Supplementary Material (ESI) for New Journal of Chemistry

Electronic Supporting Information

An *ab-initio* and DFT study of some homolytic substitution reactions of acyl radicals at sulfur, selenium and tellurium.

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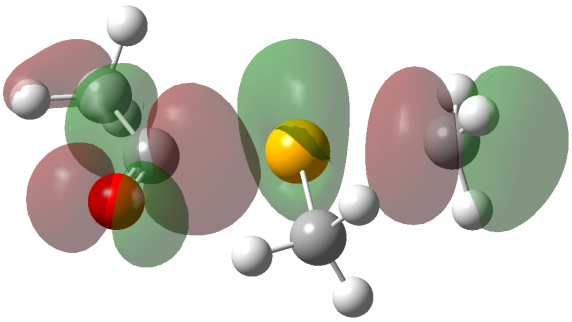
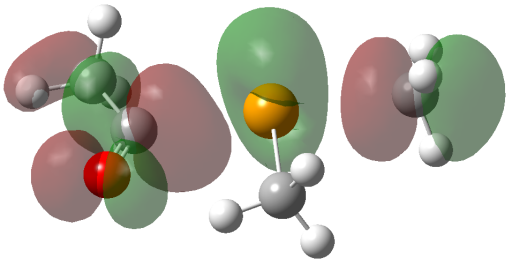
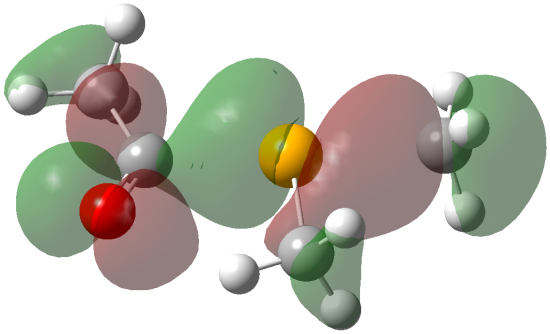
Fig. S1 and Gaussian Archive entries for the optimised transition structures **12**, **13** and higher-level calculated single-point energies (13 pages).



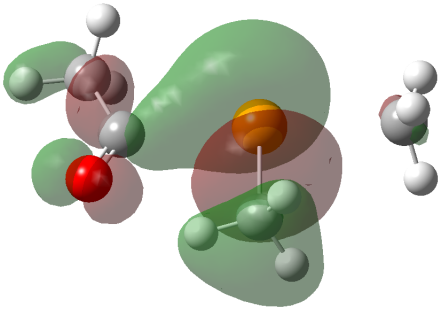
12 (X=Se)
SOMO - σ^*_{Se-C} 394 kJ mol^{-1}



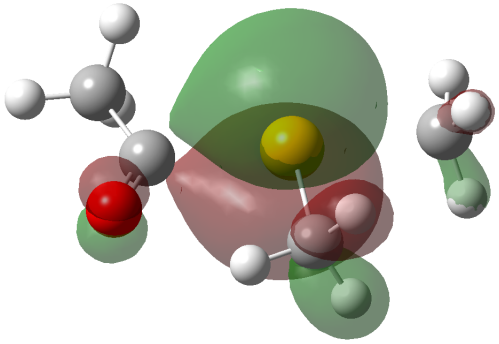
12 (X=Te)
SOMO - σ^*_{Te-C} 420 kJ mol^{-1}



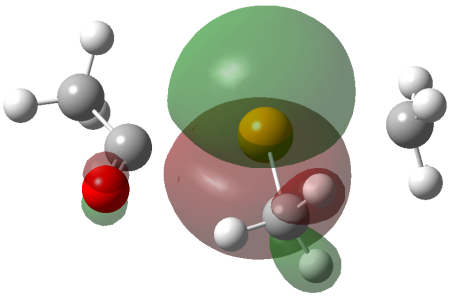
12 (X=Se)
LP_{Se} – SOMO 1817 kJmol^{-1}



12 (X=Te)
LP_{Te} – SOMO 28 kJ mo^{-1}



12 (X=Se)
LP_{Se} - $\pi^*_{C=O}$ 59 kJ mol^{-1}



12 (X=Te)
LP_{Te} - $\pi^*_{C=O}$ 121 kJ mol^{-1}

Fig. S1 BHandHLYP/6-311G** (Se) and BHandHLYP/DZP (Te) generated Kohn-Sham orbitals for transition states **12** (X = Se, Te)

Gaussian Archive Entries for Transition States 12, 13

Transition State 12 (X=S)

UHF/6-311G**


```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET16\FTS\UHF\6-311G(d,p)\C4H9O1S1(2)
\SONIA\27-Jun-2007\0\\#UHF/6-311G** OPT=(TS,READFC,NOEIGEN) FREQ=NORAM
AN GEOM=CHECKPOINT GUESS=CHECK\\ts of acyl rad attacking dimethyl sulf
ide\\0,2\C,0.8149822891,0.0004570875,-1.2438930363\C,0.7680481207,-0.0
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82547811,0.8846257973,2.2955696934\H,0.6793144587,-0.8851219476,2.2951
136739\O,1.9713160063,0.0011700042,-1.1023831261\C,0.047162372,0.00016
06981,-2.5373912736\H,-0.5871203686,-0.8779511823,-2.5719242113\H,0.73
76594517,0.0010692189,-3.3716131532\H,-0.5888491966,0.8770379906,-2.57
14136087\C,-2.1153360468,-0.000647986,1.8906530157\H,-1.9724139338,-0.
9063278761,2.4590352963\H,-3.0164685668,-0.0013280373,1.2995154073\H,-
1.9732776213,0.9056375093,2.4582809501\S,-0.5339967768,-0.0004555305,0
.4127002548\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-629.0727707\S2
=0.887606\S2-1=0.\S2A=0.754754\RMSD=5.255e-09\RMSF=5.999e-06\Dipole=-0
.633605,-0.0002881,-0.0787454\PG=C01 [X(C4H9O1S1)]\\@
```


MP2/6-311G**


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\\#MP2=Direct/6-311G** opt=(ef,ts,readfc) freq=noraman geom=checkpoint
 guess=check\\nbo on acyl rad attacking dimethylsulfide\\0,2\C\C,1,B1\
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,1,B6,6,A5,2,D4,0\H,7,B7,1,A6,6,D5,0\H,7,B8,1,A7,6,D6,0\H,7,B9,1,A8,6,
D7,0\C,2,B10,1,A9,6,D8,0\H,11,B11,2,A10,1,D9,0\H,11,B12,2,A11,1,D10,0\
H,11,B13,2,A12,1,D11,0\S,2,B14,1,A13,6,D12,0\\B1=2.70707069\B2=1.08865
564\B3=1.08984875\B4=1.09131034\B5=1.20787849\B6=1.51375226\B7=1.09445
38\B8=1.091857\B9=1.09144277\B10=2.77327144\B11=1.08952007\B12=1.08809
359\B13=1.0909329\B14=1.80580092\A1=76.47345511\A2=149.41086709\A3=94.
8605372\A4=81.37918453\A5=124.77411957\A6=108.73573701\A7=108.4971488\
A8=111.51272822\A9=88.52161407\A10=79.22234768\A11=144.12888779\A12=92
.16080149\A13=44.51902936\D1=106.10568441\D2=-108.54209895\D3=53.66316
547\D4=-175.98212648\D5=76.29204818\D6=-41.41716797\D7=-163.4438578\D8
=212.9676103\D9=113.00547802\D10=-0.13297046\D11=-134.2424591\D12=190.
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```


MP2(Full)/6-311G**


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oint guess=check\\TS of acyl rad at dimethylsulfide\\0,2\C,-0.12285579
53,0.1390451328,0.1287162322\C,0.0359858421,-0.1363378393,2.8127964885
\H,0.9954915731,-0.5162682422,2.467360081\H,0.1241146937,0.9341248175,
3.003547676\H,-0.2609371501,-0.6561073451,3.7230167504\O,0.9070375991,
0.7417328345,0.3128551581\C,-0.8142041839,0.0019805164,-1.2084967536\H
,-1.5535762319,-0.8002085588,-1.1972619408\H,-0.0572815204,-0.18534213
79,-1.972188409\H,-1.3151608209,0.9456164162,-1.4439781553\C,-2.731852
1747,-0.0442694374,2.9091903164\H,-2.7755719037,-0.892436994,3.5932334
707\H,-3.6326457718,0.0422742692,2.3057649785\H,-2.4804231054,0.889124
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D=3.031e-09\RMSF=6.579e-06\Thermal=0.\Dipole=-0.4751853,-0.1188699,0.0
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ROMP2/6-311G// MP2/6-311G****

MP2= -629.0519071

QCISD/6-311G//MP2/6-311G****

QCISD=-630.0649213

CCSD(T)/6-311G// MP2/6-311G****

CCSD(T)=-630.1008284

MP2/cc-pVDZ

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62008,3.5044766529\H,-0.5926215327,-0.8880665858,3.172610507\O,1.09455
15697,-0.6509644408,0.1111038538\C,-0.4358171384,0.4743357237,-1.39994
38409\H,-1.2575393537,-0.2172717674,-1.6503698299\H,0.3449241716,0.404
70345,-2.171996679\H,-0.8474944341,1.4931304756,-1.343148391\C,-2.6529
49795,0.953029831,2.6725818589\H,-2.9565152948,-0.0416726206,3.0307443
457\H,-3.4317856861,1.4292373828,2.0615888752\H,-2.3082961507,1.608682
5326,3.486914966\S,-1.0483534821,0.7021772922,1.3956099144\\Version=IA
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901e-09\RMSF=1.867e-06\Thermal=0.\Dipole=-0.3873663,0.1507935,-0.13398
76\PG=C01 [X(C4H9O1S1)]\\@

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

MP2=-629.9145761

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

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

CCSD(T)=-630.0093782

MP2/aug-cc-pVDZ

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\\#MP2=Direct/aug-cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=ch
eckpoint guess=check\\ts of acyl rad attacking dimethyl sulfide\\0,2\C
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.5920667826,3.6865538817\H,-0.3126383883,-0.9686519784,2.7953751021\O,
0.4678172564,-1.109543363,0.2251561629\C,-0.5016711893,0.4907745885,-1
.3265798593\H,-1.2721294533,-0.1743734766,-1.7502014422\H,0.3769538068
,0.4623969823,-1.9883580094\H,-0.8955905282,1.5153014293,-1.2630797294
\C,-2.5775102419,0.9444198669,2.5724098348\H,-2.7516253486,-0.10103546
41,2.8577101402\H,-3.3485802634,1.3402499113,1.9014375872\H,-2.3830403
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MP2=-629.977006

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

QCISD=-630.0391706

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

CCSD(T)=-630.0768008

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rad attacking dimethylsulfide\\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,1,B6,6,A5,2,D4,0\H,7,B7,1
,A6,6,D5,0\H,7,B8,1,A7,6,D6,0\H,7,B9,1,A8,6,D7,0\C,2,B10,1,A9,6,D8,0\H
,11,B11,2,A10,1,D9,0\H,11,B12,2,A11,1,D10,0\H,11,B13,2,A12,1,D11,0\S,2
,B14,1,A13,6,D12,0\\B1=2.84289586\B2=1.08056098\B3=1.08205545\B4=1.082
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B10=2.8329792\B11=1.08003491\B12=1.0785877\B13=1.08007237\B14=1.811203
98\A1=62.84785391\A2=125.28065088\A3=124.03503411\A4=83.3011134\A5=126
.66778429\A6=108.77047658\A7=109.7983953\A8=109.68858777\A9=93.51713\A
10=84.88767949\A11=143.72032761\A12=84.9719345\A13=45.45839214\D1=95.7
5183863\D2=-96.33090595\D3=0.5351334\D4=-178.85672929\D5=113.88310878\
D6=-6.61464918\D7=-128.39385143\D8=180.09958994\D9=122.36627039\D10=-0
.37274376\D11=-123.23803087\D12=179.49452221\\Version=IA64L-G03RevD.01
\State=2-A\HF=-631.0883725\S2=0.781425\S2-1=0.\S2A=0.750285\RMSD=5.076
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\PG=C01 [X(C4H9O1S1)]\\@

QCISD/6-311G**//BHandHLYP/6-311G**

QCISD=-630.0647946

CCSD(T)/6-311G**//BHandHLYP/6-311G**

CCSD(T)=-630.0999262

BHandHLYP/cc-pVDZ

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(2)\SONIA\27-Jun-2007\0\\#BHANDHLYP/CC-PVDZ OPT=(TS,READFC,NOEIGEN) FR
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hyl sulfide\\0,2\C,0.7794520519,0.0003482752,-1.1885283992\C,0.7660265
627,0.0002500676,1.6563364868\H,1.7331604474,0.0008063929,1.1556117932
\H,0.6708196806,0.8917328182,2.2778995643\H,0.6718007639,-0.8913899415
,2.2778237461\O,1.9532425646,0.0008986569,-1.0493241631\C,0.0320258538
,0.0002270083,-2.4875645369\H,-0.6116181009,-0.8817224098,-2.528263262
9\H,0.7328221536,0.0006344492,-3.3236890154\H,-0.6123249312,0.88167258
58,-2.5279796917\C,-2.0654163732,-0.000814887,1.82828034\H,-1.93347482
72,-0.9120055789,2.4106198146\H,-2.9818789696,-0.0012855492,1.24212635
54\H,-1.9342470199,0.9106474069,2.4103698276\S,-0.5270955178,-0.000396
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ole=-0.5306728,-0.0000925,-0.1415106\PG=C01 [X(C4H9O1S1)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET10\FTS\UBHandHLYP\Aug-CC-pVDZ\C4H9
O1S1(2)\SONIA\27-Jun-2007\0\\#BHANDHLYP/AUG-CC-PVDZ OPT=(TS,READFC,NOE
IGEN) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\ts of acyl rad attacki
ng dimethyl sulfide\\0,2\C,0.7741837472,0.0004004632,-1.1885334103\C,0
.7669935291,0.0001999196,1.6641119166\H,1.7363311898,0.0006589,1.17387
59356\H,0.6673951673,0.8901824952,2.2822340089\H,0.6682147533,-0.88989
95086,2.2821966358\O,1.9497577716,0.0010174709,-1.0526948236\C,0.02347
13093,0.0001670697,-2.4844962895\H,-0.6182611631,-0.8804768172,-2.5225
636258\H,0.7210064173,0.0004220748,-3.3201026205\H,-0.6188242511,0.880
4043262,-2.5225220378\C,-2.0587989287,-0.000876008,1.8173493835\H,-1.9
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274073233\H,-1.9293782115,0.9085973505,2.3975621827\S,-0.5226104249,-0
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05\Dipole=-0.612812,-0.0002218,-0.0837504\PG=C01 [X(C4H9O1S1)]\\@

Transition State 12 (X=Se)

UHF/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET10\FTS\UHF\6-311G(d,p)\C4H9O1Se1(2
)\SONIA\26-Jun-2007\0\\#UHF/6-311G** OPT=(TS,READFC,NOEIGEN) FREQ=NORA
MAN GEOM=CHECKPOINT GUESS=CHECK\\ts of acyl rad attacking dimethyl sel
enide\\0,2\C,0.8759169584,0.9333208134,-1.1980152681\C,0.3138670311,0.
549042548,1.7917999622\H,0.9880870687,1.3245273324,1.4628112456\H,-0.5
221275922,0.9847516909,2.3195769685\H,0.8361395557,-0.1495933209,2.429
3085988\Se,-0.3391858425,-0.3862427649,0.2071665573\O,1.5538609801,1.7
850083998,-0.7872979581\C,0.6600242702,0.5360174087,-2.6338762175\H,0.
9505848844,-0.5004397157,-2.7594229478\H,1.2463788819,1.1756142378,-3.
2824336175\H,-0.3945546968,0.6227187076,-2.8679103998\C,-1.6299409255,
-1.8043456707,1.5294729858\H,-0.9102400384,-2.3020390619,2.1588670475\
H,-2.1095066923,-2.4480809125,0.8110748125\H,-2.3025345732,-1.13948274
48,2.0465602352\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-2631.34595
55\S2=0.921126\S2-1=0.\S2A=0.755887\RMSD=7.741e-09\RMSF=6.020e-06\Dipo
le=-0.3511877,-0.4447743,-0.25005\PG=C01 [X(C4H9O1Se1)]\\@

MP2/6-311G**

1\1\GINC-AC38\FTS\UMP2-FC\6-311G(d,p)\C4H9O1Se1(2)\SXH563\15-Aug-2007\
0\\#MP2=Direct/6-311G** opt=(ts,readfc,noeigen) freq=noraman geom=chec
kpoint guess=check\\ts of acyl rad attacking dimethylselenide\\0,2\C,-
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2.962808985\H,0.9457383441,-0.0000029114,2.4490356905\H,-0.115701636,0
.893685356,3.5791678938\H,-0.1156986533,-0.8936814738,3.5791782638\Se,
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2102863752\C,-0.7066471315,0.0000081988,-1.3101762527\H,-1.3445299708,
-0.8848591137,-1.3747635189\H,0.0337572941,-0.0000222082,-2.1123484505
\H,-1.3444684869,0.8849191897,-1.3747780389\C,-2.9553232812,-0.0000024
704,3.2363797613\H,-2.774370035,-0.9125304733,3.8007691934\H,-3.904985
1259,-0.0000079926,2.7072273436\H,-2.7743736303,0.9125339153,3.8007567
108\\Version=IA64L-G03RevD.01\State=2-A\HF=-2631.3417181\MP2=-2632.258
7644\PUHF=-2631.3539122\PMP2-0=-2632.2679853\S2=0.852385\S2-1=0.801477
\S2A=0.753387\RMSD=3.490e-09\RMSF=6.541e-06\Thermal=0.\Dipole=-0.39849
81,0.00001,-0.1990953\PG=C01 [X(C4H9O1Se1)]\\@

MP2(Full)/6-311G**

1\1\GINC-X141\FTS\UMP2-FU\6-311G(d,p)\C4H9O1Se1(2)\SXH563\22-Mar-2010\
0\\#MP2(Full)/6-311G** opt=(ts,noeigen,readfc) freq=noraman geom=check
point guess=check\\TS of acyl rad at dimethylsulfide\\0,2\C,0.01322394
44,-0.0000446754,-0.0621827832\C,0.0163737799,-0.000018867,2.863686157
4\H,0.9762360044,-0.0000944324,2.3464686698\H,-0.080550504,0.893350122
1,3.4799285668\H,-0.0806319604,-0.8933060935,3.4800340143\O,1.19509680
39,-0.0000783566,0.1104445907\C,-0.6929142429,0.0000607553,-1.39724449
37\H,-1.3316333546,-0.8839393893,-1.4573836885\H,0.0412732482,-0.00033
05488,-2.2045009249\H,-1.3308612299,0.8846091712,-1.4575830641\C,-2.91
49375079,0.0001668892,3.1468767843\H,-2.7327420993,-0.912015048,3.7106
514237\H,-3.8657095657,0.0001739766,2.6205500266\H,-2.7326559363,0.912
4121796,3.7105204852\Se,-1.3793428963,-0.0000423114,1.5128682113\\Vers
ion=EM64L-G03RevE.01\State=2-A\HF=-2631.3415868\MP2=-2632.7322675\PUHF
=-2631.3537118\PMP2-0=-2632.7414121\S2=0.850635\S2-1=0.800197\S2A=0.75
3299\RMSD=3.559e-09\RMSF=6.458e-06\Thermal=0.\Dipole=-0.3922546,0.0001
206,-0.1969785\PG=C01 [X(C4H9O1Se1)]\\@

ROMP2/6-311G**//MP2/6-311G**

MP2=-2632.2625312

QCISD/6-311G**//MP2/6-311G**

QCISD=-2632.3264818

CCSD(T)/6-311G**//MP2/6-311G**

CCSD(T)=-2632.3616776

MP2/cc-pVDZ

```
 1\1\GINC-AC58\FTS\UMP2-FC\CC-pVDZ\C4H9O1Se1(2)\SXH563\16-Aug-2007\0\\#
 MP2=Direct/cc-pvdz opt=(ts,readfc,noeigen) freq=noraman geom=checkpoin
 t guess=check\\ts of acyl rad attacking dimethylselenide\\0,2\C,-0.016
 7794985,0.0053861637,0.0491104397\C,-0.0139772992,-0.0572171543,2.9640
 167053\H,0.9557463776,-0.0324093793,2.4443942049\H,-0.157515652,0.8677
 600443,3.5421304329\H,-0.0664279753,-0.9291149038,3.6325095282\Se,-1.3
 998731082,-0.2024767142,1.6068136384\O,1.1647127484,0.1534910836,0.226
 4100563\C,-0.7169369156,0.0111495166,-1.2967301794\H,-1.4321978991,-0.
 8242134343,-1.3479725562\H,0.0269893272,-0.0571174413,-2.1046988447\H,
 -1.2837772432,0.9524148582,-1.3858949355\C,-2.9409766356,0.0110023645,
 3.2100141929\H,-2.7547726345,-0.8269311366,3.8967073226\H,-3.902103712
 5,-0.0688084121,2.6857348913\H,-2.7802142973,0.9971158767,3.6666517173
 \\Version=IA64L-G03RevD.01\State=2-A\HF=-2631.3070792\MP2=-2632.193438
 3\PUHF=-2631.3187669\PMP2-0=-2632.2022344\S2=0.846756\S2-1=0.79796\S2A
 =0.753126\RMSD=9.567e-09\RMSF=1.152e-06\Thermal=0.\Dipole=-0.394904,0.
 0464202,-0.2044422\PG=C01 [X(C4H9O1Se1)]\\@
```

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

```
MP2=-2632.1977108
```

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

```
QCISD=-2632.2646313
```

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

```
CCSD(T)=-2632.2948229
```

MP2/aug-cc-pVDZ

```
1\1\GINC-AC25\FTS\UMP2-FC\Aug-CC-pVDZ\C4H9O1Se1(2)\SXH563\17-Jan-2008\
 0\\#MP2/aug-cc-pvdz opt=(ts,calcfc,noeigen) freq=noraman\\TS of acyl r
 ad attacking dimethylselenide\\0,2\C,0.,0.,0.\C,0.,0.,2.86473077\H,1.0
 490931736,0.,2.5440934693\H,-0.3527373383,1.0324404784,2.9951988421\H,
 -0.1214433059,-0.5690991872,3.7957984564\Se,-1.0633812928,-0.890468507
 ,1.4923012449\O,0.832485592,0.8630605384,0.2162171076\C,-0.4877607066,
 -0.4012802386,-1.3786689454\H,-1.0550843004,-1.3421383109,-1.343235214
 2\H,0.3810959441,-0.4974627828,-2.0466860285\H,-1.139593164,0.39952511
 36,-1.7645645472\C,-2.7894029279,-0.8776861596,2.9236983779\H,-2.49102
 02694,-1.5875119956,3.7068246937\H,-3.6492351814,-1.2182390732,2.33615
 61427\H,-2.885376693,0.1564737799,3.27594554\\Version=IA64L-G03RevD.01
 \State=2-A\HF=-2631.3203492\MP2=-2632.2605564\PUHF=-2631.330266\PMP2-0
 =-2632.2680331\S2=0.833847\S2-1=0.791828\S2A=0.752583\RMSD=5.441e-09\R
 MSF=3.447e-06\Thermal=0.\Dipole=-0.4316543,-0.2799689,-0.0293462\Polar
 =104.7059532,16.3551003,76.2158436,-27.5390952,-8.2673721,123.2672477\
 PG=C01 [X(C4H9O1Se1)]\\@
```

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

```
MP2=-2632.2649116
```

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

```
QCISD=-2632.328592
```

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

```
CCSD(T)=-2632.3656707
```

BHandHLYP/6-311G**

```
 1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET2\FTS\UBHandHLYP\6-311G(d,p)\C4H9O
 1Se1(2)\SONIA\26-Jun-2007\0\\#BHANDHLYP/6-311G** OPT=(TS,READFC,NOEIGE
 N) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\ts of acyl rad attacking
 dimethyl selenide\\0,2\C,0.8290486438,0.8833731984,-1.1337791587\C,0.3
 154270524,0.5491877108,1.7741229944\H,0.9910856345,1.3269098538,1.4481
 446091\H,-0.5251368694,0.9798976504,2.2998009048\H,0.834033994,-0.1549
 477916,2.4094464856\Se,-0.3251298921,-0.3717505307,0.1826716999\O,1.51
```

57479072,1.7454185483,-0.7237871714\C,0.6310104724,0.5072461162,-2.571
8924049\H,0.9223945965,-0.5280311713,-2.7122481371\H,1.2236126545,1.15
56553245,-3.2062099074\H,-0.4211438568,0.5938351059,-2.8206446613\C,-1
.589250749,-1.7604652584,1.47902835\H,-0.8758348066,-2.2638998124,2.11
24471706\H,-2.0712002565,-2.4068000872,0.7636159482\H,-2.2667905355,-1
.1025000156,2.0002284763\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-2
634.39889\S2=0.78969\S2-1=0.\S2A=0.750342\RMSD=5.764e-09\RMSF=5.268e-0
6\Dipole=-0.2926464,-0.3780119,-0.2849421\PG=C01 [X(C4H9O1Se1)]\\@

QCISD/6-311G**// BHandHLYP/6-311G**

QCISD=-2632.3257076

CCSD(T)/6-311G**// BHandHLYP/6-311G**

CCSD(T)=-2632.3604868

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FTS\UBHandHLYP\CC-pVDZ\C4H9O1Se1
(2)\SONIA\26-Jun-2007\0\\#BHANDHLYP/CC-PVDZ OPT=(TS,READFC,NOEIGEN) FR
EQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\ts of acyl rad attacking dimet
hyl selenide\\0,2\C,0.828490492,0.8830571663,-1.1301202639\C,0.3157350
835,0.5491888294,1.7703220082\H,0.996202105,1.3318812308,1.4362766044\
H,-0.5297963702,0.9854073649,2.3025488035\H,0.8399766172,-0.1583000847
,2.413054986\Se,-0.3264777139,-0.3734400136,0.1818914809\O,1.518843509
1,1.7495847105,-0.7190394681\C,0.632273237,0.5089659135,-2.5697519305\
H,0.9242280518,-0.5346685991,-2.7103738256\H,1.2290952966,1.1619420015
,-3.209215607\H,-0.428148837,0.5945637558,-2.819479064\C,-1.587309736,
-1.7584457733,1.4758683077\H,-0.869675562,-2.2676502937,2.1166081291\H
,-2.0755890781,-2.4126766335,0.7572014596\H,-2.2719324809,-1.096812778
4,2.0034751784\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-2634.354663
8\S2=0.789511\S2-1=0.\S2A=0.750336\RMSD=8.283e-09\RMSF=9.174e-05\Dipol
e=-0.2776943,-0.3617662,-0.3021311\PG=C01 [X(C4H9O1Se1)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FTS\UBHandHLYP\Aug-CC-pVDZ\C4H9O
1Se1(2)\SONIA\26-Jun-2007\0\\#BHANDHLYP/AUG-CC-PVDZ OPT=(TS,READFC,NOE
IGEN) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\ts of acyl rad attacki
ng dimethyl selenide\\0,2\C,0.8260861573,0.8798813448,-1.1331897478\C,
0.3127542925,0.5465378473,1.7798275967\H,0.9933798847,1.3307794502,1.4
598931975\H,-0.5336029309,0.9780786937,2.3084098269\H,0.8328948019,-0.
1628987661,2.4186552363\Se,-0.3245315693,-0.3709167367,0.1838924378\O,
1.51823285,1.7482245111,-0.7255500111\C,0.6254805994,0.5008280816,-2.5
697948613\H,0.9163033429,-0.5411679339,-2.7055291228\H,1.2188814157,1.
1494015302,-3.212445942\H,-0.4336020007,0.5859969932,-2.8144335006\C,-
1.5821336155,-1.7532191951,1.4657949954\H,-0.8668924116,-2.2617586819,
2.1043276907\H,-2.0667961642,-2.4032416723,0.7458626055\H,-2.265479983
4,-1.0939851262,1.9914893133\\Version=x86-Linux-G03RevB.04\State=2-A\H
F=-2634.3737707\S2=0.788233\S2-1=0.\S2A=0.750335\RMSD=7.425e-09\RMSF=2
.478e-05\Dipole=-0.331849,-0.4224356,-0.258775\PG=C01 [X(C4H9O1Se1)]\\
@

Transition State 12 (X=Te)

UHF/DZP

1\1\GINC-AC21\FTS\UHF\Gen\C4H9O1Te1(2)\SXH563\24-Jan-2008\0\\#uhf/gen
pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\\TS calc on acyl rad
attacking dimethyltellurium\\0,2\C,-0.0276614348,-0.0222422975,-0.0496
723684\C,0.1800326983,-0.0750670628,1.443233874\O,1.1948472794,-0.1608
370304,2.0077041986\H,0.9304652964,-0.0766153381,-0.5527140373\H,-0.53
67201858,0.9008068839,-0.3019522731\H,-0.6596671701,-0.8511539453,-0.3
468093081\Te,-1.8991067952,0.0389755878,2.703396156\C,-0.7865525097,-0
.0855476725,4.5278375641\H,0.2584151295,-0.1525030574,4.2631280776\H,-
0.9639715553,0.8013922796,5.1187772942\H,-1.088633704,-0.9674463989,5.
0740541736\C,-4.0353191916,0.1545393971,4.0921981778\H,-4.8155100263,0

.2276807496,3.3534533274\H,-3.8856079444,1.0429701115,4.6828675977\H,-
4.0132339449,-0.7741848352,4.6377286708\\Version=IA64L-G03RevD.01\Stat
e=2-A\HF=-239.4063434\S2=0.945607\S2-1=0.\S2A=0.757797\RMSD=5.177e-09\
RMSF=6.553e-06\Thermal=0.\Dipole=-0.5586354,0.0494822,-0.3911546\PG=C0
1 [X(C4H9O1Te1)]\\@

MP2/DZP

1\1\GINC-AC27\FTS\UMP2-FC\Gen\C4H9O1Te1(2)\SXH563\24-Jan-2008\0\\#MP2/
gen pseudo=read opt=(ts,readfc,noeigen) freq=noraman geom=checkpoint g
uess=check\\TS calc on acyl rad attacking dimethyltellurium\\0,2\C,-0.
0815798861,0.0274858481,0.0722983594\C,-0.1303223595,0.0074749563,1.58
82028481\O,0.8211073919,0.2264998702,2.292741808\H,0.9589985314,0.0092
871267,-0.2588290756\H,-0.5647835138,0.9464178135,-0.273209132\H,-0.63
29772153,-0.8235076535,-0.3352538632\Te,-2.1559650842,-0.3920186979,2.
-0.0274271254,4.2794626131\H,-1.8104156933,0.7727012057,4.8279675154\H
,-1.629615252,-0.9984407603,4.993229813\C,-4.436527031,0.0717326035,3.
4872884252\H,-5.137228585,-0.14169248,2.686588422\H,-4.3893886779,1.11
15379795,3.7938046795\H,-4.4239514795,-0.654275492,4.2957587988\\Versi
on=IA64L-G03RevD.01\State=2-A\HF=-239.4027006\MP2=-240.2975438\PUHF=-2
39.4120074\PMP2-0=-240.3047824\S2=0.841496\S2-1=0.800051\S2A=0.752958\
RMSD=9.331e-09\RMSF=5.292e-07\Thermal=0.\Dipole=-0.4411036,0.0301638,-
0.3627878\PG=C01 [X(C4H9O1Te1)]\\@

ROMP2/DZP//MP2/DZP

MP2=-240.2974199

QCISD/DZP//MP2/DZP

QCISD=-240.3654383

CCSD(T)/DZP//MP2/DZP

CCSD(T)=-240.3991742

BHandHLYP/DZP

1\1\GINC-AC25\FTS\UBHandHLYP\Gen\C4H9O1Te1(2)\SXH563\24-Jan-2008\0\\#B
HandHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\\TS calc
on acyl rad attacking dimethyltellurium\\0,2\C,-0.0515930282,0.016380
0757,0.0557914606\C,-0.0999071293,0.0008584694,1.559589788\O,0.8431088
17,0.1331823293,2.2601099981\H,0.980622776,0.0165909049,-0.2743168642\
H,-0.5537026668,0.910514597,-0.3008516078\H,-0.5772454331,-0.844429632
5,-0.3434110191\Te,-2.1636464906,-0.2575234441,2.4267143145\C,-1.36613
76057,-0.0705002761,4.3938028173\H,-0.291184467,-0.0231203745,4.282016
3681\H,-1.7365503541,0.8344776284,4.853702059\H,-1.6456566073,-0.93315
30267,4.9816134581\C,-4.5119865803,0.0421859608,3.5180137143\H,-5.1745
876125,-0.0560268007,2.675343766\H,-4.4520816395,1.0247010709,3.953993
9183\H,-4.5044487209,-0.7863830707,4.2069652058\\Version=IA64L-G03RevD
.01\State=2-A\HF=-240.9103418\S2=0.790391\S2-1=0.\S2A=0.750391\RMSD=5.
609e-09\RMSF=5.581e-06\Thermal=0.\Dipole=-0.5395936,0.0259599,-0.40716
48\PG=C01 [X(C4H9O1Te1)]\\@

QCISD/DZP//BHandHLP/DZP

QCISD=-240.3643043

CCSD(T)/DZP//BHandHLP/DZP

CCSD(T)=-240.3974393

Transition State 13 (X=S, R=Et)

BHandHLYP/6-311G**

1\1\GINC-AC29\FTS\UBHandHLYP\6-311G(d,p)\C5H11O1S1(2)\SXH563\30-Jul-20
09\0\\#BHandHLYP/6-311G** opt=(ts,calcfc,noeigen) freq=noraman\\calc o
n acyl radical attacking ethylmethylsulfide\\0,2\C,-0.042114129,-0.007
4577628,0.0857404\C,-0.0244555683,0.0074361637,2.9364917329\H,0.928199
4749,0.0028167786,2.4267289571\H,-0.1073179607,0.9003616989,3.54241658
95\H,-0.1026109793,-0.8696057893,3.5657124949\O,1.1273952923,-0.006577

012,0.2126196013\C,-0.8035284079,0.011660466,-1.2042165879\H,-1.548628
2764,-0.7756049594,-1.2006731673\H,-0.1213019529,-0.1104643611,-2.0367
15672\H,-1.3237812667,0.9606310783,-1.2861181049\C,-2.8501826184,-0.00
60018997,3.1457204225\H,-2.6460236266,-0.8943661537,3.7283242002\H,-2.
6560292349,0.8963148603,3.7099673395\C,-4.1714528877,-0.0208222667,2.4
34890408\H,-4.2854099782,0.851480255,1.7981528926\H,-4.996068951,-0.01
89185058,3.145616106\H,-4.2747745107,-0.906718504,1.8153086594\S,-1.33
74985206,-0.014294606,1.688627683\\Version=IA64L-G03RevD.01\State=2-A\
HF=-670.3884782\S2=0.782457\S2-1=0.\S2A=0.750296\RMSD=4.455e-09\RMSF=7
.649e-07\Thermal=0.\Dipole=-0.6644427,0.0278227,-0.0488606\PG=C01 [X(C
5H11O1S1)]\\@

Transition State 13 (X=S, R=*i*-Pr)

BHandHLYP/6-311G**

1\1\GINC-AC22\FTS\UBHandHLYP\6-311G(d,p)\C6H13O1S1(2)\SXH563\30-Jul-20
09\0\\#BHandHLYP/6-311G** opt=(ts,calcfc,noeigen) freq=noraman\\calc o
n acyl radical attacking ipropylmethylsulfide\0,2\C,-0.0185492899,-0.00
01085831,0.0880812024\C,-0.0117819953,0.0004924328,2.9495254035\H,0.92
8123047,0.000354565,2.4162459451\H,-0.0704527435,0.8865540214,3.566772
2991\H,-0.0704929022,-0.8852976633,3.5671602419\O,1.1503996231,-0.0001
753957,0.2153134171\C,-0.7836314517,-0.0003590939,-1.1993985868\H,-1.4
218146309,-0.8768287084,-1.2318465048\H,-0.0986006607,0.0001271852,-2.
0388548415\H,-1.4229147838,0.8753077071,-1.2316446104\C,-2.9382244609,
0.000166261,3.1110421836\C,-2.9208746641,-1.27322478,3.9132182395\C,-2
.9204589705,1.2730675659,3.9139861407\H,-3.8296570098,1.3541951525,4.5
114925556\H,-2.083264339,1.3020584859,4.6053217568\H,-2.8654310926,2.1
472758853,3.2741126234\H,-3.8300165842,-1.3543377013,4.5108125864\H,-2
.8662955974,-2.1470669691,3.2728099448\H,-2.0835850887,-1.3029854051,4
.6044094792\H,-3.7378451904,0.0005233472,2.3809418485\S,-1.3423107175,
0.0002646241,1.7194300127\\Version=IA64L-G03RevD.01\State=2-A\HF=-709.
68656\S2=0.786131\S2-1=0.\S2A=0.750339\RMSD=9.466e-09\RMSF=3.446e-06\T
hermal=0.\Dipole=-0.7341016,-0.0001328,0.0115347\PG=C01 [X(C6H13O1S1)]
\\@

Transition State 13 (X=S, R=*t*-Bu)

BHandHLYP/6-311G**

1\1\GINC-AC2\FTS\UBHandHLYP\6-311G(d,p)\C7H15O1S1(2)\SXH563\30-Jul-200
9\0\\#BHandHLYP/6-311G**opt=(ts,calcfc,noeigen) freq=noraman\\calc on
acyl radical attacking tButylmethylsulfide\\0,2\C,-0.0464143017,-0.000
1257629,0.0672211541\C,-0.0438391365,-0.000219091,2.9448252242\H,0.889
6656838,-0.0001705791,2.3999989768\H,-0.0927101883,0.8857756465,3.5630
465803\H,-0.092699476,-0.886309802,3.5629091204\O,1.1218148153,-0.0001
271184,0.1927451191\C,-0.8197730241,-0.0000276165,-1.2148311221\H,-1.4
593698773,-0.8756381673,-1.241235382\H,-0.1419651491,-0.0002496424,-2.
0604002816\H,-1.4588899987,0.8759335897,-1.2413435407\C,-3.0052442912,
0.0000501185,3.100343439\C,-4.1863371627,-0.0000859466,2.1607728623\H,
-4.1868505858,0.880205881,1.5249750222\H,-5.11617417,0.0000317398,2.72
97880431\H,-4.1868855734,-0.8805914111,1.5252722782\C,-2.9248043996,-1
.2623290374,3.9229232787\C,-2.9248042188,1.2626699166,3.9225527012\H,-
3.8122604845,1.3501379636,4.5523487073\H,-2.0640164125,1.2681007594,4.
5828046475\H,-2.8789384768,2.1441118556,3.2911028356\H,-3.8123079313,-
1.3496593889,4.5526719735\H,-2.8788470448,-2.143952833,3.2917326637\H,
-2.0640699162,-1.267524438,4.5832464032\S,-1.3870047464,-0.000132724,1
.7299655172\\Version=IA64L-G03RevD.01\State=2-A\HF=-748.9873507\S2=0.7
87968\S2-1=0.\S2A=0.750358\RMSD=3.197e-09\RMSF=5.981e-06\Thermal=0.\Di
pole=-0.7463141,0.000085,0.0076998\PG=C01 [X(C7H15O1S1)]\\@

Transition State 13 (X=Se, R=Et)

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET22\FTS\UBHandHLYP\6-311G(d,p)\C5H1
1O1Se1(2)\SONIA\22-Jul-2008\0\\#BHANDHLYP/6-311G** OPT=(TS,READFC,NOEI
GEN) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\ts of acyl rad attackin
g ethylmethyl selenide\\0,2\C,1.3203223035,-0.0296596291,-1.4800316507
\C,1.3033571919,0.0196773988,1.5021671036\H,2.244603028,0.0072021163,0
.9718554841\H,1.2245495979,0.9168845474,2.1001455075\H,1.217551492,-0.
8566384967,2.1294447729\Se,-0.1191354148,0.0033109148,0.1717261241\O,2
.4804973592,-0.0311409189,-1.2918986877\C,0.6281027161,-0.0488872481,-
2.8101009351\H,-0.0104619323,-0.9238994415,-2.8644927638\H,1.360897544
,-0.064981906,-3.6083701141\H,-0.0035065994,0.8288898683,-2.8934487976
\C,-1.6803683629,0.036359561,1.7990420391\H,-1.4419407291,-0.852561134
5,2.3659011551\H,-1.4348978662,0.9416442787,2.336220567\C,-3.033915498
,0.0309958064,1.1536095896\H,-3.1731605367,0.9003200059,0.5180420289\H
,-3.8219309536,0.0465435484,1.9059485135\H,-3.1800679167,-0.8577624702
,0.5471380497\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-2673.6985969
\S2=0.79123\S2-1=0.\S2A=0.750362\RMSD=4.822e-09\RMSF=4.229e-05\Dipole=
-0.6590898,0.0008455,-0.1069286\PG=C01 [X(C5H11O1Se1)]\\@

Transition State 13 (X=Se, R=*i*-Pr)

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET8\FTS\UBHandHLYP\6-311G(d,p)\C6H13
O1Se1(2)\SONIA\24-Jul-2008\0\\#BHANDHLYP/6-311G** OPT=(TS,READFC,NOEIG
EN) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\ts of acyl rad attacking
 ipropylmethyl selenide\\0,2\C,1.2490354769,0.0240327268,-1.9427050832
\C,1.4038011389,0.0417787599,1.0454168271\H,2.2946085615,0.0624618565,
0.4343441766\H,1.3570275662,0.931243247,1.6571174079\H,1.4037959873,-0
.8432868036,1.6652324407\Se,-0.1172267834,-0.0038788667,-0.1726792903\
O,2.4175345825,0.0553659114,-1.82507821\C,0.4745340407,-0.0022488546,-
3.2260457109\H,-0.1406660372,-0.895245964,-3.2481916191\H,1.152960136,
0.0117650639,-4.0713836712\H,-0.186843563,0.8568643437,-3.2562050121\C
,-1.6549045638,-0.0368272705,1.4841505056\C,-1.5039067807,-1.302478481
6,2.2827733806\C,-1.570974763,1.2422678738,2.2711341209\H,-2.390507578
6,1.2943462929,2.9904768655\H,-0.6469133311,1.305251728,2.8388001901\H
,-1.6370436119,2.1141569064,1.6297791383\H,-2.3197320235,-1.3910742385
,3.002759592\H,-1.5238042635,-2.182463468,1.6494312018\H,-0.5779473166
,-1.311509877,2.8507687791\H,-2.525007842,-0.0627034321,0.8404478187\\
Version=x86-Linux-G03RevB.04\State=2-A\HF=-2712.9970144\S2=0.794945\S2
-1=0.\S2A=0.750407\RMSD=6.937e-09\RMSF=5.010e-05\Dipole=-0.712588,-0.0
188179,-0.0082024\PG=C01 [X(C6H13O1Se1)]\\@

Transition State 13 (X=Se, R=*t*-Bu)

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET10\FTS\UBHandHLYP\6-311G(d,p)\C7H1
5O1Se1(2)\SONIA\24-Jul-2008\0\\#BHANDHLYP/6-311G** OPT=(TS,READFC,NOEI
GEN) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\ts of acyl rad attackin
g t-butylmethyl selenide\\0,2\C,1.5052126494,0.0217951952,-2.012315837
2\C,1.6638648796,0.029665088,0.9918317122\H,2.5454815547,0.0434210592,
0.3671272772\H,1.6375906221,0.9181110651,1.6063925745\H,1.667434175,-0
.8570599781,1.609421435\Se,0.1255922152,0.0017648639,-0.2037785317\O,2
.6735266896,0.0415996002,-1.8999169427\C,0.7178750796,0.0063631487,-3.
2875111046\H,0.0935899304,-0.8803913119,-3.3038002168\H,1.3862535734,0
.0161407602,-4.1411321277\H,0.0641114286,0.8715512675,-3.3068088676\C,
-1.4341643725,-0.02161847,1.4271977071\C,-2.7132586178,-0.0445904917,0
.6274118517\H,-2.8047121075,0.8334610774,-0.0047933663\H,-3.5717796466
,-0.0578495128,1.3007197763\H,-2.7750514043,-0.9274734694,-0.001651421
8\C,-1.2308710042,-1.2782044006,2.2360420448\C,-1.2733603451,1.2439709
571,2.2315552254\H,-2.0691015752,1.3075911778,2.9774775228\H,-0.330788
0638,1.2707960944,2.7682113646\H,-1.3367220636,2.1269741546,1.60438518
92\H,-2.0240778449,-1.3659513021,2.9822155586\H,-1.264392435,-2.165064
0887,1.6120161209\H,-0.287974591,-1.271345325,2.7727552054\\Version=x8
6-Linux-G03RevB.04\State=2-A\HF=-2752.2973968\S2=0.796742\S2-1=0.\S2A=
0.750426\RMSD=6.025e-09\RMSF=2.438e-05\Dipole=-0.7272404,-0.0122384,-0

.0108113\PG=C01 [X(C7H15O1Se1)]\\@

Transition State 13 (X=Te, R=Et)

BHandHLYP/DZP

1\1\GINC-AC18\FTS\UBHandHLYP\Gen\C5H11O1Te1(2)\SXH563\29-Jul-2009\0\\#
BHandHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\\calc o
n acyl radical attacking ethylmethyltelluride\\0,2\C,0.041634071,0.000
7600002,-0.0475810355\C,0.1103997804,0.053823721,3.0700455581\H,1.0264
487369,0.0241931275,2.4960073994\H,0.1027701098,0.9187535858,3.7181078
061\H,0.0046861655,-0.8512746638,3.6514724616\O,1.1959886692,-0.095986
612,0.1765365121\C,-0.5756398275,-0.0219472717,-1.4190316117\H,-1.1674
735253,-0.9264222485,-1.5187511784\H,0.2038993764,-0.0036151671,-2.171
9641871\H,-1.2401365866,0.8269149468,-1.5382536633\C,-3.0544418414,-0.
0326480089,3.5981013845\H,-2.7360929546,-0.9754291002,4.0175240984\H,-
2.7328589481,0.8168582011,4.1836494729\Te,-1.4876963187,0.196484696,1.
6664002467\C,-4.4682605627,0.0155700893,3.1053452291\H,-5.1682683416,-
0.0578204816,3.9383886518\H,-4.6807133591,0.9455287613,2.5867195499\H,
-4.6831541552,-0.8058941739,2.4289687192\\Version=IA64L-G03RevD.01\Sta
te=2-A\HF=-280.2101601\S2=0.795457\S2-1=0.\S2A=0.750467\RMSD=4.178e-09
\RMSF=2.436e-06\Thermal=0.\Dipole=-0.783327,-0.0458432,-0.08051\PG=C01
[X(C5H11O1Te1)]\\@

Transition State 13 (X=Te, R=*i*-Pr)

BHandHLYP/DZP

1\1\GINC-AC29\FTS\UBHandHLYP\Gen\C6H13O1Te1(2)\SXH563\30-Jul-2009\0\\#
BHandHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\\calc o
n acyl radical attacking ipropylmethyltelluride\\0,2\C,0.0130564595,0.
0003537839,-0.1313904928\C,0.0312343047,-0.0044584711,3.0065169475\H,0
.9366912453,-0.0029697135,2.4153827022\H,-0.0085455619,0.882077443,3.6
229690295\H,-0.007217922,-0.8927079375,3.6205631387\O,1.1655487501,0.0
010441841,0.1063537402\C,-0.6013465452,0.0026880052,-1.5029297808\H,-1
.2315775152,-0.8737820074,-1.6098230961\H,0.1773976306,0.0034348895,-2
.2572687107\H,-1.2304248006,0.8803311564,-1.6070598541\C,-3.2209426044
,-0.0008754853,3.4537512821\C,-3.0694156064,-1.2711870849,4.246326891\
C,-3.072076104,1.2733698191,4.2404387262\H,-3.8481215259,1.3301279874,
5.0068976933\H,-2.1159483282,1.319774907,4.7542546233\H,-3.1625996164,
2.1519032912,3.6116763197\H,-3.84585574,-1.3263358691,5.012502591\H,-3
.1574064863,-2.1528583303,3.6215872317\H,-2.1135493496,-1.3128581913,4
.7610250583\H,-4.110886956,-0.0032587299,2.8370933782\Te,-1.5922006782
,-0.0038115977,1.6210440751\\Version=IA64L-G03RevD.01\State=2-A\HF=-31
9.5088356\S2=0.801668\S2-1=0.\S2A=0.750545\RMSD=9.291e-09\RMSF=2.011e-
06\Thermal=0.\Dipole=-0.7623018,0.0014453,-0.0883027\PG=C01 [X(C6H13O1
Te1)]\\@

Transition State 13 (X=Te, R=*t*-Bu)

BHandHLYP/DZP

1\1\GINC-AC7\FTS\UBHandHLYP\Gen\C7H15O1Te1(2)\SXH563\30-Jul-2009\0\\#B
HandHLYP/gen pseudo=read opt=(ts,calcfc,noeigen) freq=noraman\\calc on
acyl radical attacking tButylmethyltelluride\\0,2\C,0.0416266906,0.05
52144606,-0.091017907\C,0.174033834,-0.0619275954,3.0623158142\H,1.043
6371889,-0.0098097724,2.4218430266\H,0.1455458474,0.8005722957,3.71284
00893\H,0.2012323181,-0.9722523899,3.6441372007\O,1.1998845279,0.08443
81057,0.1028336278\C,-0.6396104771,0.0829635021,-1.4291418691\H,-1.243
9954425,-0.8116438629,-1.5335140137\H,0.0981491208,0.1380805446,-2.222
0081506\H,-1.3038693369,0.9395690754,-1.4672463273\C,-3.0946502274,-0.
198732618,3.6107536782\Te,-1.5269618147,-0.0654181389,1.7714200835\C,-
4.4398658708,-0.2118495537,2.9227555529\H,-5.2336795953,-0.2716226982,
3.6699061629\H,-4.6055055004,0.6910422066,2.3425856653\H,-4.5477660132
,-1.0678286528,2.2632738196\C,-2.8945033933,1.0306968536,4.464813307\C

,-2.8126696158,-1.4835564504,4.352767628\H,-1.9060524662,1.0618021671,
4.9112077288\H,-3.6176721056,1.0259141556,5.2844104707\H,-3.0430376333
,1.9438101201,3.8983670262\H,-2.9045232526,-2.3503894082,3.7071412484\
H,-3.5313345572,-1.5979940587,5.1683377338\H,-1.8224415829,-1.49057356
53,4.796268994\\Version=IA64L-G03RevD.01\State=2-A\HF=-358.808577\S2=0
.803306\S2-1=0.\S2A=0.750568\RMSD=6.523e-09\RMSF=5.799e-06\Thermal=0.\
Dipole=-0.7423255,-0.0230089,-0.1154301\PG=C01 [X(C7H15O1Te1)]\\@