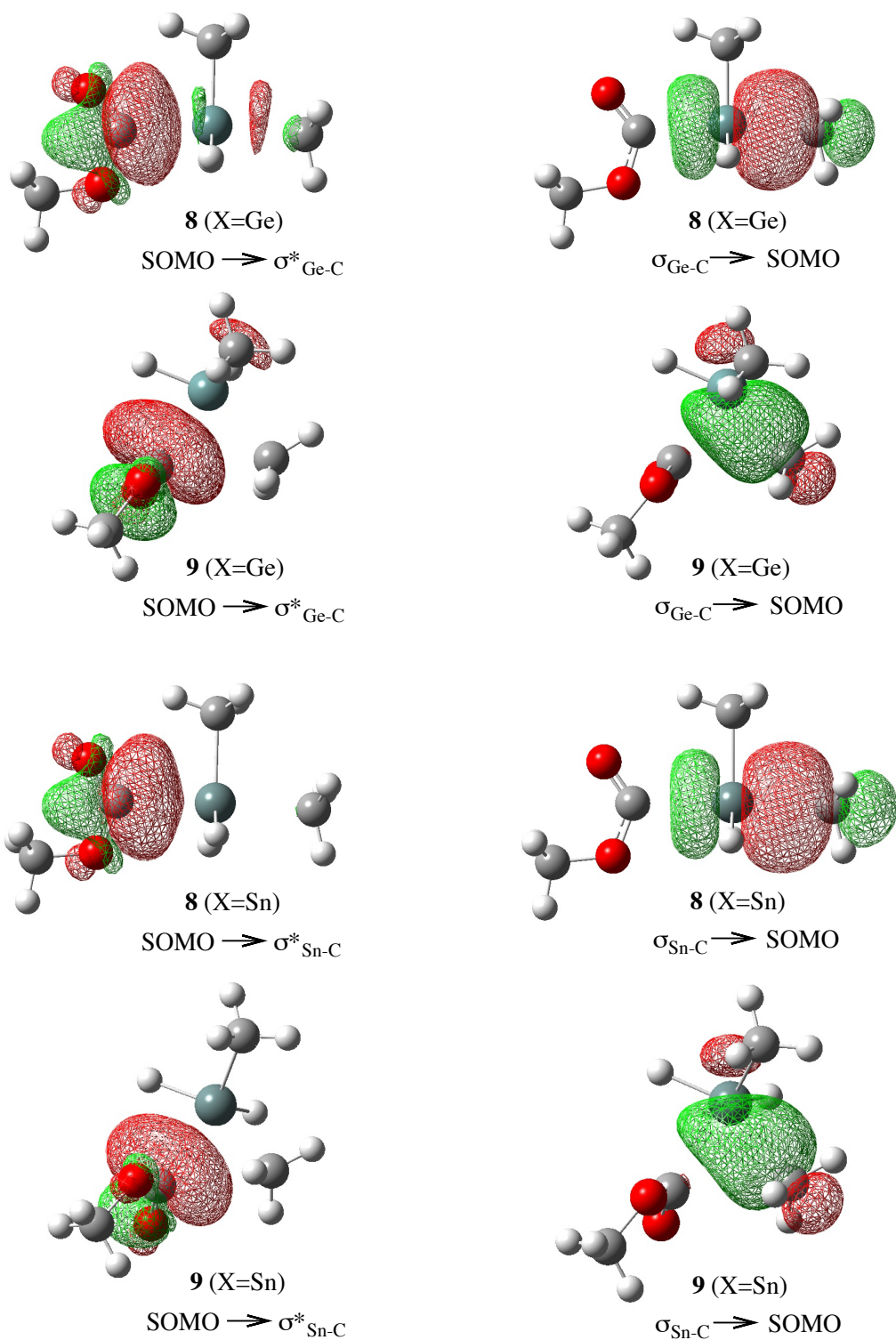


Fig. S1 Gauss View representations of key BHandHLYP/DZP generated orbitals for transition states **8** (X=Ge, Sn) and **9** (X=Ge, Sn).

Table S4. BHandHLYP calculated geometric features^a of the transition states **10** (X=Si, Ge, Sn, R=Et, *i*-Pr, *t*-Bu) and **11** (X=Si, Ge, Sn, R=Et, *i*-Pr, *t*-Bu).

X	R	Basis Set	10			11		
			r ₁	r ₂	θ	r ₁	r ₂	θ
Si	Et	6-311G(d,p)	2.098	2.075	166.2	2.048	2.067	80.5
		DZP	2.098	2.076	167.2	2.050	2.064	80.9
	<i>i</i> -Pr	6-311G(d,p)	2.126	2.086	163.9	2.093	2.061	83.9
		DZP	2.124	2.086	164.6	2.091	2.058	83.2
	<i>t</i> -Bu	6-311G(d,p)	2.150	2.092	163.7	2.094	2.090	86.1
		DZP	2.149	2.091	164.4	2.098	2.089	85.8
Ge	Et	6-311G(d,p)	2.217	2.173	171.6	2.200	2.159	76.9
		DZP	2.219	2.178	171.4	2.202	2.157	75.8
		SDB- aug-cc-pVTZ	2.240	2.183	171.6	2.218	2.200	75.0
	<i>i</i> -Pr	6-311G(d,p)	2.247	2.183	168.8	2.242	2.160	78.8
		DZP	2.248	2.186	168.7	2.240	2.161	79.3
		SDB- aug-cc-pVTZ	2.268	2.193	168.7	2.270	2.178	79.3
	<i>t</i> -Bu	6-311G(d,p)	2.271	2.193	167.9	2.264	2.195	81.9
		DZP	2.272	2.195	168.1	2.260	2.201	81.3
		SDB- aug-cc-pVTZ	2.294	2.203	168.4	2.284	2.209	81.5
Sn	Et	DZP	2.402	2.332	176.6	2.420	2.357	71.3
		SDB- aug-cc-pVTZ	2.425	2.346	176.8	2.438	2.362	71.3
	<i>i</i> -Pr	DZP	2.434	2.336	174.1	2.443	2.350	76.6
		SDB- aug-cc-pVTZ	2.458	2.346	174.0	2.454	2.360	76.4
	<i>t</i> -Bu	DZP	2.456	2.346	172.4	2.475	2.360	78.8
		SDB- aug-cc-pVTZ	2.484	2.356	172.7	2.502	2.371	78.6

^a Distances in Å and angle in degrees.

Table S6. Calculated energy barriers^a for the ($\Delta E_1^\ddagger$, $\Delta E_2^\ddagger$) for the reactions depicted in Scheme 4, and transition state frequencies (ν)^b of **10** and **11**.

X	R	10						11				
		Basis Set	$\Delta E_1^\ddagger$	$\Delta E_1^\ddagger + \text{ZPE}$	$\Delta E_2^\ddagger$	$\Delta E_2^\ddagger + \text{ZPE}$	ν	$\Delta E_1^\ddagger$	$\Delta E_1^\ddagger + \text{ZPE}$	$\Delta E_2^\ddagger$	$\Delta E_2^\ddagger + \text{ZPE}$	ν
Si	Et	6-311G(d,p)	90.8	89.5	87.5	95.2	853i	100.4	98.9	97.1	104.6	454i
Si	Et	DZP	91.0	87.7	85.8	93.7	821i	101.3	99.1	97.9	105.2	424i
Si	<i>i</i> -Pr	6-311G(d,p)	83.9	83.6	102.0	109.4	886i	93.9	93.3	111.9	119.1	449i
Si	<i>i</i> -Pr	DZP	84.2	83.9	100.9	108.3	820i	93.1	92.7	113.7	120.1	429i
Si	<i>t</i> -Bu	6-311G(d,p)	78.3	78.1	113.3	118.6	898i	97.7	97.3	132.7	137.9	486i
Si	<i>t</i> -Bu	DZP	79.5	78.9	112.5	118.0	863i	98.0	97.9	134.6	138.2	436i
Ge	Et	6-311G(d,p)	83.7	82.0	97.6	105.1	678i	104.1	102.8	106.2	113.7	412i
Ge	Et	DZP	85.8	84.3	94.7	102.4	720i	102.4	103.2	101.3	111.2	401i
Ge	Et	SDB- ^c	83.7	82.0	97.6	102.6	721i	104.1	102.8	106.2	113.8	412i
Ge	<i>i</i> -Pr	6-311G(d,p)	78.3	77.5	100.7	107.7	705i	95.9	95.6	118.3	125.7	420i
Ge	<i>i</i> -Pr	DZP	78.2	77.2	100.2	107.0	745i	96.8	92.9	113.2	120.7	424i
Ge	<i>i</i> -Pr	SDB- ^c	75.8	74.5	110.2	116.9	741i	94.2	93.4	128.7	135.7	431i
Ge	<i>t</i> -Bu	6-311G(d,p)	72.1	71.3	110.6	115.5	712i	86.9	97.4	135.5	141.6	445i
Ge	<i>t</i> -Bu	DZP	72.0	71.6	108.3	113.4	753i	84.7	95.4	130.9	137.2	453i
Ge	<i>t</i> -Bu	SDB- ^c	69.1	68.7	119.8	125.7	748i	85.3	95.6	140.0	151.7	460i
Sn	Et	DZP	65.2	63.2	68.7	75.9	727i	69.9	69.1	72.4	80.9	375i
Sn	Et	SDB- ^c	60.3	58.5	72.6	79.9	714i	66.1	65.3	78.3	86.7	389i
Sn	<i>i</i> -Pr	DZP	56.0	55.0	81.7	88.3	771i	56.4	57.4	81.1	89.8	380i
Sn	<i>i</i> -Pr	SDB- ^c										
Sn	<i>t</i> -Bu	DZP	49.9	49.1	92.6	96.9	808i	59.8	61.8	101.6	108.7	358i
Sn	<i>t</i> -Bu	SDB- ^c										

^aEnergies in kJ mol⁻¹. ^bFrequencies in cm⁻¹.

Gaussian Archive Entries for Transition States 8 – 11

Transition State 8 (X=Si)

HF/6-311G(d,p)

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET17\FTS\UHF\6-311G(d,p)\C4H11O2Si1(
2)\SONIA\31-May-2004\0\#\UHF/6-311G** OPT=(TS,READFC,NOEIGEN) FREQ=NOR
AMAN GEOM=CHECKPOINT GUESS=CHECK\ts of oxyacyl rad attacking disulfid
e\0,2\C,0.6395665591,0.0264115718,-0.8104791248\C,0.7876021221,-0.002
227298,2.2181124019\H,1.7631542274,0.028166135,1.7494272955\H,0.682720
7341,0.8657408988,2.8632082283\H,0.72922304,-0.8865627577,2.8466181187
\O,1.815272752,0.0564455144,-0.7834211959\C,-2.2312088836,-0.087823124
2,2.2645806685\H,-2.1030302417,-0.9905757687,2.8462230868\H,-3.1395875
802,-0.1059819566,1.6805045624\H,-2.1527000508,0.8065595762,2.86760430
85\C,0.5897222065,0.0520519939,-3.1485386812\O,-0.0960130354,0.0200347
569,-1.9017390222\H,-0.1788270533,0.0406823157,-3.9055122505\H,1.18457
54195,0.9518194712,-3.2279677978\H,1.2304900188,-0.8135451717,-3.24805
18614\H,-1.1155274212,1.2680396951,0.4120684508\H,-1.0429530735,-1.336
0001019,0.3826491924\Si,-0.5946934126,-0.0264759548,0.9337470589\Ver
sion=x86-Linux-G03RevB.04\State=2-A\HF=-596.5151773\S2=0.810181\S2-1=0.
\S2A=0.751898\RMSD=7.319e-09\RMSF=7.985e-06\Dipole=-0.60755,-0.0137217
,-0.2016664\PG=C01 [X(C4H11O2Si1)]\@
```

HF/DZP

```
1\1\GINC-GOMBERG06\FTS\UHF\Gen\C4H11O2Si1(2)\SHORVAT\03-Apr-2012\0\#\U
HF/gen pseudo=read opt=(ts,calcf, noeigen) freq=noraman\TS of oxyacyl
radical attacking SiMe2\0,2\C,-0.9888179902,0.2958830083,0.0000062489
\C,1.7495892083,1.5601345213,-0.0004357266\H,0.9434001591,2.282165981,
0.0012048142\H,2.3709772478,1.7249255636,0.8750359481\H,2.3675678053,1
.7253135174,-0.8782605855\O,-1.402926683,1.3966124293,-0.0003741932\C,
2.9527880315,-1.1893468874,0.0001142679\H,3.4577280195,-0.8629039768,-
0.8987647779\H,2.7690463078,-2.2536130912,0.0006203305\H,3.4581791911,
-0.8621182175,0.8984540057\C,-3.1393270906,-0.6220719465,0.0002553287\
O,-1.7265533212,-0.7940394814,0.0003428166\H,-3.5552391012,-1.61749204
82,0.0005535386\H,-3.4530100172,-0.0815846196,0.8830017445\H,-3.452966
7542,-0.0821305383,-0.8828403983\H,0.7777116461,-0.8609776046,1.292619
3742\H,0.77744193,-0.8618886159,-1.2916235045\Si,1.0881604111,-0.20402
09936,0.0002507682\Version=AM64L-G09RevC.01\State=2-A\HF=-311.3541784
\S2=0.81254\S2-1=0.\S2A=0.751994\RMSD=1.951e-09\RMSF=4.223e-06\Dipole=
0.0477487,-0.6447942,0.000736\Quadrupole=5.6895919,-4.8492154,-0.8403
765,2.6301814,-0.0011412,0.001478\PG=C01 [X(C4H11O2Si1)]\@
```

MP2/6-311G(d,p)

```
1\1\GINC-AC24\FTS\UMP2-FC\6-311G(d,p)\C4H11O2Si1(2)\SXH563\16-Jan-2008
\0\#\MP2/6-311G** opt=(ts,readfc, noeigen) freq=noraman geom=checkpoint
guess=check\TS of oxyacyl rad attacking dimethylsilane\0,2\C,-0.009
8625945,-0.0000620916,0.0056881509\C,0.0078573244,0.0000136972,2.97401
71638\H,1.0164692014,0.0002846665,2.5547150446\H,-0.1172079615,0.88227
45859,3.6083210621\H,-0.1169736588,-0.8827757954,3.6076389844\O,1.1945
819403,-0.0001267996,0.0719126178\C,-2.9579985457,0.0007689855,2.85016
16519\H,-2.8721580555,-0.9069315558,3.447339364\H,-3.8494648251,0.0008
315798,2.2259472793\H,-2.8718601776,0.908600447,3.4470956744\C,0.11275
33695,-0.000356272,-2.332435937\O,-0.7088553369,-0.0001747725,-1.1477
07383\H,-0.5867251144,-0.0004191763,-3.1660772505\H,0.744899589,0.8888
212989,-2.3578718368\H,0.7448082805,-0.8896043302,-2.3576617932\H,-1.8
069455426,1.3090771672,1.1020835357\H,-1.8076219739,-1.3082452085,1.10
21908667\Si,-1.2774142762,0.0002987861,1.5993291275\Version=IA64L-G03
RevD.01\State=2-A\HF=-596.5171794\MP2=-597.6122869\PUHF=-596.5224546\
MP2-0=-597.615839\S2=0.779824\S2-1=0.760104\S2A=0.75061\RMSD=1.070e-09
\RMSF=1.253e-06\Thermal=0.\Dipole=-0.5237376,0.0000091,-0.0973542\PG=C
01 [X(C4H11O2Si1)]\@
```

MP2/DZP

```
1\1\GINC-GOMBERG09\FTS\UMP2-FC\Gen\C4H11O2Si1(2)\SHORVAT\12-Jun-2012\0
```

```

\\#MP2/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\\TS of oxy
acyl radical attacking SiMe2\\0,2\\C,-0.9374233232,0.2832308252,0.022356
144\\C,1.7461572693,1.4945084337,-0.0703522219\\H,0.9657654508,2.2256507
141,0.150856054\\H,2.5711624904,1.6091927574,0.6365582272\\H,2.13560019,
1.687810734,-1.0744754753\\O,-1.3561109488,1.4118424125,0.0916355533\\C,
2.9002431786,-1.217910016,-0.0693001075\\H,3.3724124818,-0.8649047999,-
0.9856974895\\H,2.7206458051,-2.2910488232,-0.0790077236\\H,3.4214545758
,-0.8889619462,0.8293515791\\C,-3.1304993507,-0.5357922377,0.0105987538
\\O,-1.7162852121,-0.8162672228,-0.0319439491\\H,-3.6164786832,-1.507541
733,-0.0390859496\\H,-3.3886499567,-0.0201170412,0.9370813442\\H,-3.4206
108534,0.0866035684,-0.8375013366\\H,0.8388414688,-0.9039167924,1.31849
18948\\H,0.7636142839,-0.9845151543,-1.2693859313\\Si,1.0326411336,-0.24
74136788,-0.001837366\\Version=AM64L-G09RevC.01\\State=2-A\\HF=-311.3564
003\\MP2=-312.4493475\\PUHF=-311.3618061\\PMP2-0=-312.4530101\\S2=0.781129
\\S2-1=0.760803\\S2A=0.750651\\RMSD=7.398e-09\\RMSF=1.612e-06\\Dipole=0.129
6976,-0.5146236,-0.0492338\\PG=C01 [X(C4H11O2Si1)]\\@

```

MP2/cc-pVDZ

```

1\\1\\GINC-AC25\\FTS\\UMP2-FC\\CC-pVDZ\\C4H11O2Si1(2)\\SXH563\\17-Jan-2008\\0\\
#MP2/cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint gues
s=check\\TS of oxyacyl rad attacking dimethylsilane\\0,2\\C,-0.00465762
19,-0.0000167708,-0.0088785869\\C,-0.0051675272,0.0000240057,2.95627585
43\\H,1.0012339336,-0.0005187767,2.507917105\\H,-0.1228705485,0.89125760
49,3.5951267804\\H,-0.1236949747,-0.8908465009,3.5954782862\\O,1.2037564
975,0.0001094774,0.074911489\\C,-2.9680687265,0.00064576,2.9134651209\\H
,-2.8548552617,-0.9154569292,3.5107281853\\H,-3.8868511406,0.0010258464
,2.3121967334\\H,-2.854213526,0.9165448089,3.5109240566\\C,0.1503956751,
-0.0003584941,-2.3499206818\\O,-0.6931601608,-0.000277254,-1.1755613511
\\H,-0.5383196033,-0.0005626747,-3.2037452498\\H,0.7900620829,0.89520567
35,-2.3672152108\\H,0.790260338,-0.895786181,-2.3669484934\\H,-1.8639838
671,1.3073876523,1.0737636683\\H,-1.8647294088,-1.3064296881,1.07372917
89\\Si,-1.3168545174,0.0003276525,1.5816317816\\Version=IA64L-G03RevD.0
1\\State=2-A\\HF=-596.448237\\MP2=-597.4854554\\PUHF=-596.453465\\PMP2-0=-5
97.4890091\\S2=0.780598\\S2-1=0.76076\\S2A=0.750626\\RMSD=5.407e-09\\RMSF=1
.802e-06\\Thermal=0.\\Dipole=-0.4931111,-0.0000787,-0.0693998\\PG=C01 [X(
C4H11O2Si1)]\\@

```

MP2/aug-cc-pVDZ

```

1\\1\\GINC-AC25\\FTS\\UMP2-FC\\CC-pVDZ\\C4H11O2Si1(2)\\SXH563\\17-Jan-2008\\0\\
#MP2/cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint gues
s=check\\TS of oxyacyl rad attacking dimethylsilane\\0,2\\C,-0.00465762
19,-0.0000167708,-0.0088785869\\C,-0.0051675272,0.0000240057,2.95627585
43\\H,1.0012339336,-0.0005187767,2.507917105\\H,-0.1228705485,0.89125760
49,3.5951267804\\H,-0.1236949747,-0.8908465009,3.5954782862\\O,1.2037564
975,0.0001094774,0.074911489\\C,-2.9680687265,0.00064576,2.9134651209\\H
,-2.8548552617,-0.9154569292,3.5107281853\\H,-3.8868511406,0.0010258464
,2.3121967334\\H,-2.854213526,0.9165448089,3.5109240566\\C,0.1503956751,
-0.0003584941,-2.3499206818\\O,-0.6931601608,-0.000277254,-1.1755613511
\\H,-0.5383196033,-0.0005626747,-3.2037452498\\H,0.7900620829,0.89520567
35,-2.3672152108\\H,0.790260338,-0.895786181,-2.3669484934\\H,-1.8639838
671,1.3073876523,1.0737636683\\H,-1.8647294088,-1.3064296881,1.07372917
89\\Si,-1.3168545174,0.0003276525,1.5816317816\\Version=IA64L-G03RevD.0
1\\State=2-A\\HF=-596.448237\\MP2=-597.4854554\\PUHF=-596.453465\\PMP2-0=-5
97.4890091\\S2=0.780598\\S2-1=0.76076\\S2A=0.750626\\RMSD=5.407e-09\\RMSF=1
.802e-06\\Thermal=0.\\Dipole=-0.4931111,-0.0000787,-0.0693998\\PG=C01 [X(
C4H11O2Si1)]\\@

```

BHandHLYP/6-311G(d,p)

```

1\\1\\GINC-AC19\\FTS\\UBHandHLYP\\6-311G(d,p)\\C4H11O2Si1(2)\\SXH563\\16-Jan-2
008\\0\\#BHandHLYP/6-311G** opt=(ts,calcfc,noeigen) freq=noraman\\TS of
oxyacyl rad attacking dimethylsilane\\0,2\\C,0.,0.,0.\\C,0.,0.,2.968874
76\\H,0.9981937531,0.,2.546706197\\H,-0.1161729911,0.8760614313,3.599943
3074\\H,-0.1163107789,-0.8762886177,3.5996029949\\O,1.1854528307,0.00005
88789,0.0844877729\\C,-2.9691579726,0.0007363417,2.8736229382\\H,-2.8818
646428,-0.9003070322,3.4652947588\\H,-3.8516160988,0.0009900546,2.25110

```

38423\H,-2.8813874747,0.9016959332,3.4653524425\C,0.1197908561,-0.0003
900195,-2.3383532115\O,-0.6668405759,-0.0002185015,-1.1462699164\H,-0.
5868178986,-0.0006118452,-3.1548256793\H,0.7455779912,0.8827555589,-2.
3769966246\H,0.7457455109,-0.8834314608,-2.376657273\H,-1.796731646,1.
3023689119,1.0829970095\H,-1.7974186907,-1.3014740333,1.0829366547\Si,
-1.2921605292,0.0003296118,1.6060586926\\Version=IA64L-G03RevD.01\Stat
e=2-A\HF=-598.8025892\S2=0.766878\S2-1=0.\S2A=0.750164\RMSD=7.028e-09\
RMSF=2.811e-06\Thermal=0.\Dipole=-0.0404435,-0.5558795,0.0001382\Polar
=123.1154774,-0.0128646,63.8348327,-51.8334141,0.0160344,139.4841603\PG
=C01 [X(C4H11O2Si1)]\\@

BHAndHLYP/DZP

1\1\GINC-GOMBERG07\FTS\ROBHandHLYP\Gen\C4H11O2Si1(2)\SHORVAT\03-Apr-20
12\0\#BHAndHLYP/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman
geom=checkpoint guess=check\\TS of oxyacyl radical attacking SiMe2\\0,2
\C,-0.9415736636,0.2748546412,0.0000086336\C,1.7255242163,1.5399553826
, -0.0001414375\H,0.9115536208,2.2549863788,-0.0001378463\H,2.344462519
5,1.7071015411,0.8760031769\H,2.3443495362,1.7069806026,-0.8763888379\
O,-1.3705392723,1.382788949,0.0000079201\C,2.9204735803,-1.1558763724,
0.0000993419\H,3.4164064983,-0.8188040563,-0.9000693135\H,2.749161404,
-2.222130829,0.0001676046\H,3.4163931373,-0.8186874082,0.9002319465\C,
-3.1089422725,-0.6105113834,0.0000371638\O,-1.6956883578,-0.8165403743
,0.0000186715\H,-3.5479891706,-1.5970290492,0.0000506999\H,-3.40980312
32,-0.0600836926,0.8829851902\H,-3.4098281924,-0.0600973782,-0.8829109
181\H,0.7973015539,-0.8998134957,1.294987886\H,0.7972866299,-0.9000501
42,-1.2948123586\Si,1.0552003557,-0.214196314,0.0000224769\\Version=AM
64L-G09RevC.01\State=2-A\HF=-313.171385\RMSD=6.844e-09\RMSF=6.942e-07\
Dipole=0.0539932,-0.5619234,0.0000045\Quadrupole=5.4662444,-4.5524531,
-0.9137913,2.3911994,-0.0000558,-0.0000342\PG=C01 [X(C4H11O2Si1)]\\@

BHAndHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET23\FTS\UBHandHLYP\CC-pVDZ\C4H11O2S
i1(2)\SONIA\25-Jul-2007\0\#BHAndHLYP/CC-PVDZ OPT=(TS,READFC,NOEIGEN)
FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\ts of oxyacyl rad attacking
disulfide\\0,2\C,0.614421609,0.0257939895,-0.7816153434\C,0.7742885739
, -0.003037878,2.1766320713\H,1.7449752975,0.0291439132,1.6769893785\H,
0.6729682036,0.8712783515,2.8261423023\H,0.7215364347,-0.8956263106,2.
806757661\O,1.8066065627,0.0587359495,-0.7574869649\C,-2.1917639112,-0
.086302843,2.2987241662\H,-2.0289218636,-0.9973036121,2.874744833\H,-3
.1251550673,-0.1058218658,1.7385238552\H,-2.0790872792,0.8192114531,2.
8950322772\C,0.6281382527,0.0523226509,-3.1198202284\O,-0.1085576675,0
.0181382565,-1.8980891307\H,-0.1152218928,0.0405162484,-3.914544777\H,
1.2338218577,0.9586579031,-3.1761535753\H,1.2832771703,-0.8174213906,-
3.1960285543\H,-1.1943375623,1.2662075129,0.4087122296\H,-1.1222415263
, -1.3393518056,0.3796306678\Si,-0.6090365772,-0.0269385401,0.891519890
9\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-598.7204878\S2=0.767633\
S2-1=0.\S2A=0.750171\RMSD=2.277e-09\RMSF=2.362e-06\Dipole=-0.5207044,-
0.0132059,-0.1112212\PG=C01 [X(C4H11O2Si1)]\\@

BHAndHLYP/aug-cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET22\FTS\UBHandHLYP\Aug-CC-pVDZ\C4H1
1O2Si1(2)\SONIA\26-Jul-2007\0\#BHAndHLYP/AUG-CC-PVDZ OPT=(TS,READFC,N
OEIGEN) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\ts of oxyacyl rad at
tacking disulfide\\0,2\C,0.6139433338,0.0257786656,-0.7848957167\C,0.7
789555497,-0.0030189665,2.193874335\H,1.7567688492,0.0292270145,1.7155
149507\H,0.6710498161,0.8679344932,2.8426767679\H,0.7195682718,-0.8927
257661,2.8231921396\O,1.8080820722,0.0585940984,-0.7640383116\C,-2.194
287711,-0.0861665025,2.2737939405\H,-2.044265796,-0.994883607,2.852086
6531\H,-3.1183229039,-0.1053323203,1.7037273313\H,-2.0943577951,0.8162
708859,2.8723891969\C,0.6116118053,0.0519705341,-3.1304200241\O,-0.114
4470704,0.0180717544,-1.8972319145\H,-0.1412463202,0.0398951934,-3.912
5043043\H,1.2122811812,0.9578271103,-3.1888316556\H,1.261412969,-0.817
7538647,-3.2087130927\H,-1.1660651615,1.2713693793,0.4145939839\H,-1.0
937320258,-1.3428511157,0.3853130978\Si,-0.5981077833,-0.0266919007,0.
905471538\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-598.7445865\S2=0

.767733\S2-1=0.\S2A=0.75018\RMSD=4.429e-09\RMSF=1.367e-06\Dipole=-0.58
74975,-0.0150552,-0.1072638\PG=C01 [X(C4H11O2Si1)]\@

B3LYP/6-311G(d,p)

1\1\GINC-GOMBERG18\FTS\UB3LYP\6-311G(d,p)\C4H11O2Si1(2)\SHORVAT\05-Mar-
2012\0\#B3LYP/6-311G** opt=(ts,calcfc,noeigen) freq=noraman\TS of o
xyacyl radical attacking SiMe2\0,2\C,-0.9678881226,0.286596772,-0.0000
281529\C,1.7344233447,1.5380545076,-0.0000272312\H,0.9234709691,2.2688
826171,-0.0000865914\H,2.3586615445,1.699086994,0.8821984449\H,2.35872
23159,1.6990096542,-0.8822239065\O,-1.4068359062,1.4079191044,-0.00008
5939\C,2.9972079284,-1.1674176565,0.0000957417\H,3.4715909876,-0.81087
7477,-0.9112188681\H,2.8112541295,-2.2376671701,0.0001305045\H,3.47155
8001,-0.8108126552,0.9114021229\C,-3.168011731,-0.5990152918,-0.000024
8739\O,-1.7377908322,-0.8176306562,0.0000093441\H,-3.6124609715,-1.591
4139298,0.0000117252\H,-3.4667492237,-0.0426817445,0.889539315\H,-3.46
67188087,-0.0427609621,-0.8896487901\H,0.8380870113,-0.9371435901,1.29
63950047\H,0.8381346051,-0.9372358739,-1.296301721\Si,1.0170937588,-0.
2120456419,0.0000238711\Version=AM64L-G09RevC.01\State=2-A\HF=-599.02
70225\S2=0.757087\S2-1=0.\S2A=0.75003\RMSD=4.241e-09\RMSF=9.166e-06\Di
pole=0.0542538,-0.4899039,0.0000243\Quadrupole=5.4752396,-4.4387092,-1
.0365303,2.4588082,0.000001,0.0001999\PG=C01 [X(C4H11O2Si1)]\@

B3LYP/cc-pVDZ

1\1\GINC-GOMBERG19\FTS\ROB3LYP\CC-pVDZ\C4H11O2Si1(2)\SHORVAT\06-Mar-20
12\0\#B3LYP/cc-pVDZ opt=(ts,readfc,noeigen) freq=noraman geom=checkpo
int guess=check\TS of oxyacyl radical attacking SiMe2\0,2\C,-0.973408
2094,0.2803408602,-0.0000287797\C,1.724947187,1.5257899352,-0.00002647
45\H,0.8933237533,2.2474622952,-0.0000810242\H,2.3516527163,1.69181832
61,0.8905719111\H,2.3517080179,1.6917465178,-0.8905991339\O,-1.4099769
419,1.4081272893,-0.0000881673\C,3.029532577,-1.1539543553,0.000095522
1\H,3.4976453715,-0.7816307615,-0.9197281202\H,2.860584129,-2.23696806
1,0.000133089\H,3.4976121406,-0.7815616181,0.9199080219\C,-3.178486080
7,-0.5809431473,-0.0000260494\O,-1.7546104887,-0.8214128145,0.00000933
99\H,-3.6451748789,-1.5736215744,0.0000113736\H,-3.4748459697,-0.01349
87302,0.8952705258\H,-3.4748153403,-0.0135805613,-0.895384599\H,0.8421
29311,-0.9785261891,1.2996780497\H,0.8421748954,-0.9786194551,-1.2995
806596\Si,1.0137568905,-0.2381209563,0.0000251748\Version=AM64L-G09Re
vC.01\State=2-A\HF=-598.932102\RMSD=5.037e-09\RMSF=7.339e-05\Dipole=0.
1195654,-0.4622869,0.0000251\Quadrupole=5.2754996,-4.1851611,-1.090338
5,2.2606396,0.000005,0.000186\PG=C01 [X(C4H11O2Si1)]\@

M05-2X/6-311G(d,p)

1\1\GINC-GOMBERG08\FTS\ROM052X\6-311G(d,p)\C4H11O2Si1(2)\SHORVAT\01-Oct-
2012\0\#M052X/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=ch
eckpoint guess=check\TS of oxyacyl radical attacking SiMe2\0,2\C,-0.9
445743252,0.2699263722,0.0049917351\C,1.7257433788,1.5283144769,-0.004
6338074\H,0.9094220263,2.2456399975,0.0499454066\H,2.4003091757,1.6771
861807,0.8375962429\H,2.2909374684,1.6949170954,-0.9214596775\O,-1.383
9242914,1.3832019428,0.0164141554\C,2.9490179631,-1.1443590076,0.00773
8843\H,3.4249457029,-0.7809177824,-0.8975730767\H,2.7857937435,-2.2157
217027,0.0026010398\H,3.4233671378,-0.7894526914,0.9171914444\C,-3.127
3559392,-0.5929266349,-0.0101507994\O,-1.7057077471,-0.830672663,-0.01
00517935\H,-3.5853700062,-1.5750841179,-0.022873441\H,-3.4104922893,-0.
0420804037,0.8836148682\H,-3.4067893535,-0.0210839787,-0.8918576052\H
,0.8061313672,-0.9326866828,1.3135238084\H,0.8036932293,-0.9511948768,
-1.2844392918\Si,1.0386017589,-0.2301585236,0.0095819486\Version=AM64
L-G09RevC.01\State=2-A\HF=-598.928119\RMSD=9.075e-09\RMSF=2.582e-06\Di
pole=0.1349334,-0.5272436,-0.0107956\Quadrupole=5.8194686,-4.650248,-1
.1692205,2.348964,0.0340402,-0.0471765\PG=C01 [X(C4H11O2Si1)]\@

M05-2X/DZP

1\1\GINC-GOMBERG05\FTS\ROM052X\Gen\C4H11O2Si1(2)\SHORVAT\02-Oct-2012\0
\#M052X/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=che
ckpoint guess=check\TS of oxyacyl radical attacking SiMe2\0,2\C,-0.94
23919127,0.2684524775,0.0078216668\C,1.7204477859,1.5188745109,-0.0087
592121\H,0.9014038561,2.2314788819,0.0609857298\H,2.40915466,1.6673074

019,0.8216723491\H,2.2686742855,1.6879138352,-0.935245106\O,-1.3780326
 026,1.3828435477,0.0312468841\C,2.9545341661,-1.1350904482,0.010899378
 \H,3.4270720984,-0.7669815646,-0.8943619755\H,2.8002532491,-2.20772188
 21,0.0060316919\H,3.4260753652,-0.7750496464,0.9198076925\C,-3.1283589
 584,-0.5854717335,-0.0146947344\O,-1.7078026608,-0.8290665775,-0.01915
 17658\H,-3.5904740308,-1.5655179068,-0.0388602695\H,-3.4084243481,-0.0
 442456766,0.8858961971\H,-3.406725848,-0.0016751781,-0.8888997818\H,0.
 807646434,-0.941454557,1.3147983999\H,0.8034402883,-0.9729509486,-1.27
 16560224\Si,1.0372571728,-0.2387975356,0.0126288785\\Version=AM64L-G09
 RevC.01\State=2-A\HF=-313.315853\RMSD=2.141e-09\RMSF=2.009e-06\Dipole=
 0.146632,-0.5308812,-0.0170578\Quadrupole=5.7944878,-4.6674072,-1.1270
 806,2.2845998,0.0556822,-0.0898941\PG=C01 [X(C4H11O2Si1)]\@

M05-2X/aug-cc-pVDZ

1\1\GINC-GOMBERG04\FTS\ROM052X\Aug-CC-pVDZ\C4H11O2Si1(2)\SHORVAT\02-Oct-2012\0\#M052X/aug-cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\\TS of oxyacyl radical attacking SiMe2\\0,2\C,-0.9509569837,0.2645506302,0.0049653818\C,1.7282747977,1.5320335904,-0.005741091\H,0.9048868862,2.250062828,0.0250023301\H,2.383972584,1.6833809368,0.8574154182\H,2.3197529975,1.6899323198,-0.9134333273\O,-1.3887615949,1.3847859342,0.0200722026\C,2.9605068487,-1.1420870219,0.0063919206\H,3.4356887195,-0.7763206348,-0.9050726137\H,2.8006808861,-2.2194852865,0.004355277\H,3.4345040561,-0.7797537867,0.9197783197\C,-3.1388470683,-0.5900356049,-0.0073845517\O,-1.7163718705,-0.8358267225,-0.0114078741\H,-3.6025107117,-1.575938339,-0.0219439235\H,-3.4154030785,-0.0373796644,0.8935695674\H,-3.4158732177,-0.0110625622,-0.8914777769\H,0.8033547303,-0.9461567943,1.3143946181\H,0.8014320653,-0.9599354946,-1.2950946099\Si,1.0494189539,-0.2379173277,0.0057707327\\Version=AM64L-G09RevC.01\State=2-A\HF=-598.8682327\RMSD=3.970e-09\RMSF=1.432e-06\Dipole=0.1872285,-0.5391238,-0.009764\Quadrupole=5.544618,-4.4283027,-1.1163152,2.5318302,0.0354891,-0.057065\PG=C01 [X(C4H11O2Si1)]\@

M06-2X/6-311G(d,p)

1\1\GINC-GOMBERG05\FTS\ROM062X\6-311G(d,p)\C4H11O2Si1(2)\SHORVAT\02-Oct-2012\0\#M062X/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\\TS of oxyacyl radical attacking SiMe2\\0,2\C,-0.9462112258,0.2678678656,0.0104788227\C,1.7182714835,1.5139788709,-0.0085454926\H,0.9063572026,2.2355253909,0.0902537669\H,2.4368165634,1.6596799082,0.7994267973\H,2.2374469968,1.6900992998,-0.9530302709\O,-1.3799844835,1.3835897567,0.0300404766\C,2.9625631684,-1.1346543484,0.0134581464\H,3.4327229993,-0.7598135666,-0.8930146463\H,2.8093021828,-2.209812957,0.0040193265\H,3.4313995093,-0.7756622308,0.9268836887\C,-3.1318289547,-0.584109339,-0.0189864504\O,-1.7181591965,-0.8276156943,-0.01643585\H,-3.5999401167,-1.5641535507,-0.0455201271\H,-3.4222839646,-0.0408591858,0.8806569398\H,-3.4113481531,0.0015546424,-0.8951791036\H,0.8250631566,-0.9442762048,1.3202003177\H,0.8188198139,-0.9790987753,-1.2632012947\Si,1.0247420186,-0.2393928817,0.018654953\\Version=AM64L-G09RevC.01\State=2-A\HF=-598.8255855\RMSD=6.076e-09\RMSF=2.546e-06\Dipole=0.1692886,-0.5241587,-0.0194613\Quadrupole=5.4949994,-4.4959192,-0.9990802,2.1923721,0.0625107,-0.0792895\PG=C01 [X(C4H11O2Si1)]\@

M06-2X/DZP

1\1\GINC-GOMBERG04\FTS\ROM062X\Gen\C4H11O2Si1(2)\SHORVAT\04-Oct-2012\0\#M062X/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\\TS of oxyacyl radical attacking SiMe2\\0,2\C,-0.9483210189,0.2678863714,0.0142138835\C,1.7117748089,1.5027743822,-0.013313368\H,0.8981755151,2.2197821001,0.1015186005\H,2.4451009289,1.6508095417,0.7806398767\H,2.2124790283,1.6833115431,-0.9669267196\O,-1.3779998783,1.3844505085,0.0479972512\C,2.9749774727,-1.1262942608,0.0165609459\H,3.4428046944,-0.7480718047,-0.8898682998\H,2.8326507418,-2.2030633989,0.0078222253\H,3.4431372783,-0.7628129675,0.9286492494\C,-3.136

8178042,-0.5756526166,-0.0245393296\O,-1.7238814869,-0.8246133929,-0.0267007844\H,-3.6086560116,-1.5534394464,-0.0652026598\H,-3.4246428179,-0.0445338116,0.8831637392\H,-3.4147654284,0.0239592855,-0.8917457826\H,0.8245831584,-0.9491608089,1.3210066171\H,0.8145712222,-1.0012125442,-1.245579885\Si,1.0285785974,-0.25127168,0.0224824088\\Version=AM64L-G09RevC.01\State=2-A\HF=-313.2266628\RMSD=1.437e-09\RMSF=3.446e-06\Dipole=0.157681,-0.5286395,-0.0265931\Quadrupole=5.3932775,-4.5056505,-0.8876271,2.1594513,0.089507,-0.1259786\PG=C01 [X(C4H11O2Si1)]\@

M06-2X/aug-cc-pVDZ

1\1\GINC-GOMBERG17\FTS\ROM062X\Aug-CC-pVDZ\C4H11O2Si1(2)\SHORVAT\03-Oct-2012\0\#M062X/aug-cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\\TS of oxyacyl radical attacking SiMe2\\0,2\C,-0.9508788715,0.2614413498,0.0175252127\C,1.718403591,1.5155712989,-0.0174019139\H,0.9046125908,2.2361730591,0.1174706315\H,2.4743766923,1.6569242719,0.763121033\H,2.197985686,1.6924575175,-0.9883987351\O,-1.3832496941,1.3836407844,0.061966428\C,2.9747951315,-1.1312478769,0.0222748262\H,3.4438694402,-0.7488168242,-0.8883128911\H,2.8253094143,-2.2123856957,0.0110661464\H,3.440612058,-0.7678865366,0.9420630268\C,-3.1426522242,-0.5791335474,-0.0283153652\O,-1.728449481,-0.8327081552,-0.03429312\H,-3.6175094623,-1.5611619102,-0.0760162336\H,-3.4256070069,-0.0510209559,0.8886309843\H,-3.4177768125,0.0308716649,-0.8953329698\H,0.826771642,-0.9502345393,1.3373899906\H,0.8185605034,-1.0013015755,-1.2581303676\Si,1.0345758028,-0.2483353296,0.0248533168\\Version=AM64L-G09RevC.01\State=2-A\HF=-598.7682841\RMSD=3.969e-09\RMSF=2.663e-06\Dipole=0.2290442,-0.5318174,-0.0320864\Quadrupole=5.2170127,-4.2793274,-0.9376853,2.3601925,0.1164348,-0.165047\PG=C01 [X(C4H11O2Si1)]\@

ROMP2/6-311G(d,p)//MP2/6-311G(d,p)

MP2=-597.6112994

ROMP2/DZP//MP2/DZP

MP2= -312.3688802

ROMP2/cc-pVDZ//MP2/cc-pVDZ

MP2= -597.482795

ROMP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ

MP2= -597.559794

ROMP2/6-311G(d,p)//BHandHLYP/6-311G(d,p)

MP2= -597.6078545

ROMP2/DZP//BHandHLYP/DZP

MP2=-312.3722014

ROMP2/cc-pVDZ//BHandHLYP/cc-pVDZ

MP2=-597.4802053

ROMP2/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ

MP2= -597.5563435

ROMP2/6-311G(d,p)//B3LYP/6-311G(d,p)

MP2=-597.6125858

QCISD/6-311G(d,p)//MP2/6-311G(d,p)

MP2= -597.692746

QCISD/DZP//MP2/DZP

QCISD=-312.4494892

QCISD/cc-pVDZ//MP2/cc-pVDZ

QCISD=-597.572616

QCISD/aug-cc-pVDZ//MP2/aug-cc-pVDZ

QCISD= -597.647325

QCISD/6-311G(d,p)//BHandHLYP/6-311G(d,p)

QCISD = -597.6897433

QCISD/DZP//BHandHLYP/DZP

QCISD= -312.4478845

QCISD/cc-pVDZ//BHandHLYP/cc-pVDZ

QCISD= -597.5706181

QCISD/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ

QCISD=

QCISD/6-311G(d,p)//B3LYP/6-311G(d,p)

QCISD=-597.6928928

CCSD(T)/6-311G(d,p)//MP2/6-311G(d,p)

CCSD(T)= -597.731889

CCSD(T)/DZP//MP2/DZP

CCSD(T)= -312.4881057

CCSD(T)/cc-pVDZ//MP2/cc-pVDZ

CCSD(T)= -597.605565

CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ

CCSD(T)= -597.687478

CCSD(T)/6-311G(d,p)//BHandHLYP/6-311G(d,p)

CCSD(T)= -597.7286539

CCSD(T)/DZP//BHandHLYP/DZP

CCSD(T)= -312.4862017

CCSD(T)/cc-pVDZ//BHandHLYP/cc-pVDZ

CCSD(T)= -597.6032371

CCSD(T)/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ

CCSD(T)= -597.6836225

CCSD(T)/6-311G(d,p)//B3LYP/6-311G(d,p)

CCSD(T)= -597.7310228

CCSD(T)/6-311G(d,p)//M06-2X/6-311G(d,p)

CCSD(T)=-597.7301957

CCSD(T)/6-311++G(d,p)//M06-2X/6-311G(d,p)

CCSD(T) = -597.7443368

CCSD(T)/cc-pVTZ//M06-2X/6-311G(d,p)

CCSD(T)=-597.9723458

CCSD(T)/aug-cc-pVTZ//M06-2X/6-311G(d,p)

Transition State 9 (X=Si)

HF/6-311G(d,p)

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1\1\GINC-AC28\FTS\UHF\6-311G(d,p)\C4H11O2Si1(2)\SXH563\08-Aug-2008\0\
#UHF/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint gue
ss=check\FS TS of oxyacyl radical attacking dimethylsilane\0,2\Si,-0
.0199950986,-0.0152711448,0.0041405077\C,0.0537858158,0.0395962555,2.1
58609321\H,1.4648007301,-0.005861902,0.283425019\H,-0.1400320427,1.222
0935356,-0.8039268547\O,0.1441738707,1.0338780318,2.7709916283\H,-2.33
79899555,-0.7556043114,1.1956837054\H,-2.5035657038,0.1579609351,-0.33
72793669\H,-2.2028850188,1.0352263008,1.1945670006\C,-2.040381214,0.12
29364884,0.6410225413\C,-0.205932046,-1.6234302465,-0.9727046324\H,-0.
1331179186,-2.4727936074,-0.2975758105\H,-1.1560216289,-1.6908866465,-
1.4931599661\H,0.5941126994,-1.7141745087,-1.7015411328\O,0.0713557597
,-1.184813048,2.6243670538\C,0.2583782787,-1.3425726934,4.0315327505\H
,-0.5445349124,-0.8585007703,4.5698322817\H,1.2063921134,-0.9175369083
,4.3298906242\H,0.2472192737,-2.4061190615,4.2084868655\Version=IA64L
-G03RevD.01\State=2-A\HF=-596.5160542\S2=0.808283\S2-1=0.\S2A=0.751456
\RMSD=7.958e-09\RMSF=2.286e-06\Thermal=0.\Dipole=-0.4234678,-0.9461766
,0.4898417\PG=C01 [X(C4H11O2Si1)]\@
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HF/DZP

```
1\1\GINC-GOMBERG06\FTS\UHF\Gen\C4H11O2Si1(2)\SHORVAT\03-Apr-2012\0\#U
HF/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=checkpoin
t guess=check\TS of oxyacyl radical attacking SiMe2\0,2\Si,1.30675166
97,-0.1711867005,-0.5973983154\C,-0.8120383031,-0.3874845962,-0.295758
6854\H,0.7306694559,0.3170968027,-1.9044948328\H,2.1546662115,-1.27200
55682,-1.0999621088\O,-1.4143047048,-1.3355588239,-0.627733284\H,0.603
024795,-0.4614135037,1.9960761642\H,2.167671696,-1.2004079686,1.530882
013\H,0.6368160756,-2.0645756604,1.187044246\C,1.1156119003,-1.1030497
464,1.2934104428\C,2.2449792931,1.3564982418,-0.0139748982\H,1.5367678
673,2.0993614901,0.3444633597\H,2.939877513,1.1390244773,0.7905541247\
H,2.7965797112,1.7976585175,-0.8384738893\O,-1.2916512905,0.7165837388
,0.2220858384\C,-2.7092584012,0.8009700327,0.3730507613\H,-3.061102044
2,0.0164506372,1.0284216649\H,-3.1912116074,0.7146783388,-0.5906657684
\H,-2.8978538374,1.7704352911,0.8057121674\Version=AM64L-G09RevC.01\S
tate=2-A\HF=-311.3534913\S2=0.810312\S2-1=0.\S2A=0.751636\RMSD=7.653e-
09\RMSF=3.163e-06\Dipole=-0.3915525,0.6760815,0.8036238\Quadrupole=4.0
907906,-2.7827862,-1.3080043,-3.747192,-0.7229176,-1.6351838\PG=C01 [X
(C4H11O2Si1)]\@
```

MP2/6-311G(d,p)

```
1\1\GINC-AC3\FTS\UMP2-FC\6-311G(d,p)\C4H11O2Si1(2)\SXH563\08-Aug-2008\
0\#MP2/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint
guess=check\FS TS of oxyacyl radical attacking dimethylsilane\0,2\Si
,0.0147051808,-0.0186166206,0.0691538493\C,0.0864756161,0.0263584378,2
.0739394727\H,1.532491744,-0.0500348989,0.2050749175\H,-0.1230218409,1
.2815818268,-0.6310134921\O,0.2282191359,1.0288680228,2.7228160518\H,-
2.2942053114,-0.8752624425,1.1276658983\H,-2.4908753041,0.1804828102,-
0.3356993707\H,-2.2038896174,0.9318593808,1.2850728007\C,-2.0318679909
,0.0663662447,0.6476529642\C,-0.2160952539,-1.6000618905,-0.9379751002
\H,-0.0388079131,-2.4551003331,-0.2769130873\H,-1.2180691864,-1.698006
3628,-1.361078199\H,0.5205622682,-1.645303987,-1.7445728195\O,0.035293
2428,-1.2276499886,2.5607712017\C,0.2086017101,-1.3066125626,3.9937816
879\H,-0.5767141997,-0.742225136,4.4988719741\H,1.1829439045,-0.906842
7807,4.2781216945\H,0.1400168176,-2.3656730213,4.2306910918\Version=I
A64L-G03RevD.01\State=2-A\HF=-596.5157492\MP2=-597.6135905\PUHF=-596.5
218691\MP2-0=-597.6178725\S2=0.787895\S2-1=0.764838\S2A=0.750829\RMSD
=3.193e-09\RMSF=3.394e-06\Thermal=0.\Dipole=-0.4430456,-0.789613,0.387
6863\PG=C01 [X(C4H11O2Si1)]\@
```

MP2/DZP

```
1\1\GINC-GOMBERG08\FTS\UMP2-FC\Gen\C4H11O2Si1(2)\SHORVAT\03-Apr-2012\0
\#MP2/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\TS of oxy
```

acyl radical attacking SiMe2\\0,2\\Si,1.2354928571,-0.2581614579,-0.5440884952\\C,-0.7428518351,-0.3650117093,-0.3158285205\\H,0.8651176901,0.1708305937,-1.9648639735\\H,1.9593522406,-1.4950979746,-0.9096453991\\O,-1.41615915,-1.3176590193,-0.6087576798\\H,0.5940523959,-0.1843671754,2.043740459\\H,2.8169691219,1.1225184056,0.8542289581\\H,2.8936304334,1.5691627639,-0.8691372746\\O,-1.2059067314,0.8090205318,0.156719023\\C,-2.6454637073,0.867126754,0.2672709473\\H,-3.0030666058,0.0921042951,0.9469078076\\H,-3.1051463542,0.7289290273,-0.7123755924\\H,-2.8610578371,1.8580113537,0.6600199177\\Version=AM64L-G09RevC.01\\State=2-A\\HF=-311.3533752\\MP2=-312.4498745\\PUHF=-311.3597092\\PMP2-0=-312.4543094\\S2=0.789537\\S2-1=0.765489\\S2A=0.750953\\RMSD=5.667e-09\\RMSF=1.463e-06\\Dipole=-0.2530687,0.6084786,0.6799112\\PG=C01 [X(C4H11O2Si1)]\\@

MP2/cc-pVDZ

1\\1\\GINC-AC29\\FTS\\UMP2-FC\\CC-pVDZ\\C4H11O2Si1(2)\\SXH563\\08-Aug-2008\\0\\#MP2/cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\\FS TS of oxyacyl radical attacking dimethylsilane\\0,2\\Si,0.097776082,-0.0059229644,0.0617178033\\C,0.0905269881,0.0330755038,2.0806394388\\H,1.5450368781,-0.0126445888,0.1947587462\\H,-0.134416328,1.2964195082,-0.6593254143\\O,0.2151470961,1.0331672729,2.746150157\\H,-2.3057120745,-0.8413929731,1.1698542161\\H,-2.528990807,0.1593652636,-0.3494723051\\H,-2.2126314372,0.9872295972,1.2507364525\\C,-2.0533600146,0.0879595693,0.6404903529\\C,-0.2087864545,-1.6135566795,-0.9322899416\\H,-0.0853361188,-2.4614124846,-0.2351827536\\H,-1.2015589861,-1.6947136915,-1.4023999003\\H,0.569591598,-1.6968040125,-1.7083619193\\O,0.055557763,-1.2355705894,2.5515674885\\C,0.2208639934,-1.3265164862,3.9881640726\\H,-0.5820452393,-0.7763604072,4.5015152679\\H,1.1940291511,-0.9107415573,4.289147429\\H,0.168069386,-2.3974535819,4.2186523451\\Version=IA64L-G03RevD.01\\State=2-A\\HF=-596.446005\\MP2=-597.4867195\\PUHF=-596.4523145\\PMP2-0=-597.4911786\\S2=0.790534\\S2-1=0.766428\\S2A=0.750948\\RMSD=7.319e-09\\RMSF=6.094e-07\\Thermal=0.\\Dipole=-0.4306658,-0.7895238,0.3764401\\PG=C01 [X(C4H11O2Si1)]\\@

MP2/aug-cc-pVDZ

1\\1\\GINC-AC24\\FTS\\UMP2-FC\\Aug-CC-pVDZ\\C4H11O2Si1(2)\\SXH563\\09-Aug-2008\\0\\#MP2/aug-cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\\FS TS of oxyacyl radical attacking dimethylsilane\\0,2\\Si,0.0054419088,-0.0046437221,0.0567062785\\C,0.0943246287,0.0314230903,2.0758808268\\H,1.544475287,-0.0272271953,0.2031466919\\H,-0.1236819443,1.307697613,-0.6508495298\\O,0.2013031417,1.0414066665,2.7424955255\\H,-2.3039077856,-0.8600075613,1.145309984\\H,-2.5202572042,0.1686284479,-0.3498377884\\H,-2.2163688815,0.9653007142,1.2630414984\\C,-2.0470671793,0.0795150771,0.638940228\\C,-0.2185333025,-1.6106676894,-0.9431787474\\H,-0.1406583827,-2.461092859,-0.2439631576\\H,-1.1995410033,-1.6640945674,-1.4387966778\\H,0.5767703786,-1.7179863788,-1.6964679543\\O,0.0773094364,-1.2380555426,2.5570925644\\C,0.2302529633,-1.3219552196,4.0075164863\\H,-0.5894578951,-0.7818532792,4.5004150185\\H,1.1943031069,-0.8891673306,4.3065333747\\H,0.1910557292,-2.3930935652,4.232376914\\Version=IA64L-G03RevD.01\\State=2-A\\HF=-596.4645575\\MP2=-597.5639926\\PUHF=-596.4710117\\PMP2-0=-597.5685528\\S2=0.791799\\S2-1=0.76691\\S2A=0.75102\\RMSD=7.169e-09\\RMSF=6.713e-07\\Thermal=0.\\Dipole=-0.4289179,-0.8429399,0.2631509\\PG=C01 [X(C4H11O2Si1)]\\@

BHandHLYP/6-311G(d,p)

1\\1\\GINC-AC23\\FTS\\UBHandHLYP\\6-311G(d,p)\\C4H11O2Si1(2)\\SXH563\\09-Aug-2008\\0\\#BHandHLYP/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\\FS TS of oxyacyl radical attacking dimethylsilane\\0,2\\Si,-0.06638403,-0.0228109632,0.0875003085\\C,0.0840572483,0.0115576125,2.0944394239\\H,1.4671232129,-0.0384948805,0.2699104398\\H,-0.1031802486,1.2635388437,-0.6489336288\\O,0.1809556959,1.0062214896,2.7311638541\\H,-2.3795663273,-0.7717746418,1.1043352032\\H,-2.5415557975,0.2029085264,-0.3934505059\\H,-2.2305312794,1.0159626533,1.1739314663\\C,-2.

0767383873,0.1256080281,0.5817196548\C,-0.209905961,-1.6186274459,-0.9
065606403\H,-0.1044709007,-2.4628518192,-0.2300992023\H,-1.1657766537,
-1.7089056562,-1.411336234\H,0.5852494906,-1.6836917957,-1.6416633712\
O,0.0975045197,-1.2195289983,2.5817802723\C,0.273100298,-1.3381017053,
3.9976621751\H,-0.5321074825,-0.8348822074,4.5178652814\H,1.2199863607
,-0.9045907651,4.293480383\H,0.258003244,-2.3974095765,4.2046166557\\V
ersion=IA64L-G03RevD.01\State=2-A\HF=-598.7991418\S2=0.767183\S2-1=0.\
S2A=0.750188\RMSD=7.824e-09\RMSF=1.475e-06\Thermal=0.\Dipole=-0.383043
6,-0.8851048,0.3279119\PG=C01 [X(C4H11O2Si1)]\\@

BHandHLYP/DZP

1\1\GINC-GOMBERG06\FTS\UBHandHLYP\Gen\C4H11O2Si1(2)\SHORVAT\03-Apr-201
2\0\#\BHandHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\\
TS of oxyacyl radical attacking SiMe2\\0,2\Si,1.2285374558,-0.185738912
7,-0.5337217474\C,-0.7557131414,-0.3431751942,-0.3265815194\H,0.748548
6838,0.369279914,-1.8990566277\H,1.9758146678,-1.314515318,-1.13145299
72\O,-1.3813876412,-1.2926735018,-0.6616381939\H,0.7164749709,-0.44518
08252,2.0282650167\H,2.2389281491,-1.2533827866,1.5312523426\H,0.66172
18392,-2.0493250163,1.2245477056\C,1.1872839755,-1.1099061683,1.316347
5672\C,2.1845318825,1.3439649666,0.0049832565\H,1.4723539111,2.0933473
96,0.3401521367\H,2.8691227828,1.1391189121,0.8207449723\H,2.740080604
5,1.763773998,-0.8263875158\O,-1.2613970687,0.7617652278,0.2021095083\
C,-2.6845002264,0.7986926502,0.3485288426\H,-3.015953197,-0.0048154143
0.9941298333\H,-3.1619944229,0.7031425881,-0.6184499444\H,-2.90645722
55,1.7587024847,0.7894663639\\Version=AM64L-G09RevC.01\State=2-A\HF=-3
13.1713727\S2=0.767846\S2-1=0.\S2A=0.750203\RMSD=7.201e-09\RMSF=1.869e
-06\Dipole=-0.2157456,0.644293,0.7146587\Quadrupole=4.030814,-2.657051
7,-1.3737622,-3.3504923,-0.8058867,-1.5167535\PG=C01 [X(C4H11O2Si1)]\\
@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\FTS\UBHandHLYP\CC-pVDZ\C4H11O2S
i1(2)\SONIA\26-Sep-2008\0\#\BHANDHLYP/CC-PVDZ OPT=(TS,CALCFC,NOEIGEN)
FREQ=NORAMAN\\FS ts of oxyacyl rad attacking dimethylsilane\\0,2\Si,0.2
641959772,0.4272310879,-1.2694600307\C,0.2678012063,0.4204608136,0.749
0224757\H,1.7965255628,0.4295903385,-0.9735021874\H,0.2720803683,1.732
1531249,-1.9948816044\O,0.2913854536,1.4025104729,1.4196346843\H,-2.11
8312104,-0.3589310972,-0.4313566153\H,-2.1830120361,0.6337642434,-1.94
31208652\H,-1.9881473889,1.4442167308,-0.3370231637\C,-1.7865811676,0.
5526922175,-0.9293453651\C,0.2247320729,-1.1651237475,-2.2925817336\H,
0.305210377,-2.0168418287,-1.6089784952\H,-0.7005550786,-1.2710617545,
-2.8645154067\H,1.0756747692,-1.2036176873,-2.9775620284\O,0.272958225
8,-0.8261025628,1.2083404312\C,0.3381020837,-0.9657304556,2.6304762052
\H,-0.5227237894,-0.4861405069,3.0989266782\H,1.2536765512,-0.51271849
53,3.0137595525\H,0.33176448,-2.0367045467,2.8214641487\\Version=x86-L
inux-G03RevB.04\State=2-A\HF=-598.7166837\S2=0.768071\S2-1=0.\S2A=0.75
0207\RMSD=2.565e-09\RMSF=5.422e-07\Dipole=-0.3876083,-0.8765771,0.2495
046\PG=C01 [X(C4H11O2Si1)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-AC28\FTS\UBHandHLYP\Aug-CC-pVDZ\C4H11O2Si1(2)\SXH563\08-Aug-2
008\0\#\BHandHLYP/aug-cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geo
m=checkpoint guess=check\\FS TS of oxyacyl radical attacking dimethyls
ilane\\0,2\Si,-0.080968368,-0.0265218503,0.0937688063\C,0.085572275,0.
0021688153,2.1031486237\H,1.4700932113,-0.0654160003,0.2836157315\H,-0
.0822728961,1.2756343831,-0.631118597\O,0.168568637,1.0046623507,2.743
1920433\H,-2.4134052497,-0.7720115384,1.0785595225\H,-2.5508369674,0.2
143502023,-0.4230733763\H,-2.2546832044,1.0247160421,1.1588530938\C,-2
.0951836636,0.1310354726,0.5624433091\C,-0.2169081091,-1.6198589205,-0
.9200035517\H,-0.1511915101,-2.4744911008,-0.242423846\H,-1.1632707498
, -1.6861174236,-1.4573926329\H,0.6043411232,-1.6969083752,-1.632567894
4\O,0.1223845237,-1.2301355033,2.5974548189\C,0.2967704573,-1.33585442
21,4.0169042805\H,-0.5257544095,-0.8447886344,4.5329271245\H,1.2376833
09,-0.8762038676,4.3123923822\H,0.3048245934,-2.4001329312,4.229681697
4\\Version=IA64L-G03RevD.01\State=2-A\HF=-598.7410121\S2=0.768325\S2-1
=0.\S2A=0.750215\RMSD=3.642e-09\RMSF=1.449e-06\Thermal=0.\Dipole=-0.37

86769,-0.9061936,0.2048143\PG=C01 [X(C4H11O2Si1)]\@

B3LYP/6-311G(d,p)

1\1\GINC-GOMBERG16\FTS\UB3LYP\6-311G(d,p)\C4H11O2Si1(2)\SHORVAT\20-Mar-2012\0\#B3LYP/6-311G** opt=(ts,calcfc,noeigen) freq=noraman\TS of oxyacyl radical attacking SiMe2\0,2\Si,1.2111447022,-0.1644129993,-0.5803836079\C,-0.7602090277,-0.3362653487,-0.3453893803\H,0.8261376158,0.386026356,-1.9753856128\H,1.9456097266,-1.3517768566,-1.1126914548\O,-1.3981025073,-1.2910010078,-0.6976187498\H,0.7499193196,-0.4255611606,2.0503638561\H,2.2703149842,-1.267467155,1.5269839511\H,0.6598506925,-2.0500518756,1.2449156998\C,1.2075453623,-1.1167346188,1.3455120558\C,2.1984067911,1.3514234252,0.0053797831\H,1.4931023113,2.1383555849,0.2878829428\H,2.8362490704,1.1397572806,0.8650621802\H,2.8139850888,1.7351739858,-0.8111634339\O,-1.2794690164,0.7709276262,0.2155945382\C,-2.7212780704,0.7911315869,0.3654120587\H,-3.046465506,-0.0354752482,0.9980745399\H,-3.2018654363,0.7122356643,-0.6102456558\H,-2.9488801007,1.7467897608,0.8309352896\Version=AM64L-G09RevC.01\State=2-A\HF=-599.0226509\S2=0.75787\S2-1=0.\S2A=0.750038\RMSD=4.599e-09\RMSF=3.886e-06\Dipole=-0.2005634,0.6170225,0.7423478\Quadrupole=4.1845591,-2.5486224,-1.6359366,-3.0735076,-0.8097744,-1.4449504\PG=C01 [X(C4H11O2Si1)]\@

B3LYP/cc-pVDZ

1\1\GINC-GOMBERG14\FTS\ROB3LYP\CC-pVDZ\C4H11O2Si1(2)\SHORVAT\20-Mar-2012\0\#B3LYP/cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\TS of oxyacyl radical attacking SiMe2\0,2\Si,1.2147804396,-0.1696000001,-0.5846388062\C,-0.7638913343,-0.3398098937,-0.3439944504\H,0.8269971705,0.388509486,-1.9898361517\H,1.9608358389,-1.3621600704,-1.1208463868\O,-1.4125170405,-1.2967999101,-0.6861796223\H,0.7370512169,-0.4295760543,2.0523764273\H,2.2806415655,-1.2709125151,1.5375902318\H,0.6603505459,-2.0678536965,1.2374308469\C,1.2092162182,-1.1249936859,1.3465412168\C,2.1978682302,1.3577009576,0.0059906663\H,1.4767794706,2.1452697356,0.281898517\H,2.8347215728,1.1490379258,0.8785606831\H,2.8220166863,1.7444270804,-0.8147259418\O,-1.2761261358,0.777785194,0.2130482043\C,-2.7151829959,0.7961491656,0.3660286091\H,-3.0441767359,-0.0357409831,1.0060629458\H,-3.2058539384,0.7109560515,-0.6147021339\H,-2.9475147748,1.7606862129,0.8326341446\Version=AM64L-G09RevC.01\State=2-A\HF=-598.9274696\RMSD=9.870e-09\RMSF=1.129e-06\Dipole=-0.1764735,0.5990385,0.7359625\Quadrupole=3.8376652,-2.2732832,-1.5643819,-2.896889,-0.6428767,-1.3718808\PG=C01 [X(C4H11O2Si1)]\@

M05-2X/6-311G(d,p)

1\1\GINC-GOMBERG07\FTS\UM052X\6-311G(d,p)\C4H11O2Si1(2)\SHORVAT\02-Oct-2012\0\#M052X/6-311G** opt=(ts,calcfc,noeigen) freq=noraman\TS of oxyacyl radical attacking SiMe2\0,2\Si,1.2415172492,-0.1775336503,-0.587593057\C,-0.7372315018,-0.347109168,-0.3554860657\H,0.7935700797,0.378602938,-1.9637618846\H,2.0060919079,-1.3341980516,-1.1362759021\O,-1.3881012843,-1.2880762198,-0.69637242\H,0.6742700988,-0.3964691255,1.9823266429\H,2.1996535532,-1.2532197044,1.5201263142\H,0.5980435242,-2.0280655232,1.2013505052\C,1.1465518399,-1.0975840149,1.3004640635\C,2.1753383032,1.3478786916,0.0273715657\H,1.4361036759,2.055554655,0.4063845173\H,2.8658553465,1.1082050106,0.8338000924\H,2.7170616825,1.8260772019,-0.786080203\O,-1.2263528605,0.7603626064,0.2121017884\C,-2.6615770975,0.7793516786,0.3758051815\H,-2.9702326811,-0.0499582581,1.0072567145\H,-3.1421477969,0.697500202,-0.5957332417\H,-2.8858750388,1.7309507317,0.8429533885\Version=AM64L-G09RevC.01\State=2-A\HF=-598.9280653\S2=0.761878\S2-1=0.\S2A=0.750087\RMSD=6.724e-09\RMSF=4.151e-06\Dipole=-0.176529,0.6308625,0.7639815\Quadrupole=4.2233928,-2.6006235,-1.6227693,-3.2280268,-0.9314255,-1.4609224\PG=C01 [X(C4H11O2Si1)]\@

M05-2X/DZP

1\1\GINC-GOMBERG06\FTS\UM052X\Gen\C4H11O2Si1(2)\SHORVAT\02-Oct-2012\0\#M052X/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\TS of oxyacyl radical attacking SiMe2\0,2\Si,1.2369745662,-0.1810392317,-0.5818251662\C,-0.7338036077,-0.341886502,-0.35

48481321\H,0.8063610681,0.3749900802,-1.9695514498\H,1.9964871257,-1.3
3752439,-1.1347004274\O,-1.3875210697,-1.2836335809,-0.6888668001\H,0.
6823807085,-0.411841283,1.9840889562\H,2.2138749837,-1.2574253052,1.51
8989251\H,0.6162033375,-2.0416144035,1.1960916052\C,1.1594889676,-1.10
88694271,1.301337795\C,2.1592168067,1.3477906367,0.0292551596\H,1.4090
523248,2.0540387695,0.3890159707\H,2.8381863825,1.1185150024,0.8481176
73\H,2.7100870309,1.8203937033,-0.7810149713\O,-1.2223673137,0.7693276
535,0.2074766547\C,-2.6569534736,0.7877611048,0.3740689547\H,-2.964272
4762,-0.039588211,1.0087745817\H,-3.1399239661,0.7019532663,-0.5959800
309\H,-2.8809323953,1.7409221175,0.8382083759\\Version=AM64L-G09RevC.0
1\State=2-A\HF=-313.3153316\S2=0.761871\S2-1=0.\S2A=0.750086\RMSD=5.23
4e-09\RMSF=3.514e-06\Dipole=-0.1512859,0.6245695,0.7630114\Quadrupole=
4.119199,-2.5533027,-1.5658963,-3.2923016,-0.8701225,-1.4914039\PG=C01
[X(C4H11O2Si1)]\@

M05-2X/aug-cc-pVDZ

1\1\GINC-GOMBERG17\FTS\UM052X\Aug-CC-pVDZ\C4H11O2Si1(2)\SHORVAT\02-Oct
-2012\0\#M052X/aug-cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=
checkpoint guess=check\\TS of oxyacyl radical attacking SiMe2\\0,2\Si,1
.2357057229,-0.1778671122,-0.5702412678\C,-0.7467100938,-0.3369081573,
-0.3485453939\H,0.7778816097,0.4090858024,-1.9520993023\H,1.9784957556
, -1.3384789097,-1.158574487\O,-1.3954497722,-1.2926216714,-0.676861737
3\H,0.7097588523,-0.4044704258,2.0079469857\H,2.2321842518,-1.26613287
45,1.5146365062\H,0.6163619692,-2.0417902529,1.2144665117\C,1.17048514
37,-1.1083850427,1.3123700691\C,2.1917407488,1.3482478237,0.0318887089
\H,1.4578925065,2.0611755413,0.426263304\H,2.8956152247,1.0982110895,0
.8303779224\H,2.7235113156,1.8263170952,-0.7944686861\O,-1.2486441911,
0.7791755868,0.1978160648\C,-2.6857413873,0.7821159443,0.3577563037\H,
-2.9853152069,-0.0484490132,1.0009259838\H,-3.1623863122,0.6809436116,
-0.6197431672\H,-2.9228471373,1.7421009648,0.8147236813\\Version=AM64L
-G09RevC.01\State=2-A\HF=-598.8683777\S2=0.76301\S2-1=0.\S2A=0.750104\
RMSD=8.409e-09\RMSF=2.165e-06\Dipole=-0.0766044,0.6620357,0.7749358\Qu
adрупole=4.0419926,-2.5154901,-1.5265025,-3.2778555,-0.8304962,-1.4619
25\PG=C01 [X(C4H11O2Si1)]\@

M06-2X/6-311G(d,p)

1\1\GINC-GOMBERG07\FTS\UM062X\6-311G(d,p)\C4H11O2Si1(2)\SHORVAT\02-Oct
-2012\0\#M062X/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=che
ckpoint guess=check\\TS of oxyacyl radical attacking SiMe2\\0,2\Si,1.23
87620186,-0.1752641512,-0.6027946856\C,-0.7366619917,-0.3442217811,-0.
3640531252\H,0.8164536266,0.3781182051,-1.9764736536\H,1.991885458,-1.
3488005983,-1.1209179362\O,-1.3847778424,-1.2828114586,-0.7166244843\H
,0.6722403345,-0.3656159978,1.9786161151\H,2.1951328321,-1.2376881744,
1.521973425\H,0.5856896019,-2.0091432532,1.2162936779\C,1.1403463902,-
1.0779337,1.3015147531\C,2.1813323821,1.3383007974,0.0238125093\H,1.44
74899098,2.0437215313,0.4238066576\H,2.8825123895,1.089365284,0.820964
3432\H,2.7156128796,1.8323168823,-0.7879512244\O,-1.2317404175,0.75498
17209,0.216725654\C,-2.6602174572,0.7697856316,0.3808518855\H,-2.97519
61901,-0.0781642946,0.9890666924\H,-3.1477718724,0.7163778629,-0.59250
30893\H,-2.8885530516,1.7089454939,0.8763304855\\Version=AM64L-G09RevC
.01\State=2-A\HF=-598.8245877\S2=0.759677\S2-1=0.\S2A=0.750061\RMSD=3.
363e-09\RMSF=4.368e-06\Dipole=-0.1653489,0.5993213,0.7143606\Quadrupol
e=4.0419778,-2.5191149,-1.5228629,-3.1266789,-0.998856,-1.4210199\PG=C
01 [X(C4H11O2Si1)]\@

M06-2X/DZP

1\1\GINC-GOMBERG17\FTS\UM062X\Gen\C4H11O2Si1(2)\SHORVAT\03-Oct-2012\0\
\#M062X/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=chec
kpoint guess=check\\TS of oxyacyl radical attacking SiMe2\\0,2\Si,1.242
1381596,-0.1786943454,-0.591571131\C,-0.7378723159,-0.346045602,-0.360
4397265\H,0.8016676893,0.3932631603,-1.9578544074\H,1.984502365,-1.341

9134964,-1.1337566517\O,-1.3846126377,-1.2861296252,-0.7102096316\H,0.6782596866,-0.3758237674,1.9844035828\H,2.2018640759,-1.2396483785,1.5230976197\H,0.5961768109,-2.0150802818,1.2162881721\C,1.1469295836,-1.0813167713,1.300393791\C,2.1819122682,1.3352496014,0.023769092\H,1.4430537862,2.0421819247,0.4119269866\H,2.8784822871,1.0954277659,0.8275633306\H,2.719276692,1.824043516,-0.7890333372\O,-1.2325550756,0.7564668001,0.2134361602\C,-2.6614388544,0.7727739221,0.375523236\H,-2.9777413697,-0.0707827225,0.9891043278\H,-3.1476856713,0.7127896785,-0.5981202196\H,-2.8898184796,1.7155086215,0.8641168063\\Version=AM64L-G09RevC.01\State=2-A\HF=-313.2247517\S2=0.758577\S2-1=0.\S2A=0.750048\RMSD=6.513e-09\RMSF=3.285e-06\Dipole=-0.1655435,0.5934191,0.6912767\Quadrupole=4.0315631,-2.5113604,-1.5202026,-3.2027054,-1.0054632,-1.3790981\PG=C01 [X(C4H11O2Si1)]\\@

M06-2X/aug-cc-pVDZ

1\1\GINC-GOMBERG04\FTS\UM062X\Aug-CC-pVDZ\C4H11O2Si1(2)\SHORVAT\03-Oct-2012\0\#M062X/aug-cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\\TS of oxyacyl radical attacking SiMe2\\0,2\Si,1.2317462434,-0.1731247421,-0.5888645161\C,-0.7463835625,-0.3369554841,-0.3524410654\H,0.8017974981,0.4106558201,-1.965748277\H,1.966056322,-1.3518554813,-1.1433063573\O,-1.3917340493,-1.2935697676,-0.6845511348\H,0.7156472079,-0.3795191549,2.006133465\H,2.2323391692,-1.254665492,1.5043269203\H,0.6067515214,-2.0257414252,1.2240572397\C,1.1674742786,-1.0922020415,1.3098490166\C,2.1933717821,1.3386158471,0.0318326873\H,1.4620800009,2.0481838403,0.4431289243\H,2.9033870908,1.0796577662,0.8248064343\H,2.7218310587,1.8342031886,-0.7891065663\O,-1.2540939024,0.7752381948,0.2000497711\C,-2.6845559224,0.7763081424,0.3605428177\H,-2.9899164415,-0.0624923956,0.9947619343\H,-3.1683621051,0.6879153609,-0.6176949319\H,-2.92489719,1.7316178239,0.8308616381\\Version=AM64L-G09RevC.01\State=2-A\HF=-598.7673045\S2=0.759995\S2-1=0.\S2A=0.750064\RMSD=8.188e-09\RMSF=3.398e-06\Dipole=-0.0678538,0.6321971,0.7250692\Quadrupole=3.8685748,-2.4449126,-1.4236621,-3.1886892,-0.8825944,-1.3985228\PG=C01 [X(C4H11O2Si1)]\\@

ROMP2/6-311G(d,p)//MP2/6-311G(d,p)

MP2= -597.6129587

ROMP2/DZP//MP2/DZP

MP2= -312.4491527

ROMP2/cc-pVDZ//MP2/cc-pVDZ

MP2= -597.4858232

ROMP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ

MP2= -597.5632828

ROMP2/6-311G(d,p)//BHandHLYP/6-311G(d,p)

MP2= -597.614392

ROMP2/DZP//BHandHLYP/DZP

MP2= -312.4511812

ROMP2/cc-pVDZ//BHandHLYP/cc-pVDZ

MP2= -597.4877634

ROMP2/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ

MP2= -597.5649115

ROMP2/6-311G(d,p)//B3LYP/6-311G(d,p)

MP2= -597.6108168

QCISD/6-311G(d,p)//MP2/6-311G(d,p)

QCISD= -597.688973

QCISD/DZP//MP2/DZP

QCISD=-312.4464955

QCISD/cc-pVDZ//MP2/cc-pVDZ

QCISD=-597.570020

QCISD/aug-cc-pVDZ//MP2/aug-cc-pVDZ

QCISD= -597.649128

QCISD/6-311G(d,p)//BHandHLYP/6-311G(d,p)

QCISD = -597.6866344

QCISD/DZP//BHandHLYP/DZP

QCISD= -237.2895951

QCISD/cc-pVDZ//BHandHLYP/cc-pVDZ

QCISD= -597.5706181

QCISD/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ

QCISD= -

QCISD/6-311G(d,p)//B3LYP/6-311G(d,p)

QCISD=-597.7342169

CCSD(T)/6-311G(d,p)//MP2/6-311G(d,p)

CCSD(T)= -597.728180

CCSD(T)/DZP//MP2/DZP

CCSD(T)= -312.5648479

CCSD(T)/cc-pVDZ//MP2/cc-pVDZ

CCSD(T)= -597.603069

CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ

CCSD(T)= -597.689121

CCSD(T)/6-311G(d,p)//BHandHLYP/6-311G(d,p)

CCSD(T)= -597.7259527

CCSD(T)/DZP//BHandHLYP/DZP

CCSD(T)= -312.5624466

CCSD(T)/cc-pVDZ//BHandHLYP/cc-pVDZ

CCSD(T)= -597.6001486

CCSD(T)/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ

CCSD(T)= -597.679854

CCSD(T)/6-311G(d,p)//B3LYP/6-311G(d,p)

CCSD(T)= -597.7276139

CCSD(T)/6-311G(d,p)//M06-2X/6-311G(d,p)

CCSD(T)=-597.7419621

CCSD(T)/6-311++G(d,p)//M06-2X/6-311G(d,p)

CCSD(T)=-597.7274471

CCSD(T)/cc-pVTZ//M06-2X/6-311G(d,p)

CCSD(T)=-597.9704782

CCSD(T)/aug-cc-pVTZ//M06-2X/6-311G(d,p)

CCSD(T)=-597.9999432

Transition State 8 (X=Ge)

HF/6-311G(d,p)

```
1\1\GINC-AC55\FTS\UHF\6-311G(d,p)\C4H11Ge1O2(2)\SXH563\26-Jul-2007\1\
# uhf/6-311G** opt=(ef,ts,calcfc,noeigen) freq=noraman geom=checkpoint
guess=check\single point on BS TS Sulfur\0,2\C\C,1,B1\H,2,B2,1,A1\H
,2,B3,1,A2,3,D1,0\H,2,B4,1,A3,3,D2,0\O,1,B5,2,A4,3,D3,0\C,2,B6,1,A5,6,
D4,0\H,7,B7,2,A6,1,D5,0\H,7,B8,2,A7,1,D6,0\H,7,B9,2,A8,1,D7,0\C,1,B10,
6,A9,2,D8,0\O,1,B11,6,A10,11,D9,0\H,11,B12,1,A11,6,D10,0\H,11,B13,1,A1
2,6,D11,0\H,11,B14,1,A13,6,D12,0\Ge,2,B15,1,A14,6,D13,0\H,1,B16,6,A15,
12,D14,0\H,7,B17,2,A16,1,D15,0\B1=3.11013598\B2=1.08127895\B3=1.08449
622\B4=1.08449058\B5=1.17535891\B6=3.10409088\B7=1.08035465\B8=1.07935
641\B9=1.08035573\B10=2.33781292\B11=1.31474069\B12=1.07876716\B13=1.0
8153474\B14=1.08153501\B15=1.966398\B16=2.63079779\B17=2.70353112\A1=6
3.75589959\A2=125.33051098\A3=125.40292801\A4=84.78572918\A5=92.246342
39\A6=84.07756933\A7=145.93568238\A8=84.0659457\A9=92.87240556\A10=125
.70746011\A11=135.7683631\A12=94.02418093\A13=94.02463059\A14=46.64493
635\A15=133.93525752\A16=62.71956055\D1=96.19198477\D2=-96.16182065\D3
=0.00552691\D4=-179.94403381\D5=123.00266036\D6=-0.02036643\D7=-123.02
445276\D8=-180.0256513\D9=-0.0010462\D10=180.00235246\D11=-54.93791575
\D12=54.94227199\D13=180.05410437\D14=135.55855817\D15=-33.47556368\
Version=IA64L-G03RevD.01\State=2-A\HF=-2382.8930853\S2=0.839165\S2-1=0.
\S2A=0.753272\RMSD=2.595e-09\RMSF=4.048e-06\Thermal=0.\Dipole=-0.53284
39,0.0001854,-0.1828183\PG=C01 [X(C4H11Ge1O2)]\@
```

HF/DZP

```
1\1\GINC-GOMBERG18\FTS\UHF\Gen\C4H11Ge1O2(2)\SHORVAT\16-Apr-2012\0\#U
HF/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\TS of MeO2CGe
H2Me\0,2\C,1.3206003145,0.3213485883,-0.0014891446\C,-1.4684040532,1.
7002775577,-0.0001209423\H,-0.6097571726,2.3576924291,-0.0016822647\H,
-2.0742130543,1.893678353,-0.8788237657\H,-2.0720659169,1.8950587455,0
.8797568607\O,1.7441370047,1.417589904,-0.00317496\C,-2.9496140283,-1.
0313306307,0.0030033669\H,-3.4109264549,-0.6537064624,0.9041137404\H,-
2.8440307912,-2.1055747076,0.0037387145\H,-3.412309641,-0.6550626707,-
0.8979650354\C,3.4566296588,-0.6287209502,-0.0020600666\O,2.0401750991
,-0.7791488747,-0.0007050966\H,3.8571816538,-1.630355693,-0.0011633931
\H,3.7770294377,-0.0943173154,-0.8860666006\H,3.7784893969,-0.09215336
09,0.8801034561\Ge,-0.8914583151,-0.1798738921,0.0006682298\H,-0.59723
33373,-0.8962129762,1.330825239\H,-0.5993518007,-0.8979060439,-1.32904
23378\Version=AM64L-G09RevC.01\State=2-A\HF=-311.2174508\S2=0.837247\
S2-1=0.\S2A=0.753147\RMSD=5.707e-09\RMSF=1.367e-05\Dipole=-0.0754887,-
0.5731626,0.0008123\Quadrupole=5.7605469,-4.8822463,-0.8783006,-3.4029
454,-0.0012418,0.0076469\PG=C01 [X(C4H11Ge1O2)]\@
```

MP2/6-311G(d,p)

```
1\1\GINC-AC12\FTS\UMP2-FC\6-311G(d,p)\C4H11Ge1O2(2)\SXH563\04-Feb-2008
\0\#MP2/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint
guess=check\TS of oxyacyl rad attacking dimethylgermane\0,2\C,-0.00
78408179,0.0000228514,0.0038313973\C,-0.011550998,-0.0000119843,3.0290
425166\H,0.9704623982,0.0000163429,2.5526650284\H,-0.1250619205,0.8867
606817,3.6571057488\H,-0.1251654629,-0.8870316774,3.6567411173\O,1.191
6574498,-0.0001783833,0.1088655486\C,-3.0213303182,0.0006504209,3.1354
005364\H,-2.8646577897,-0.9088539845,3.7130945347\H,-3.9578466612,0.00
08264744,2.5820277597\H,-2.8643069946,0.9101044061,3.7130784032\C,0.16
75347342,-0.0000611677,-2.3307350423\O,-0.6815421676,0.0001078367,-1.1
611340994\H,-0.514249671,0.0000371621,-3.1779745551\H,0.7992420234,0.8
```

895815255,-2.3399276637\H,0.7989385599,-0.8899196434,-2.3398905071\Ge,
-1.4079759617,0.0003239933,1.6407255398\H,-1.9847361079,-1.3300099369,
1.1121410347\H,-1.984133408,1.3309312553,1.1121740305\\Version=IA64L-G
03RevD.01\State=2-A\HF=-2382.893947\MP2=-2383.9887609\PUHF=-2382.90029
73\PM2-0=-2383.9932146\S2=0.791732\S2-1=0.766425\S2A=0.751067\RMDS=4.
407e-09\RMSE=1.087e-04\Thermal=0.\Dipole=-0.4205449,0.0000525,-0.11737
2\PG=C01 [X(C4H11Ge1O2)]\@

MP2/DZP

1\1\GINC-GOMBERG05\FTS\UMP2-FC\Gen\C4H11Ge1O2(2)\SHORVAT\17-Apr-2012\0
\\#MP2/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=check
point guess=check\\TS of MeO2CGeH2Me\\0,2\C,1.2587978277,0.2951108384,
-0.0011746667\C,-1.4416257559,1.6660725945,-0.0002338823\H,-0.57024558
97,2.3233281026,-0.0023232005\H,-2.0537941543,1.8529911921,-0.88566809
2\H,-2.0506171755,1.8545564104,0.8870659096\O,1.7067154163,1.412400012
4,-0.0026978325\C,-2.8996056908,-0.9815391086,0.0023387937\H,-3.347666
5137,-0.5830357889,0.9112403588\H,-2.8281625278,-2.0670104572,0.003112
2325\H,-3.3487954212,-0.5844032201,-0.9066030865\C,3.4206365449,-0.601
3550993,-0.0015014582\O,1.9940158145,-0.8319537223,-0.0003493427\H,3.8
696300996,-1.5918112196,-0.0006768889\H,3.71325304,-0.0425494454,-0.89
18379676\H,3.7143681215,-0.0405637701,0.8872179016\Ge,-0.8396445347,-0
.2105731982,0.0004753503\H,-0.6253285994,-0.963431895,1.3359525802\H,-
0.6270529014,-0.9649502255,-1.3344207109\\Version=AM64L-G09RevC.01\Sta
te=2-A\HF=-311.2184857\MP2=-312.308404\PUHF=-311.2246176\PM2-0=-312.3
126927\S2=0.790031\S2-1=0.765613\S2A=0.750987\RMDS=6.894e-09\RMSE=5.25
5e-06\Dipole=-0.0850735,-0.4367884,0.0006276\PG=C01 [X(C4H11Ge1O2)]\@

MP2/cc-pVDZ

1\1\GINC-AC5\FTS\UMP2-FC\CC-pVDZ\C4H11Ge1O2(2)\SXH563\05-Feb-2008\0\\#
MP2/cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess
=check\\TS of oxyacyl rad attacking dimethylgermane\\0,2\C,-0.01438418
45,0.0000143645,0.0091138901\C,-0.0164448704,0.0000054487,3.0174069862
\H,0.9686371626,-0.0002420663,2.5254214668\H,-0.1240386246,0.894380750
4,3.6519023799\H,-0.1244609216,-0.8942767019,3.6519613874\O,1.19059296
44,-0.0002214222,0.1179287161\C,-3.0153452703,0.0006156647,3.146238283
6\H,-2.8556253059,-0.9161949087,3.7302779582\H,-3.9676330272,0.0008243
421,2.5999462823\H,-2.8552343966,0.9173457684,3.7302972941\C,0.1763552
241,-0.0000250811,-2.3283823619\O,-0.6857795099,0.0001447937,-1.165411
5404\H,-0.4997532579,0.0001081223,-3.1921413478\H,0.8159213606,0.89566
7424,-2.3347414503\H,0.8155683452,-0.8959695641,-2.3347414786\Ge,-1.41
78369313,0.0002917246,1.6313842596\H,-2.0068214659,-1.3262231023,1.105
3813359\H,-2.0062804045,1.3270506158,1.105389267\\Version=IA64L-G03Rev
D.01\State=2-A\HF=-2382.844116\MP2=-2383.9017251\PUHF=-2382.8502203\PM
P2-0=-2383.9059952\S2=0.789864\S2-1=0.765558\S2A=0.75098\RMDS=4.715e-0
9\RMSE=3.034e-06\Thermal=0.\Dipole=-0.4019716,0.0000781,-0.1009094\PG=

MP2/aug-cc-pVDZ

1\1\GINC-AC21\FTS\UMP2-FC\Aug-CC-pVDZ\C4H11Ge1O2(2)\SXH563\05-Feb-2008
\0\\#MP2/aug-cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpo
int guess=check\\TS of oxyacyl rad attacking dimethylgermane\\0,2\C,-0
.0206215895,0.0000103258,0.0138202111\C,-0.013192373,0.0000062408,3.03
50468564\H,0.9783058037,-0.0002238396,2.560074804\H,-0.1275961046,0.89
34226984,3.6674283978\H,-0.1279938354,-0.8933299573,3.667469344\O,1.19
13322599,-0.0002399847,0.1196162471\C,-3.0122924107,0.0006168986,3.127
0749727\H,-2.8578978333,-0.9153110699,3.7111523528\H,-3.9585615532,0.0
008165875,2.5740813908\H,-2.857515864,0.9164752727,3.7111604662\C,0.16
88708602,-0.0000210641,-2.3421974471\O,-0.6948948235,0.0001535253,-1.1
64651763\H,-0.5182469438,0.0001237759,-3.1950216583\H,0.8016119152,0.8
979338259,-2.3424079461\H,0.8012406751,-0.8982374374,-2.3424139382\Ge,
-1.4093552275,0.0002891623,1.6447023231\H,-1.9831483533,-1.3341152573,
1.1111480698\H,-1.9826077159,1.3349264698,1.111148645\\Version=IA64L-G
03RevD.01\State=2-A\HF=-2382.8627926\MP2=-2383.985515\PUHF=-2382.86893
21\PM2-0=-2383.9897885\S2=0.789671\S2-1=0.765194\S2A=0.751002\RMDS=9.
836e-09\RMSE=1.366e-05\Thermal=0.\Dipole=-0.5065502,0.0001065,-0.06640

47\PG=C01 [X(C4H11Ge1O2)]\@

BHandHLYP/6-311G(d,p)

1\1\GINC-GOMBERG01\FTS\ROBHandHLYP\6-311G(d,p)\C4H11Ge1O2(2)\SHORVAT\17-Apr-2012\0\#\BHandHLYP\6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\TS of MeO2CGeH2Me\0,2\C,1.2544551473,0.3011308841,-0.0010581372\C,-1.4452744863,1.6757630283,-0.0003773579\H,-0.5799186442,2.3255665928,-0.001314931\H,-2.0499712868,1.8650438605,-0.8798751489\H,-2.0490308062,1.8663118937,0.8794919969\O,1.6887377842,1.4053523483,-0.00219242\C,-2.8858856689,-0.9929943709,0.0024992461\H,-3.3446150401,-0.6117902794,0.903639579\H,-2.792492815,-2.0685569005,0.0031498533\H,-3.3457922585,-0.6129821638,-0.8985445912\C,3.409096322,-0.6128152872,-0.0017025127\O,1.9909544351,-0.7992271315,-0.0006621978\H,3.8337752714,-1.6054756617,-0.0011916395\H,3.7155619801,-0.0673246852,-0.8856457225\H,3.7166758838,-0.0659387993,0.8809965535\Ge,-0.8586101249,-0.1960811124,0.0006440742\H,-0.605562728,-0.9313702722,1.3267832381\H,-0.6072249651,-0.9333299435,-1.3247238826\Version=AM64L-G09RevC.01\State=2-A\HF=-2386.232041\RMSD=6.526e-09\RMSF=1.446e-05\Dipole=-0.0156905,-0.4782527,0.0003839\Quadrupole=5.4297632,-4.5568731,-0.8728901,-3.1567499,-0.0015004,0.0048573\PG=C01 [X(C4H11Ge1O2)]\@

BHandHLYP/DZP

1\1\GINC-GOMBERG18\FTS\UBHandHLYP\Gen\C4H11Ge1O2(2)\SHORVAT\16-Apr-2012\0\#\BHandHLYP/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\TS of MeO2CGeH2Me\0,2\C,1.267339135,0.3023236243,-0.0010956633\C,-1.4472312521,1.6797043217,-0.0003490767\H,-0.581781173,2.3301481859,-0.0013159644\H,-2.0517821936,1.8737954354,-0.87929142\H,-2.0508000718,1.8750755231,0.8789830217\O,1.7024791036,1.4065048688,-0.002343686\C,-2.9051667762,-1.0022924479,0.0025049105\H,-3.3605686569,-0.6188301344,0.9043276554\H,-2.8099127877,-2.0776446751,0.030605914\H,-3.3617943156,-0.6198685039,-0.8991389541\C,3.4214258614,-0.6127852125,-0.0016812812\O,2.0035268094,-0.7985037664,-0.0005983771\H,3.8460167415,-1.6054953492,-0.0010689488\H,3.728322372,-0.0673855511,-0.8855740322\H,3.7294646308,-0.0658057322,0.8808367926\Ge,-0.858744744,-0.1927928118,0.0006389887\H,-0.612110279,-0.9314770056,1.3353843371\H,-0.6138044038,-0.933388769,-1.3333628937\Version=AM64L-G09RevC.01\State=2-A\HF=-313.0386868\S2=0.772804\S2-1=0.\S2A=0.750245\RMSD=9.941e-09\RMSF=1.789e-06\Dipole=-0.0307754,-0.5002145,0.0004617\Quadrupole=5.4687423,-4.5883985,-0.8803438,-3.0904981,-0.0013609,0.0052521\PG=C01 [X(C4H11Ge1O2)]\@

BHandHLYP/cc-pVDZ

1\1\GINC-AC57\FTS\UBHandHLYP\CC-pVDZ\C4H11Ge1O2(2)\SXH563\27-Jul-2007\0\#\BHandHLYP/cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\single point on BS TS Sulfur\0,2\C,-0.0452972581,0.0001710535,0.0422201461\C,-0.0123759463,-0.0001033013,3.0676912247\H,0.9542030388,0.0006484439,2.5615711533\H,-0.1052124255,0.8867664576,3.6986374813\H,-0.1039336945,-0.8872249708,3.6984704109\O,1.141838542,0.010410167,0.1422204851\C,-3.0527035879,-0.0023967147,3.2183949429\H,-2.9017177447,-0.9116528279,3.7990137427\H,-3.9882259955,-0.0030417999,2.6618533288\H,-2.903086946,0.9069619945,3.7992080326\C,0.1025686047,0.0005010105,-2.2904474993\O,-0.7040347885,-0.0002116851,-1.1111560558\H,-0.5945353696,0.0000589292,-3.1260200566\H,0.7349304867,0.8896520387,-2.3194679653\H,0.7362574093,-0.8876993471,-2.3196341775\Ge,-1.438368553,-0.001026699,1.718728534\H,-1.998970265,-1.3284785856,1.1716446987\H,-2.0009417186,1.3257083203,1.1719314925\Version=IA64L-G03RevD.01\State=2-A\HF=-2386.1731498\S2=0.77326\S2-1=0.\S2A=0.750242\RMSD=8.418e-09\RMSF=2.240e-06\Thermal=0.\Dipole=-0.4415239,-0.0003194,-0.1542531\PG=C01 [X(C4H11Ge1O2)]\@

BHandHLYP/aug-cc-pVDZ

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1\1\GINC-AC17\FTS\UBHandHLYP\Aug-CC-pVDZ\C4H11Ge1O2(2)\SXH563\30-Jul-2
007\0\#\BHandHLYP/aug-cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geo
m=checkpoint guess=check\single point on BS TS Sulfur\0,2\C,-0.04126
14743,0.0001676399,0.0383653074\C,-0.0084703636,-0.0001072923,3.086059
8182\H,0.964665575,0.0006595072,2.5997324285\H,-0.1067046416,0.8837590
464,3.7159867895\H,-0.1053940697,-0.8842340321,3.7158242838\O,1.147904
2596,0.0010444207,0.1362526381\C,-3.054908426,-0.0023885216,3.20318956
14\H,-2.9129968889,-0.9091063056,3.7850597398\H,-3.9824619026,-0.00302
39968,2.6392268808\H,-2.9143463133,0.9044265004,3.7852357385\C,0.09261
32016,0.0005013602,-2.3026291626\O,-0.7048554399,-0.0002119794,-1.1117
412658\H,-0.6141780971,0.0000570218,-3.1265655374\H,0.7199638497,0.889
3830726,-2.3335899424\H,0.721287958,-0.8874381375,-2.3337675953\Ge,-1.
4293603143,-0.0010360533,1.7335114324\H,-1.974559122,-1.3307469154,1.1
772248832\H,-1.976544002,1.3279679985,1.1774839208\Version=IA64L-G03R
evD.01\State=2-A\HF=-2386.1970816\S2=0.7733\S2-1=0.\S2A=0.75025\RMSD=7
.897e-09\RMSF=2.115e-06\Thermal=0.\Dipole=-0.5124252,-0.0003662,-0.146
6004\PG=C01 [X(C4H11Ge1O2)]\@

```

ROMP2/6-311G(d,p)//MP2/6-311G(d,p)

MP2= -2383.985591

ROMP2/DZP//MP2/DZP

MP2= -312.3051025

ROMP2/cc-pVDZ//MP2/cc-pVDZ

MP2= -2383.8985023

ROMP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ

MP2= -2383.9824832

ROMP2/6-311G(d,p)//BHandHLYP/6-311G(d,p)

MP2= -2383.9831571

ROMP2/DZP//BHandHLYP/DZP

MP2= -312.3024063

QCISD/6-311G(d,p)//MP2/6-311G(d,p)

QCISD= -2384.066092

QCISD/DZP//MP2/DZP

QCISD= -312.3872224

QCISD/cc-pVDZ//MP2/cc-pVDZ

QCISD= -2383.9863233

QCISD/aug-cc-pVDZ//MP2/aug-cc-pVDZ

QCISD= -2384.109930

QCISD/6-311G(d,p)//BHandHLYP/6-311G(d,p)

QCISD = -2384.0645407

QCISD/DZP//BHandHLYP/DZP

QCISD= -312.3856618

QCISD/cc-pVDZ//BHandHLYP/cc-pVDZ

QCISD= -2383.9843622

CCSD(T)/6-311G(d,p)//MP2/6-311G(d,p)

CCSD(T)= -2384.1061756

CCSD(T)/DZP//MP2/DZP

CCSD(T)= -312.4265955

CCSD(T)/cc-pVDZ//MP2/cc-pVDZ

CCSD(T)= -2384.0206317

CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ

CCSD(T)=

CCSD(T)/6-311G(d,p)//BHandHLYP/6-311G(d,p)

CCSD(T)=-2384.104195

CCSD(T)/DZP//BHandHLYP/DZP

CCSD(T)= -312.4247982

CCSD(T)/cc-pVDZ//BHandHLYP/cc-pVDZ

CCSD(T)= -2384.0184423

Transition State 9 (X=Ge)

HF/6-311G(d,p)

1\1\GINC-AC21\FTS\UHF\6-311G(d,p)\C4H11Ge1O2(2)\SXH563\10-Aug-2008\0\#\UHF/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\FS TS of oxyacyl radical attacking dimethylgermane\0,2\Ge,0.0278631324,0.0187363457,-0.0644990392\C,0.0660214616,0.0556454972,2.2268938483\H,1.5591450944,0.089056241,0.2363359564\H,-0.1706107445,1.2618835342,-0.9520246721\O,0.1182993473,1.0356927926,2.8648712742\H,-2.3551637264,-0.6931958107,1.2395594947\H,-2.5679110308,0.1728074351,-0.3228206232\H,-2.2197720344,1.1037647519,1.1772588016\C,-2.0936280274,0.1719875849,0.6491527959\C,-0.1859076519,-1.6894260013,-1.0176135264\H,-0.1133950053,-2.5095415509,-0.310337159\H,-1.1463382928,-1.7498442823,-1.5172255495\H,0.6015356561,-1.8054599528,-1.7546500874\O,0.1028326572,-1.1802554186,2.6615891436\C,0.2556245571,-1.370090635,4.0689333392\H,-0.5735336673,-0.9202427386,4.5972248893\H,1.183904783,-0.9295355432,4.4047556698\H,0.266796494,-2.4378555508,4.2189569797\Version=IA64L-G03RevD.01\State=2-A\HF=-2382.8924711\S2=0.844124\S2-1=0.\S2A=0.752751\RMSD=6.967e-09\RMSF=3.089e-06\Thermal=0.\Dipole=-0.3933686,-0.9604248,0.3988492\PG=C01 [X(C4H11Ge1O2)]\@

HF/DZP

1\1\GINC-GOMBERG19\FTS\UHF\Gen\C4H11Ge1O2(2)\SHORVAT\16-Apr-2012\0\#\UHF/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\FS TS of MeTeCO2Me\0,2\Ge,1.1213718182,-0.1708284306,-0.4645225078\C,-1.1489681121,-0.3773789005,-0.2115449508\H,0.5975267503,0.2038829801,-1.8917986713\H,2.0508048044,-1.3635900104,-0.7704361649\O,-1.7500990422,-1.3458649669,-0.4771628101\H,0.1656128864,-0.2545575441,2.1772502277\H,1.7614098285,-1.0415579526,1.9097609396\H,0.2473246714,-1.9319918789,1.5202052162\C,0.7285094025,-0.9698159505,1.5966408853\C,2.0642199144,1.4542214221,0.1207361471\H,1.3379591504,2.216919396,0.3844141122\H,2.6934655971,1.265488699,0.9834064066\H,2.6798883737,1.8367686582,-0.6865140077\O,-1.6295886996,0.7759704262,0.1838113864\C,-3.0504909117,0.8911564821,0.2743861571\H,-3.4371395319,0.1752427596,0.9863415095\H,-3.4995288991,0.7211342287,-0.694136659\H,-3.2398940005,1.8988225826,0.6082107839\Version=AM64L-G09RevC.01\State=2-A\HF=-311.2176665\S2=0.84193\S2-1=0.\S2A=0.752579\RMSD=5.080e-09\RMSF=1.270e-06\Dipole=-0.3865785,0.7627301,0.719697\Quadrupole=4.2840817,-3.1981855,-1.0858962,-4.2044166,-0.7174686,-1.3908015\PG=C01 [X(C4H11Ge1O2)]\@

MP2/6-311G(d,p)

1\1\GINC-GOMBERG04\FTS\UMP2-FC\6-311G(d,p)\C4H11Ge1O2(2)\SHORVAT\18-Apr-2012\0\#\MP2/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\GS of MeTeCO2Me\0,2\Ge,1.0215219809,-0.1680520456,-0.4359067041\C,-1.0653904002,-0.3497785214,-0.2705919945\H,0.6250673628,0.3257089097,-1.9021646805\H,1.7989943432,-1.4415543955,-0.8189997

977\O,-1.6940109916,-1.3186414526,-0.5993022376\H,0.2253108019,-0.0738
 514606,2.1652719573\H,1.7603315229,-1.0149237861,1.9312038655\H,0.1603
 230439,-1.7943907983,1.5887205882\C,0.727982266,-0.8654362508,1.611182
 2108\C,2.0613155908,1.4070596192,0.1369929796\H,1.3572624612,2.1843540
 998,0.4484846081\H,2.7128043617,1.1638486895,0.9788494173\H,2.65759156
 54,1.7874728419,-0.6950674072\O,-1.5690555789,0.801356502,0.2067804421
 \C,-3.0140608903,0.8223919177,0.2835606152\H,-3.3660026693,0.027915081
 5,0.9432707462\H,-3.44504936,0.689176394,-0.7096528576\H,-3.2625514103
 ,1.8013666556,0.6864162488\\Version=AM64L-G09RevC.01\State=2-A\HF=-238
 2.8889105\MP2=-2383.9880891\PUHF=-2382.8969968\PM2=0=-2383.9939586\S2
 =0.807531\S2-1=0.775375\S2A=0.751881\RMSD=8.041e-09\RMSF=4.541e-06\Dip
 ole=-0.36749,0.6235119,0.6483372\PG=C01 [X(C4H11Ge1O2)]\@

MP2/DZP

1\1\GINC-GOMBERG19\FTS\UMP2-FC\Gen\C4H11Ge1O2(2)\SHORVAT\16-Apr-2012\O
 \#MP2/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=check
 point guess=check\GS of MeTeCO2Me\0,2\Ge,1.0290119971,-0.1624722315,
 -0.4481870663\C,-1.0695479434,-0.3560783896,-0.2656200856\H,0.62059797
 71,0.3335915595,-1.9080583583\H,1.8161570165,-1.4357945073,-0.82139724
 23\O,-1.6989945399,-1.3226440215,-0.5969815933\H,0.2205183068,-0.07468
 57018,2.1652559609\H,1.7498245008,-1.0229242098,1.9193638766\H,0.14458
 03459,-1.7941590301,1.5855230888\C,0.7159309744,-0.867683391,1.6071640
 273\C,2.0680676627,1.4097134334,0.1336328687\H,1.3640825978,2.20837262
 59,0.3854600531\H,2.6770915991,1.1876132561,1.0120619992\H,2.708642418
 4,1.7564953773,-0.6803541282\O,-1.5684764888,0.7948655424,0.2156461153
 \C,-3.0133298809,0.8191764115,0.2938804683\H,-3.3666649661,0.025536548
 6,0.9538376327\H,-3.4456092971,0.6863558605,-0.6987756854\H,-3.2594982
 804,1.7987428674,0.6965960685\\Version=AM64L-G09RevC.01\State=2-A\HF=-
 311.2145201\MP2=-312.3084223\PUHF=-311.2224654\PM2=0=-312.3142072\S2=
 0.806939\S2-1=0.775419\S2A=0.751718\RMSD=5.213e-09\RMSF=3.690e-06\Dipo
 le=-0.3918335,0.6137174,0.6582757\PG=C01 [X(C4H11Ge1O2)]\@

MP2/cc-pVDZ

1\1\GINC-GOMBERG13\FTS\UMP2-FC\CC-pVDZ\C4H11Ge1O2(2)\SHORVAT\14-May-20
 12\O\#MP2/cc-pvdz opt=(ts,calcfc,noeigen) freq=noraman\GS of MeTeCO2
 Me\0,2\Ge,1.023703,-0.221176,-0.37141\C,-1.055187,-0.37668,-0.231862\H,
 0.673054,0.101977,-1.898982\H,1.820539,-1.521994,-0.595115\O,-1.6933
 84,-1.373524,-0.464563\H,0.180314,0.149112,2.198033\H,1.739523,-0.8083
 1,2.102034\H,0.137923,-1.638905,1.804752\C,0.705879,-0.70054,1.740081\H,
 2.039145,1.419101,0.037953\H,1.315157,2.235742,0.200855\H,2.649528,1.
 301076,0.946872\H,2.686587,1.689914,-0.811123\O,-1.556725,0.831189,0.
 110958\C,-3.005207,0.865941,0.160384\H,-3.379748,0.145894,0.903362\H,-
 3.427767,0.622353,-0.825811\H,-3.260509,1.892525,0.449758\\Version=AM6
 4L-G09RevC.01\State=2-A\HF=-2382.8387802\MP2=-2383.9004609\PUHF=-2382.
 8465562\PM2=0=-2383.9060876\S2=0.805007\S2-1=0.77402\S2A=0.751765\RMS
 D=8.492e-09\RMSF=6.223e-07\Dipole=-0.3554345,0.6824417,0.5632242\Polar
 =110.693217,0.6715966,79.0460184,9.3692215,-4.5647031,97.3979961\PG=C0
 1 [X(C4H11Ge1O2)]\@

MP2/aug-cc-pVDZ

1\1\GINC-AC9\FTS\UMP2-FC\Aug-CC-pVDZ\C4H11Ge1O2(2)\SXH563\12-Aug-2008\O
 \#MP2/aug-cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoi
 nt guess=check\FS TS of oxyacyl radical attacking dimethylgermane\0,
 2\Ge,0.0115696839,0.0064292171,0.0489501101\C,0.1241156386,0.052571378
 ,2.1242043021\H,1.608847951,-0.0587731324,0.1915648337\H,-0.0879534235
 ,1.3671297814,-0.6682026153\O,0.225844925,1.0616289895,2.7914034533\H,
 -2.3172650812,-0.8902175811,1.126223399\H,-2.5823735877,0.156725629,-0.
 3474230225\H,-2.2549511114,0.9326057249,1.2711999025\C,-2.0856650663,
 0.0602331157,0.6282696343\C,-0.2234697921,-1.6416398147,-1.0107211124\H,
 -0.2070928746,-2.4965981006,-0.3150963103\H,-1.1866671542,-1.6371420
 655,-1.5415993652\H,0.5995761959,-1.7576965859,-1.7303806529\O,0.10094
 219,-1.2169713938,2.6021655848\C,0.2346288283,-1.3035848384,4.05455609
 19\H,-0.5911708712,-0.7637205727,4.5373667402\H,1.1950141833,-0.871823
 2286,4.3666435843\H,0.1918323685,-2.3750298236,4.2772369781\\Version=I

A64L-G03RevD.01\State=2-A\HF=-2382.8578508\MP2=-2383.9849292\PUHF=-2382.865551\PMF2=0=-2383.9904662\S2=0.803877\S2-1=0.773015\S2A=0.75177\RM
SD=6.604e-09\RMSF=1.883e-06\Thermal=0.\Dipole=-0.383745,-0.8409033,0.2344827\PG=C01 [X(C4H11Ge1O2)]\@

BHandHLYP/6-311G(d,p)

1\1\GINC-GOMBERG19\FTS\UBHandHLYP\6-311G(d,p)\C4H11Ge1O2(2)\SHORVAT\18-Apr-2012\0\#\BHandHLYP/6-311G** opt=(ts,readfc,noeigen) freq=noraman
geom=checkpoint guess=check\FS TS of MeTeCO2Me\0,2\Ge,1.0325648358,-0.171550825,-0.37342855\C,-1.1008297131,-0.3445547575,-0.2547060632\H,0.5516855657,0.3421830694,-1.8092291027\H,1.8229121267,-1.3983790388,-0.8479885194\O,-1.6988370117,-1.3161107606,-0.5629201311\H,0.259142218,-0.1608120085,2.2041682879\H,1.7932695258,-1.0519941843,1.9432808311\H,0.2270459014,-1.8423329546,1.5767694081\C,0.7709160504,-0.9100194053,1.6164246333\C,2.0795778056,1.4137193846,0.1379129424\H,1.3963273768,2.1952952616,0.4536158361\H,2.7536354416,1.1896914517,0.9563438598\H,2.6472983306,1.7760263881,-0.7108265976\O,-1.6178750176,0.7919904975,0.1726538448\C,-3.0487021316,0.8487664274,0.245695404\H,-3.4169169717,0.0952785922,0.9303240683\H,-3.4774529337,0.6876613408,-0.7351203385\H,-3.2813773989,1.8391635211,0.6060781868\Version=AM64L-G09RevC.01\State=2-A\HF=-2386.2310745\S2=0.773304\S2-1=0.\S2A=0.750331\RMSD=2.294e-09\RMSF=2.584e-06\Dipole=-0.3610844,0.7226509,0.6431603\Quadrupole=4.6078355,-3.0997174,-1.5081181,-3.6719405,-0.78633,-1.2590923\PG=C01 [X(C4H11Ge1O2)]\@

BHandHLYP/DZP

1\1\GINC-GOMBERG05\FTS\UBHandHLYP\Gen\C4H11Ge1O2(2)\SHORVAT\03-Apr-2012\0\#\BHandHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\GS of MeTeCO2Me\0,2\Ge,1.0419435268,-0.1659876754,-0.398436516\C,-1.1017539927,-0.3528486861,-0.2521878758\H,0.5609144435,0.3362538465,-1.8388025528\H,1.8440229076,-1.4081799886,-0.8358289224\O,-1.7007048134,-1.3236559363,-0.5609568217\H,0.2372294967,-0.1448767105,2.1937554848\H,1.7777671825,-1.0309345677,1.9375467489\H,0.213843474,-1.8332964639,1.5784119543\C,0.7527133652,-0.8981676121,1.6150529246\C,2.0863925622,1.4157367677,0.1331226761\H,1.4014031223,2.2031068807,0.4316253775\H,2.7450000037,1.1968326935,0.9656289222\H,2.6726854842,1.7745330023,-0.7050057187\O,-1.6173715493,0.7820582179,0.1824289661\C,-3.0480759694,0.8393686278,0.2589802975\H,-3.4153486877,0.0809037346,0.9386240099\H,-3.479073706,0.6859403973,-0.7220936245\H,-3.2792028501,1.8272354723,0.6271826698\Version=AM64L-G09RevC.01\State=2-A\HF=-313.0337786\S2=0.773354\S2-1=0.\S2A=0.750312\RMSD=6.559e-09\RMSF=5.714e-06\Dipole=-0.3771348,0.7106825,0.6618964\Quadrupole=4.5847275,-3.09434,-1.4903875,-3.6863363,-0.7963955,-1.2638735\PG=C01 [X(C4H11Ge1O2)]\@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET13\FTS\UBHandHLYP\CC-pVDZ\C4H11Ge1O2(2)\SONIA\16-Sep-2008\0\#\BHANDHLYP/CC-PVDZ OPT=(TS,READFC,NOEIGEN) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\calc on the FS TS of oxyacyl rad attacking dimethylgermane\0,2\C,-0.098261389,0.6794283923,0.7224542833\O,-0.1421525708,0.6661898613,1.9086077012\H,2.1613108252,0.5987835441,-1.0164729177\H,2.722063791,-1.1078074736,-0.7991095909\H,2.4080046858,-0.0694244599,0.6493279715\C,2.1374044214,-0.286776257,-0.3831065196\H,0.4142154291,-1.4779140556,-1.9503923505\H,0.391525339,-2.3119639844,0.4781631902\C,-1.8716687815,-1.025573053,-0.6141622185\H,-2.3297364642,-0.9350734128,0.3727939086\H,-2.1545319751,-0.1739007794,-1.236370063\H,-2.1939386448,-1.9540057202,-1.0925393329\C,-0.4435228034,2.9868897021,0.6271907703\H,-1.3672776818,2.9428217178,1.2059642682\H,-0.5161168134,3.7402360209,-0.1540585197\H,0.3910070435,3.2040111956,1.2955977271\O,-0.2242146567,1.744892734,-0.0525174756\Ge,0.1456469875,-1.1208823769,-0.4598713747\Version=x86-Linux-G03RevB.04\State=2-A\HF=-2386.1661495\S2=0.774033\S2-1=0.\S2A=0.750318\RMSD=6.579e-09\RMSF=4.952e-07\Dipole=-0.0083667,0.8880729,-0.3334488\PG=C01 [X(C4H11Ge1O2)]\@

BHandHLYP/aug-cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET16\FTS\UBHandHLYP\Aug-CC-pVDZ\C4H11Ge1O2(2)\SONIA\17-Sep-2008\0\#BHANDHLYP/AUG-CC-PVDZ OPT=(TS,READFC,NOEIGEN) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\calc on the FS TS of oxyacyl rad attacking dimethylgermane\0,2\C,-0.0890320103,0.678179624,0.7299823464\O,-0.1238641566,0.6553686903,1.9188771279\H,2.1309506216,0.5631058685,-1.1470779891\H,2.7107843437,-1.1066305523,-0.7807921737\H,2.4053107845,0.0540576016,0.5674752314\C,2.1273096222,-0.256768714,-0.4351933783\H,0.4506987059,-1.5743794483,-1.9079426292\H,0.3797918372,-2.2717410186,0.5493475518\C,-1.8639086522,-1.0106250789,-0.6676932946\H,-2.3553650995,-0.86423306,0.2932549899\H,-2.1130221439,-0.1888859792,-1.3382900038\H,-2.1931597203,-1.9504468997,-1.1115763803\C,-0.4366883417,2.9932964723,0.6547507583\H,-1.3551819269,2.9426016824,1.2356225633\H,-0.514431088,3.7454734257,-0.123672727\H,0.4016987179,3.2051373902,1.31504735\O,-0.2201165373,1.7514525209,-0.0331931581\Ge,0.1368027129,-1.1322850787,-0.4477483167\Version=x86-Linux-G03RevB.04\State=2-A\HF=-2386.1900578\S2=0.774383\S2-1=0.\S2A=0.750316\RMSD=5.382e-09\RMSF=3.031e-06\Dipole=0.0165902,0.8448152,-0.4433066\PG=C01 [X(C4H11Ge1O2)]\@

ROMP2/6-311G(d,p)//MP2/6-311G(d,p)

MP2= -2383.9878585

ROMP2/DZP//MP2/DZP

MP2= -312.308066

ROMP2/cc-pVDZ//MP2/cc-pVDZ

MP2= -2383.8996893

ROMP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ

MP2= -2383.984216

ROMP2/6-311G(d,p)//BHandHLYP/6-311G(d,p)

MP2= -2383.9935878

ROMP2/DZP//BHandHLYP/DZP

MP2= -312.312266

ROMP2/cc-pVDZ//BHandHLYP/cc-pVDZ

MP2=

ROMP2/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ

MP2=

QCISD/6-311G(d,p)//MP2/6-311G(d,p)

QCISD=

QCISD/DZP//MP2/DZP

QCISD= -312.3836201

QCISD/cc-pVDZ//MP2/cc-pVDZ

QCISD=

QCISD/aug-cc-pVDZ//MP2/aug-cc-pVDZ

QCISD=-2384.0633221

QCISD/6-311G(d,p)//BHandHLYP/6-311G(d,p)

QCISD =

QCISD/DZP//BHandHLYP/DZP

QCISD= -312.3816478

QCISD/cc-pVDZ//BHandHLYP/cc-pVDZ

QCISD= -2383.9843622

QCISD/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ

QCISD=

QCISD/6-311G(d,p)//B3LYP/6-311G(d,p)

QCISD=

CCSD(T)/6-311G(d,p)//MP2/6-311G(d,p)

CCSD(T)= -2384.102340

CCSD(T)/DZP//MP2/DZP

CCSD(T)= -312.4231

CCSD(T)/cc-pVDZ//MP2/cc-pVDZ

CCSD(T)= -2384.015991

CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ

CCSD(T)=

CCSD(T)/6-311G(d,p)//BHandHLYP/6-311G(d,p)

CCSD(T)=

CCSD(T)/DZP//BHandHLYP/DZP

CCSD(T)= -312.4210026

CCSD(T)/cc-pVDZ//BHandHLYP/cc-pVDZ

CCSD(T)=

CCSD(T)/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ

CCSD(T)=

CCSD(T)/6-311G(d,p)//B3LYP/6-311G(d,p)

CCSD(T)=

Transition State 8 (X=Sn)**HF/DZP**

```
1\1\GINC-AC32\FTS\UHF\Gen\C4H11O2Sn1(2)\SXH563\30-Jul-2007\0\#\uhf/gen
pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint gues
s=check\TS of oxyacetyl attacking Sn atom in dimethylstannane\0,2\C,
0.0982649543,-0.0002177518,-0.1652029766\C,0.0808438246,-0.0013721786,
3.1243887651\H,1.031060696,-0.0047226002,2.6079987228\H,0.003961298,0.
8810032144,3.7492631731\H,-0.0006432602,-0.8810365549,3.7524738453\O,1
.2623275685,-0.0014410241,-0.0084900066\C,-3.2283610669,0.000509835,3.
353550138\H,-3.0621067514,-0.9029539488,3.9213380917\H,-4.1658629801,0
.0024845262,2.8190130698\H,-3.0597015501,0.9019759852,3.9238025291\C,0
.2831542593,0.000550058,-2.4964133338\O,-0.5253767264,0.0008781317,-1.
3216898759\H,-0.4068594243,0.0016178659,-3.3254353276\H,0.9072844755,0
.8833403209,-2.5221002859\H,0.9054616718,-0.8835037808,-2.5228609591\H
,-2.0917352275,-1.4670181564,1.0399606049\H,-2.0895411954,1.4694425906
,1.0414851912\Sn,-1.5103505776,0.000454624,1.6855312293\Version=IA64L
-G03RevD.01\State=2-A\HF=-310.8080464\S2=0.859874\S2-1=0.\S2A=0.755061
\RMSD=4.113e-09\RMSF=3.747e-05\Thermal=0.\Dipole=-0.4696176,0.0004832,
-0.1574207\PG=C01 [X(C4H11O2Sn1)]\@
```

MP2/DZP

1\1\GINC-AC26\FTS\UMP2-FC\Gen\C4H11O2Sn1(2)\SXH563\08-Aug-2008\0\#MP2
/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint
guess=check\|S of oxyacyl radical attacking dimethylstannane\|0,2\C,-0
.015955125,0.0002194879,0.0244670163\C,-0.0755641203,-0.0002061715,3.1
287055121\H,0.8653633757,0.0007928322,2.5770481197\H,-0.1749143167,0.8
905735191,3.75156509\H,-0.1739973562,-0.8923855245,3.7497216288\O,1.17
30524442,0.0005729394,0.2073150905\C,-3.1211442914,0.0004465754,3.4978
614342\H,-2.893458039,-0.9057734825,4.0566275693\H,-4.1278063535,0.000
0881253,3.0831914407\H,-2.8938934295,0.9071086179,4.0560872331\C,0.308
3124335,-0.000165591,-2.2967922409\O,-0.6143828857,-0.0001913507,-1.18
07587437\H,-0.3198237777,-0.0004807048,-3.1842744335\H,0.9382412426,0.
890017661,-2.2649906512\H,0.9386764341,-0.890029517,-2.2646699962\H,-2
.3509530012,-1.4533192761,1.0599849601\H,-2.3505832905,1.4540146906,1.
0600945446\Sn,-1.6869641449,0.0002368462,1.6653502326\|Version=IA64L-G
03RevD.01\State=2-A\HF=-310.8071772\MP2=-311.8901664\PUHF=-310.8143884
\MP2-0=-311.895414\S2=0.805101\S2-1=0.774449\S2A=0.751995\RMSD=7.287e
-09\RMSF=1.673e-06\Thermal=0.\Dipole=-0.2373538,-0.0002021,-0.058887\P
G=C01 [X(C4H11O2Sn1)]\@

BHandHLYP/DZP

1\1\GINC-GOMBERG19\FTS\UBHandHLYP\Gen\C4H11O2Sn1(2)\SHORVAT\10-May-201
2\0\#BHandHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\|
BS TS Of oxyacyl rad attacking SnH3Me2\|0,2\C,1.553799,0.319163,-0.000
001\C,-1.243053,1.885549,-0.000015\H,-0.320761,2.452462,-0.000106\H,-1
.827202,2.123034,-0.881191\H,-1.827055,2.123089,0.881245\O,1.991673,1.
422075,-0.000012\C,-3.01865,-0.823518,-0.000056\H,-3.42764,-0.393479,0
.90238\H,-3.026749,-1.902998,-0.000021\H,-3.427561,-0.393539,-0.902555
\C,3.705529,-0.606341,-0.000018\O,2.284897,-0.78493,-0.000006\H,4.1242
41,-1.601419,0.000009\H,4.014735,-0.061843,-0.883549\H,4.014742,-0.061
79,0.883478\H,-0.518316,-1.043007,1.469579\H,-0.518268,-1.043065,-1.46
9504\Sn,-0.749169,-0.198874,0.000019\|Version=AM64L-G09RevC.01\State=2
-A\HF=-312.6264565\S2=0.777327\S2-1=0.\S2A=0.750352\RMSD=1.655e-09\RMS
F=1.387e-06\Dipole=-0.0459351,-0.4198201,-0.0000062\Polar=0.,0.,0.,
0.,0.\Quadrupole=6.0688364,-4.7879108,-1.2809255,-3.4342342,-0.0000067
,0.0000418\PG=C01 [X(C4H11O2Sn1)]\@

ROMP2/DZP//MP2/DZP

MP2= -311.8863571

ROMP2/DZP//BHandHLYP/DZP

MP2= -311.8573213

QCISD/DZP//MP2/DZP

QCISD= -311.970142

QCISD/DZP//BHandHLYP/DZP

QCISD= -311.9693089

CCSD(T)/DZP//MP2/DZP

CCSD(T)= -312.009739

CCSD(T)/DZP//BHandHLYP/DZP

CCSD(T)=-312.0082534

Transition State 9 (X=Sn)

UHF/DZP

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET16\FTS\UHF\Gen\C4H11O2Sn1(2)\SONIA
\19-Sep-2008\0\#UHF/GEN PSEUDO=READ OPT=(TS,CALCFC,NOEIGEN) FREQ=NORA
MAN GEOM=CHECKPOINT GUESS=CHECK\|FS TS of oxyacyl radical attacking dim
ethylstannane\|0,2\C,-0.0467708448,1.041226938,0.905511528\O,-0.074368
487,1.0066173623,2.0764335995\H,2.2370138189,0.8788171585,-0.962569092

7\H,2.7955393056,-0.8155531586,-0.6757403586\H,2.5037076167,0.28411096
81,0.7252544478\C,2.2496338097,0.0344884774,-0.2921091998\H,0.50098126
6,-1.4997015247,-2.0266753366\H,0.3701036032,-2.3244283053,0.657220191
\C,-2.0766153566,-0.7649945408,-0.5775023173\H,-2.5189865831,-0.627538
1687,0.4032523124\H,-2.3007789788,0.1041938619,-1.1871308604\H,-2.5220
736774,-1.6379834214,-1.0437588005\C,-0.3225729881,3.3589785757,0.7939
052329\H,-1.234295215,3.3521685963,1.3747699027\H,-0.3822594405,4.0907
457324,0.0041722481\H,0.5196115327,3.5648167436,1.4399849804\O,-0.1452
420559,2.1008084058,0.140848965\Sn,0.0593254675,-1.0449450266,-0.42851
74323\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-310.8157013\S2=0.869
075\S2-1=0.\S2A=0.753203\RMSD=4.373e-09\RMSF=3.045e-06\Dipole=0.136303
9,1.0429595,-0.3729058\PG=C01 [X(C4H11O2Sn1)]\\@

MP2/DZP

1\1\GINC-AC22\FTS\UMP2-FC\Gen\C4H11O2Sn1(2)\SXH563\11-Aug-2008\0\\#MP2
/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint
guess=check\\S of oxyacyl radical attacking dimethylstannane\\0,2\Sn,0
.160250567,-0.0106848269,-0.0602516947\C,0.1396172359,0.1145827468,2.2
67959059\H,1.871624796,-0.1689171156,0.1791020394\H,-0.0239349025,1.51
0890279,-0.8118165676\O,0.2636840606,1.1292239687,2.8961793077\H,-2.23
0787968,-1.0379524385,1.2233189636\H,-2.5827480924,0.0434478602,-0.198
7409975\H,-2.2606654032,0.7684859943,1.4335456399\C,-2.0757042139,-0.0
659586842,0.760903599\C,-0.2669249359,-1.6961769086,-1.322667998\H,-0.
2758513356,-2.606444209,-0.7167054139\H,-1.2410542184,-1.5888674124,-1
.8045997524\H,0.5066663588,-1.7974999266,-2.0875385612\O,0.0583876838,
-1.129718374,2.7686881316\C,0.1610651616,-1.189817338,4.212689208\H,-0
.6477110452,-0.61729836,4.6691902185\H,1.121438248,-0.7876419434,4.537
7192435\H,0.0784110056,-2.2455266134,4.4593871109\\Version=IA64L-G03Re
vD.01\State=2-A\HF=-310.8121202\MP2=-311.8948404\PUHF=-310.8207671\PM
P2-0=-311.9013928\S2=0.822754\S2-1=0.786959\S2A=0.751906\RMSD=1.291e-09
\RMSF=3.737e-06\Thermal=0.\Dipole=-0.4584863,-0.7793711,0.5118014\PG=C
01 [X(C4H11O2Sn1)]\\@

BHandHLYP/DZP

1\1\GINC-AC30\FTS\UBHandHLYP\Gen\C4H11O2Sn1(2)\SXH563\11-Aug-2008\0\\#
BHandHLYP/gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=ch
eckpoint guess=check\\S of oxyacyl radical attacking dimethylstannane\\
\0,2\Sn,0.123656909,-0.0206206241,-0.0618417751\C,0.1525418121,0.10264
50448,2.2964085207\H,1.8312853737,-0.1940395542,0.213294921\H,-0.02351
49156,1.5009235181,-0.819804009\O,0.2663458873,1.1153985355,2.89490118
75\H,-2.2713399822,-0.9884494688,1.2372409993\H,-2.617067664,0.0121902
386,-0.2239854124\H,-2.2816056216,0.8125649239,1.3548290379\C,-2.11023
08181,-0.0498558176,0.7297880859\C,-0.2628777844,-1.6968515174,-1.3453
67156\H,-0.2911372174,-2.606244931,-0.7544302285\H,-1.2120186413,-1.58
63512172,-1.8567133227\H,0.5300060771,-1.7897011175,-2.0787801031\O,0.
0848834517,-1.1098956803,2.8160012286\C,0.1908620441,-1.1949560467,4.2
445332015\H,-0.6134346548,-0.640004459,4.7106738199\H,1.1429481694,-0.
7966894493,4.5710401888\H,0.1164605774,-2.2459356792,4.4785723515\\Ver
sion=IA64L-G03RevD.01\State=2-A\HF=-312.6255502\S2=0.779904\S2-1=0.\S2
A=0.750344\RMSD=4.513e-09\RMSF=1.606e-06\Thermal=0.\Dipole=-0.4725731,
-0.8737723,0.4686969\PG=C01 [X(C4H11O2Sn1)]\\@

ROMP2/DZP/MP2/DZP

MP2= -311.8938784

ROMP2/DZP/BHandHLYP/DZP

MP2=

QCISD/DZP/MP2/DZP

QCISD= -311.970001

QCISD/DZP/BHandHLYP/DZP

QCISD= -311.974351

CCSD(T)/DZP//MP2/DZP

CCSD(T)= -312.0093878

CCSD(T)/DZP//BHandHLYP/DZP

CCSD(T)= -312.009184

Transition State 10 (X=Si, R=Et)

BHandHLYP/6-311G(d,p)

```
1\1\GINC-AC30\FTS\UBHandHLYP\6-311G(d,p)\C5H13O2Si1(2)\SXH563\08-Aug-2008\0\#\BHandHLYP/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\TS of oxyacyl radical attacking ethylmethylsilane\0,2\C,0.0052122978,-0.0198064357,-0.0576226337\C,-0.0442095686,0.01390245,2.9102463688\H,0.9549260962,0.0025072858,2.4917086837\H,-0.1566629693,0.8984204585,3.5303499143\H,-0.1678930395,-0.8538393257,3.5515369536\O,1.1873943736,-0.0251059869,0.051001078\C,-3.0148570744,0.0290847737,2.7788849345\H,-2.8780385063,-0.8533756543,3.3946232782\H,-2.868046497,0.9235392534,3.3746955996\C,0.1610172507,-0.0471718522,-2.3922968059\O,-0.6440271248,-0.0293041828,-1.2116726035\H,-0.5334033753,-0.0527019059,-3.2190580554\H,0.7918698751,0.832319665,-2.4308076897\H,0.7820640337,-0.9342590939,-2.4107575919\H,-1.7893072376,1.3008548159,0.9635010164\H,-1.8041568721,-1.2965940329,0.9925829027\Si,-1.3417519011,0.0059355798,1.5512317973\C,-4.3173153389,0.0278923495,2.0190457862\H,-5.1623241923,0.0405469826,2.7063518451\H,-4.406432149,0.8990501506,1.3773740609\H,-4.4164704764,-0.8565553522,1.397340675\Version=IA64L-G03RevD.01\State=2-A\HF=-638.1005867\S2=0.767047\S2-1=0.\S2A=0.750165\RMSD=6.633e-09\RMSF=6.263e-06\Thermal=0.\Dipole=-0.5527121,0.0002581,-0.2415823\PG=C01 [X(C5H13O2Si1)]\@
```

BHandHLYP/DZP

```
1\1\GINC-GOMBERG18\FTS\UBHandHLYP\Gen\C5H13O2Si1(2)\SHORVAT\19-Jul-2012\0\#\BHandHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\TS of oxyacyl radical attacking SiMe2\0,2\C,-1.3802172803,0.2480410292,-0.0000972767\C,0.8872801691,2.1456607751,-0.0000353794\H,-0.0864311605,2.6198810495,-0.0003677347\H,1.4392901345,2.4715917592,0.8763337154\H,1.4399152567,2.4715883479,-0.8760083636\O,-2.0707424015,1.2133742764,-0.0002335303\C,2.7471959797,-0.1573340179,0.00002579\H,3.1064456177,0.3513311506,-0.8880520544\H,3.1064056698,0.3514381189,0.8880590562\C,-3.2494737045,-1.1588229158,-0.0000363504\O,-1.8296402751,-0.9977625651,0.000018674\H,-3.4223837742,-2.2246304664,0.0000759493\H,-3.6801023616,-0.703106535,0.8830758314\H,-3.6800113901,-0.7033075781,-0.8832967\H,0.5879550435,-0.4489069842,1.2914680016\H,0.5880183738,-0.4489094655,-1.2915616522\Si,0.7172013786,0.2758168782,-0.0000445132\C,3.0447160447,-1.6353663788,0.0001199406\H,4.119853795,-1.8104633871,0.0001479441\H,2.6347926333,-2.125557261,0.8777807733\H,2.6348222515,-2.1256628304,-0.8774961212\Version=AM64L-G09RevC.01\State=2-A\HF=-352.4733488\S2=0.7677\S2-1=0.\S2A=0.750174\RMSD=8.816e-09\RMSF=5.046e-06\Dipole=0.1913427,-0.5813743,0.0000804\Quadrupole=4.1258853,-3.2871328,-0.8387525,4.7491941,-0.0003068,0.0005081\PG=C01 [X(C5H13O2Si1)]\@
```

Transition State 10 (X=Si, R=iPr)

BHandHLYP/6-311G(d,p)

```
1\1\GINC-AC28\FTS\UBHandHLYP\6-311G(d,p)\C6H15O2Si1(2)\SXH563\09-Aug-2008\0\#\BHandHLYP/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint guess=check\TS of oxyacyl radical attacking isopropylmethylsilane\0,2\C,0.0073777733,0.0186722734,-0.062492265\C,0.1422234581,0.048074068,2.9005852079\H,1.1023540626,0.0668320283,2.3993781365\H,0.0602570821,0.9290646659,3.5293566672\H,0.1028880334,-0.824150929,3.5454782431\O,1.1930837174,0.0479565914,-0.030562724\C,-2.9125593364,-0.026958
```

4657,2.9147177368\C,0.0040268275,-0.0018292586,-2.4023032463\O,-0.7182
 776382,-0.0087286288,-1.1686147281\H,-0.7452602579,-0.0269204551,-3.17
 92746541\H,0.6045456496,0.8959882524,-2.4811199588\H,0.647726738,-0.87
 04721797,-2.4657177252\H,-1.7423648948,1.2860619612,1.0689372894\H,-1.
 6784206866,-1.313121653,1.0917864585\Si,-1.2565805063,0.0026107121,1.6
 46337529\C,-2.972934977,1.2448530603,3.7335681893\C,-2.9110114607,-1.2
 858240741,3.7555022505\H,-3.8858268601,1.2605253689,4.3299308867\H,-2.
 1394154658,1.317161739,4.4266592839\H,-2.9726702935,2.1326475741,3.109
 9034283\H,-3.8222631839,-1.3357486162,4.352489247\H,-2.8671392986,-2.1
 832129344,3.1473060872\H,-2.0752085309,-1.3053071609,4.4493419533\H,-3
 .7191076357,-0.0529930784,2.1882474067\\Version=IA64L-G03RevD.01\State
 =2-A\HF=-677.3976454\S2=0.76765\S2-1=0.\S2A=0.75017\RMSD=3.836e-09\RMS
 F=2.837e-06\Thermal=0.\Dipole=-0.576054,-0.0157805,-0.1957209\PG=C01 [X(C6H15O2Si1)]\@

BHandHLYP/DZP

1\1\GINC-GOMBERG03\FTS\UBHandHLYP\Gen\C6H15O2Si1(2)\SHORVAT\19-Jul-201
 2\0\#BHandHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\\
 TS of oxyacyl radical attacking SiMeiPr\0,2\C,-1.7583458181,0.26379835
 32,-0.0000512787\C,0.7409451105,1.8426756569,-0.0002146468\H,-0.173138
 6533,2.4234225583,-0.0004409766\H,1.3228146749,2.1074118062,0.87667949
 35\H,1.3231074822,2.1071708504,-0.8769857569\O,-2.3170245709,1.3101870
 118,-0.0002571549\C,2.2778816981,-0.7882905166,0.0001164036\C,-3.79059
 46746,-0.8949650509,0.0001453522\O,-2.3612490805,-0.9143098415,0.00016
 75602\H,-4.0964891306,-1.9304502631,0.0003408534\H,-4.1598550505,-0.38
 85525811,0.8833956271\H,-4.1598328543,-0.3888925579,-0.8833090794\H,0.
 0869150747,-0.6732697526,1.2937127216\H,0.0869329147,-0.6735824888,-1.
 2935564214\Si,0.349835393,0.0065922518,-0.0000019797\C,3.0112576403,-0
 .398077066,1.2654612227\C,3.011259586,-0.3984887515,-1.2653542762\H,3.
 9845348777,-0.8888124348,1.2978525391\H,3.1932675598,0.6719735852,1.31
 13989359\H,2.467658486,-0.6874720057,2.1587538719\H,3.9845405528,-0.88
 9227579,-1.2975784959\H,2.4676659949,-0.6881833533,-2.1585528833\H,3.1
 932630804,0.6715478705,-1.3116474243\H,2.0551887071,-1.8509247016,0.00
 02877929\\Version=AM64L-G09RevC.01\State=2-A\HF=-391.7702123\S2=0.7682
 96\S2-1=0.\S2A=0.75018\RMSD=5.246e-09\RMSF=4.090e-06\Dipole=0.1208199,
 -0.6042379,0.0001204\Quadrupole=5.2574059,-4.0026868,-1.2547191,4.0774
 29,-0.0007297,0.0006063\PG=C01 [X(C6H15O2Si1)]\@

Transition State 10 (X=Si, R=*t*-Bu)

BHandHLYP/6-311G(d,p)

1\1\GINC-AC28\FTS\UBHandHLYP\6-311G(d,p)\C7H17O2Si1(2)\SXH563\09-Aug-2
 008\0\#BHandHLYP/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=c
 heckpoint guess=check\\TS of oxyacyl radical attacking tbu-methylsila
 ne\0,2\C,-0.0166601503,0.0101971655,-0.0591877869\C,0.0973482498,0.13
 19774573,2.8923797364\H,1.0359142179,-0.146016705,2.4288082213\H,0.184
 1652024,1.159737873,3.2335994997\H,-0.0693844553,-0.4937408394,3.76205
 85745\O,1.1678759148,-0.014056399,-0.0104769234\C,-2.990242528,-0.0379
 802289,2.9059154622\C,0.0063829406,0.0068822258,-2.3977532563\O,-0.730
 2260626,0.0269719442,-1.1719476794\H,-0.7340497459,0.0237993152,-3.183
 2968768\H,0.6507315949,0.8748722033,-2.4625558567\H,0.6074069415,-0.89
 19068738,-2.459758705\H,-1.8086399543,1.255247549,1.0282692684\H,-1.66
 97463177,-1.3355172781,1.1123358646\Si,-1.3125824157,0.0021022187,1.65
 63906048\C,-4.2098436288,-0.0201965081,2.0021306844\H,-5.1173263567,-0
 .0567025615,2.6071657832\H,-4.2530370856,0.8815189821,1.3992968962\H,-
 4.2291849879,-0.8754841994,1.3330542468\C,-2.936030677,1.1987624992,3.
 7851823563\C,-2.9416585122,-1.3127613704,3.7292352931\H,-3.8217766758,
 1.2338613155,4.4222801449\H,-2.0691638758,1.1998883718,4.4384204831\H,
 -2.9216889934,2.1120751214,3.1977893716\H,-3.8136637562,-1.3570855276,
 4.3843318058\H,-2.9590310696,-2.1985243988,3.1019326838\H,-2.062712262
 7,-1.3633839687,4.3640738756\\Version=IA64L-G03RevD.01\State=2-A\HF=-7
 16.6959203\S2=0.768129\S2-1=0.\S2A=0.750173\RMSD=4.532e-09\RMSF=4.472e
 -06\Thermal=0.\Dipole=-0.5242334,0.0180472,-0.2531517\PG=C01 [X(C7H17O
 2Si1)]\@

BHAndHLYP/DZP

```
1\1\GINC-GOMBERG08\FTS\UBHandHLYP\Gen\C7H17O2Si1(2)\SHORVAT\19-Jul-201
2\0\#\BHAndHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\
TS of oxyacyl radical attacking SiMetBu\0,2\C,1.9909480858,0.286140923
3,0.0239385101\C,-0.3287011923,2.096655942,-0.0559118604\H,0.587526831
,2.5701801433,0.2739899043\H,-0.5158335145,2.4063699213,-1.0800679009\
H,-1.152426304,2.4489969789,0.5541781947\O,2.6396689343,1.2733594923,0
.1237747064\C,-2.1543531389,-0.3889820888,0.0085960683\C,3.9068236719,
-1.0529506564,-0.0315475442\O,2.4817093444,-0.9381898249,-0.0670280542
\H,4.1165894037,-2.1088147743,-0.1140441856\H,4.3478268935,-0.51093088
5,-0.8589131697\H,4.2922244611,-0.6594325492,0.9009349011\H,0.07009984
18,-0.5025980233,-1.2609359747\H,0.0610823538,-0.4283325274,1.32191814
12\Si,-0.1567642052,0.2282116123,0.0091226312\C,-2.14358464,-1.9054252
75,-0.0614285858\H,-3.1674711857,-2.2824867878,-0.0469334915\H,-1.6738
600089,-2.2646197412,-0.9717285379\H,-1.6217843142,-2.3449397451,0.783
5999652\C,-2.822078312,0.2145528772,-1.2142034163\C,-2.8045152711,0.08
99762937,1.2942974348\H,-3.8589048384,-0.1223255716,-1.2687261013\H,-2
.8372123878,1.2993132683,-1.1798267543\H,-2.3323250125,-0.090485611,-2
.1342613093\H,-3.8480104942,-0.2292816282,1.3158962444\H,-2.3176768443
,-0.3254653256,2.171131602\H,-2.7998011572,1.1716095621,1.3840275825\
Version=AM64L-G09RevC.01\State=2-A\HF=-431.0683679\S2=0.7688\S2-1=0.\S
2A=0.750183\RMSD=7.655e-09\RMSF=7.853e-07\Dipole=-0.1001855,-0.5768929
,-0.0545071\Quadrupole=4.4817033,-3.4568122,-1.0248911,-5.2585461,-0.3
238455,-0.3587696\PG=C01 [X(C7H17O2Si1)]\@
```

Transition State 11 (X=Si, R=Et)

BHAndHLYP/6-311G(d,p)

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET14\FTS\UBHandHLYP\6-311G(d,p)\C5H1
3O2Si1(2)\SONIA\02-Oct-2008\0\#\BHAndHLYP/6-311G** OPT=(TS,READFC,NOEI
GEN) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\FS ts of oxyacyl rad at
tacking ethylmethylsilane\0,2\Si,0.5309930172,0.1193787082,-1.0689871
413\C,0.5132173264,0.1094063613,0.9793275614\H,2.0231205412,0.00577598
94,-0.7283842489\O,0.4355604119,1.1141996158,1.6036949124\H,-1.4002479
649,-1.3773269145,-0.2110664356\H,-1.853684011,0.3308268089,-0.1046309
02\C,-1.4330926425,-0.436289436,-0.7459171558\H,0.6304988516,-0.912567
7109,-2.1482778034\C,0.3818281126,1.8847531816,-1.6816728897\H,-0.5609
989226,2.0730805315,-2.1839634338\H,0.4533590425,2.5606784821,-0.83449
83905\H,1.1873051096,2.1224024686,-2.3688616148\O,0.6489845281,-1.1035
763458,1.4807876844\C,0.7341780398,-1.1945196697,2.9070751736\H,1.5848
064414,-0.6292630892,3.2661931428\H,0.8557465777,-2.2448180349,3.12413
23735\H,-0.1715187635,-0.8124923282,3.3611213992\C,-2.1595811033,-0.55
05794591,-2.0692411952\H,-2.1382394375,0.377666896,-2.6315369576\H,-3.
2058204271,-0.7974785458,-1.8951842799\H,-1.7338871956,-1.3293984964,-
2.6925126105\Version=x86-Linux-G03RevB.04\State=2-A\HF=-638.0969181\S
2=0.767479\S2-1=0.\S2A=0.750201\RMSD=9.252e-09\RMSF=6.801e-06\Dipole=-
0.4113768,-0.6192812,0.4281778\PG=C01 [X(C5H13O2Si1)]\@
```

BHAndHLYP/DZP

```
1\1\GINC-GOMBERG17\FTS\UBHandHLYP\Gen\C5H13O2Si1(2)\SHORVAT\19-Jul-201
2\0\#\BHAndHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\
TS of oxyacyl radical attacking SiMeEt\0,2\Si,-1.0110059014,0.612220800
1,0.6809412821\C,0.7829084459,-0.2537034003,0.508797851\O,1.2055153506
,-1.2077547924,1.0734067216\H,-2.4902422838,-0.2271524452,-1.107995705
8\H,-0.8128954781,-0.5024403478,-1.6075725483\C,-1.5399962992,-0.66958
52937,-0.8222943455\H,-2.0711391638,0.2060913337,1.5999899531\H,-0.130
8965899,1.3690652035,1.7278765786\C,-1.0432282206,2.1839642258,-0.3725
```

1718\H,-1.3529783257,3.0452939726,0.2061493017\H,-0.0186719392,2.33866
64862,-0.6834646981\H,-1.6681461873,2.1043620297,-1.2542226193\C,2.805
8243693,0.0595951093,-0.6159510742\H,3.3775854493,0.0954621798,0.30270
27603\H,3.2001928114,0.7584181343,-1.3382688748\H,2.8271613904,-0.9492
017506,-1.008781029\O,1.458484535,0.4703421709,-0.3757623284\C,-1.6713
148118,-2.1079464275,-0.3869073649\H,-0.7388156434,-2.5032338916,-0.00
05430184\H,-1.9780317666,-2.7344946096,-1.2229047087\H,-2.4213057411,-
2.2088016871,0.390999047\\Version=AM64L-G09RevC.01\State=2-A\HF=-352.3
998569\S2=0.767238\S2-1=0.\S2A=0.750193\RMSD=4.775e-09\RMSF=6.635e-06\
Dipole=0.185628,0.161445,-0.8283718\Quadrupole=5.0603041,-2.8762054,-2
.1840987,1.6852072,-1.9186289,1.94713\PG=C01 [X(C5H13O2Si1)]\@

Transition State 11 (X=Si, R=iPr)

BHandHLYP/6-311G(d,p)

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET23\FTS\UBHandHLYP\3-21G*\C6H15O2Si

1(2)\SONIA\02-Oct-2008\0\#BHANDHLYP/3-21G* OPT=(TS,CALCFC,NOEIGEN) FR
EQ=NORAMAN\FS ts of oxyacyl rad attacking ethylmethyilsilane\0,2\Si,0
.5856718859,0.1919206232,-1.3289695441\C,0.6871013905,0.3553586563,0.7
020946637\H,2.0569590235,-0.069371967,-1.0516989098\O,0.7054078635,1.4
258439611,1.2616299426\C,-1.2764302786,-0.5234300996,-0.9432334048\H,0
.6068079566,-0.6923098166,-2.5498882585\C,0.4014422012,1.9839339147,-1
.8410714839\H,-0.5499387698,2.1578852654,-2.3418203186\H,0.4484516274,
2.6200329178,-0.959472464\H,1.197500814,2.2800646736,-2.5209925665\O,0
.809311583,-0.8400590303,1.3220227556\C,1.0091281133,-0.7987236076,2.7
817835776\H,1.8822726707,-0.2037486049,3.0178402688\H,1.1473153275,-1.
8285405737,3.0708794936\H,0.1381076806,-0.3708835359,3.2624926332\C,-1
.2451259827,-2.0349680081,-0.724329688\C,-2.0710301902,0.2047829424,0.
1396526228\H,-0.762092735,-2.5455452443,-1.5525252345\H,-0.7077343835,
-2.263923388,0.1896544928\H,-2.262525426,-2.4169961784,-0.6345309072\H
-3.130478581,-0.0242253483,0.026152748\H,-1.7673719686,-0.128185341,1
.1279294255\H,-1.9487119843,1.2828246889,0.0859779831\H,-1.696234748,-
0.291968508,-1.9230240786\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-
673.7123146\S2=0.764808\S2-1=0.\S2A=0.750154\RMSD=5.580e-09\RMSF=6.231
e-06\Dipole=-0.3645416,-0.5441602,0.7326359\PG=C01 [X(C6H15O2Si1)]\@

BHandHLYP/DZP

1\1\GINC-GOMBERG17\FTS\UBHandHLYP\Gen\C6H15O2Si1(2)\SHORVAT\19-Jul-201
2\0\#BhandHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\\
TS of oxyacyl radical attaking SiMeiPr\0,2\Si,0.5032991618,1.11093291
27,-0.5193816465\C,-1.1111572592,-0.0263848894,-0.6811171855\O,-1.6320
762473,-0.3418571649,-1.7053724325\H,0.6805245186,-1.6062357486,-0.491
3824367\C,1.4050850013,-0.910960221,-0.0930281802\H,1.9607436309,1.304
9045916,-0.1779061477\H,0.4301071198,1.7238907421,-1.8455032532\C,-0.0
777869222,2.2069060797,0.9080238876\H,-1.1399151125,2.4192684736,0.884
3244386\H,0.1426189773,1.7315816666,1.8564017695\H,0.470480249,3.14267
45952,0.8888448664\C,-2.7983168701,-1.1444757878,0.5054250851\H,-3.594
457299,-0.5986845286,0.014553858\H,-3.0450365458,-1.3223671945,1.54195
56237\H,-2.6443150505,-2.0820563134,-0.0154703529\O,-1.5997502033,-0.3
743942504,0.5163091906\C,1.3632339422,-0.7660065566,1.3990951628\H,1.9
674605116,0.0650784168,1.7394499572\H,1.7783051366,-1.6660709172,1.855
9586194\H,0.3594316727,-0.6488263467,1.7767901941\C,2.7433620007,-1.05
25022034,-0.7507670826\H,2.6719600654,-0.9647133188,-1.8298774374\H,3.
1445778286,-2.0424321803,-0.5295034663\H,3.4485216933,-0.3123498566,-0
.3904860314\\Version=AM64L-G09RevC.01\State=2-A\HF=-391.7031935\S2=0.7
66606\S2-1=0.\S2A=0.750156\RMSD=6.718e-09\RMSF=2.712e-06\Dipole=0.3087
293,-0.7350031,0.9229334\Quadrupole=3.5440205,0.7350715,-4.279092,-0.2
519795,-3.3615694,-0.7387975\PG=C01 [X(C6H15O2Si1)]\@

Transition State 11 (X=Si, R=t-Bu)

BHandHLYP/6-311G(d,p)