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# **Understanding Homolytic Translocation Chemistry – An Ab Initio Study of Some 1,5- Silyl, Germyl and Stannyl Transfers of Synthetic Significance**

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## **Accessory Publication**

Gaussian Archive entries for the optimized structures and higher-level calculated single-point energies.

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## Transition State 3 (Y = Si, Z = CH<sub>2</sub>) SiC<sub>5</sub>H<sub>13</sub>

### SCF/6-311G\*\*

```
1\1\GINC-SATORI\POpt\UHF\6-311G(d,p)\C5H13Si1(2)\SMHORVAT\31-Jan-2001\
1\#\UHF/6-311G** SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK\calc
on the 1,5 trans of SiH3 b/w c with H ax\0,2\Si\C,1,r1\C,1,r1,2,a1\C
,2,r2,1,a2,3,d1,0\C,3,r2,1,a2,2,-d1,0\C,4,r3,2,a3,1,d2,0\H,1,r4,2,a4,4
,d3,0\H,1,r5,2,a5,4,-d4,0\H,1,r5,3,a5,5,d4,0\H,2,r6,1,a6,3,-d5,0\H,2,r
7,1,a7,3,-d6,0\H,4,r8,2,a8,1,d7,0\H,4,r9,2,a9,1,d8,0\H,6,r10,4,a10,2,d
9,0\H,6,r11,4,a11,2,d10,0\H,5,r8,3,a8,1,-d7,0\H,5,r9,3,a9,1,-d8,0\H,3,
r6,1,a6,2,d5,0\H,3,r7,1,a7,2,d6,0\|r1=2.18914325\r2=1.51307588\r3=1.52
370868\r4=1.48382986\r5=1.49534541\r6=1.08120025\r7=1.08351919\r8=1.08
80823\r9=1.09055821\r10=1.08659525\r11=1.08939265\|a1=79.80861465\|a2=11
9.34049025\|a3=113.96900182\|a4=103.45870654\|a5=83.35401905\|a6=94.511726
15\|a7=104.14789742\|a8=109.58142246\|a9=107.85050813\|a10=109.5451333\|a11
=109.66542551\|d1=52.23874676\|d2=-67.44136811\|d3=-49.31115745\|d4=155.59
192012\|d5=188.45914852\|d6=76.23639675\|d7=55.71187541\|d8=170.86409489\|d
9=183.53502482\|d10=-59.7070959\|Version=NEC-SX-4-SUPER-UX-G98RevA.7\HF
=-485.781529\|S2=0.828654\|S2-1=0.\|S2A=0.751706\|RMSD=6.073e-09\|RMSF=1.80
8e-05\|Dipole=0.6435684,0.0930211,0.7695683\|PG=C01 [X(C5H13Si1)]\|@
```

### SCF/DZP

```
1\1\GINC-SATORI\POpt\UHF\Gen\C5H13Si1(2)\SMHORVAT\01-Feb-2001\1\#\UHF/
GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK\calc
on the 1,5 trans of SiH3 b/w c with H ax\0,2\Si\C,1,r1\C,1,r1,2,a1\C
,2,r2,1,a2,3,d1,0\C,3,r2,1,a2,2,-d1,0\C,4,r3,2,a3,1,d2,0\H,1,r4,2,a4,4
,d3,0\H,1,r5,2,a5,4,-d4,0\H,1,r5,3,a5,5,d4,0\H,2,r6,1,a6,3,-d5,0\H,2,r7
,1,a7,3,-d6,0\H,4,r8,2,a8,1,d7,0\H,4,r9,2,a9,1,d8,0\H,6,r10,4,a10,2,d9
,0\H,6,r11,4,a11,2,d10,0\H,5,r8,3,a8,1,-d7,0\H,5,r9,3,a9,1,-d8,0\H,3,r
6,1,a6,2,d5,0\H,3,r7,1,a7,2,d6,0\|r1=2.18321203\r2=1.51591551\r3=1.524
87113\r4=1.47419328\r5=1.4878152\r6=1.08156726\r7=1.08378771\r8=1.0877
3638\r9=1.09019472\r10=1.0867106\r11=1.08897519\|a1=79.92399729\|a2=119.
00826956\|a3=113.90631777\|a4=103.47930376\|a5=83.45203439\|a6=95.1726393\
|a7=104.41725043\|a8=109.55298604\|a9=107.85610405\|a10=109.48245788\|a11=1
09.67397017\|d1=52.89605253\|d2=-67.71486263\|d3=-48.67871534\|d4=154.7775
596\|d5=187.76926403\|d6=75.32016147\|d7=55.37435046\|d8=170.69729612\|d9=1
83.23351743\|d10=-59.90644295\|Version=NEC-SX-4-SUPER-UX-G98RevA.7\HF=-
200.6112982\|S2=0.8297\|S2-1=0.\|S2A=0.751783\|RMSD=5.701e-09\|RMSF=2.688e-
05\|Dipole=0.5933743,0.0857084,0.7081543\|PG=C01 [X(C5H13Si1)]\|@
```

### MP2/DZP

```
1\1\GINC-SATORI\POpt\UMP2-FC\Gen\C5H13Si1(2)\SMHORVAT\01-Feb-2001\1\#\
MP2=DIRECT/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=C
HECK\calc on the 1,5 trans of SiH3 b/w c with H ax\0,2\Si\C,1,r1\C,1
,r1,2,a1\C,2,r2,1,a2,3,d1,0\C,3,r2,1,a2,2,-d1,0\C,4,r3,2,a3,1,d2,0\H,1
,r4,2,a4,4,d3,0\H,1,r5,2,a5,4,-d4,0\H,1,r5,3,a5,5,d4,0\H,2,r6,1,a6,3,-
d5,0\H,2,r7,1,a7,3,-d6,0\H,4,r8,2,a8,1,d7,0\H,4,r9,2,a9,1,d8,0\H,6,r10
,4,a10,2,d9,0\H,6,r11,4,a11,2,d10,0\H,5,r8,3,a8,1,-d7,0\H,5,r9,3,a9,1,
-d8,0\H,3,r6,1,a6,2,d5,0\H,3,r7,1,a7,2,d6,0\|r1=1.94867705\r2=1.535832
65\r3=1.53205131\r4=1.47133974\r5=1.57080567\r6=1.09465429\r7=1.097832
62\r8=1.09797339\r9=1.09823018\r10=1.09671568\r11=1.09865218\|a1=96.541
46304\|a2=112.63584804\|a3=113.51755014\|a4=108.68667611\|a5=86.32284227\|a
6=108.1262457\|a7=107.30741061\|a8=109.62234859\|a9=108.70814841\|a10=109.
07874649\|a11=109.20747355\|d1=49.10019761\|d2=-60.51881118\|d3=-63.197470
22\|d4=167.04379189\|d5=188.0704359\|d6=72.43569446\|d7=61.5996905\|d8=177.
95409824\|d9=186.06077872\|d10=-57.26603922\|Version=NEC-SX-4-SUPER-UX-G
98RevA.7\HF=-200.6038413\|MP2=-201.4239631\|PUHF=-200.6109126\|PMP2-0=-20
1.4287951\|S2=0.791386\|S2-1=0.76473\|S2A=0.751177\|RMSD=5.795e-09\|RMSF=2.
931e-05\|Dipole=0.2796137,-0.0467385,0.2493178\|PG=C01 [X(C5H13Si1)]\|@
```

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**B3LYP/DZP**

```

1\1\GINC-SATORI\POpt\UB3LYP\Gen\C5H13Si1(2)\SMHORVAT\28-Sep-2001\1\1\#B
3LYP/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK\
calc on the 1,5 trans of SiH3 b/w c with H ax\0,2\Si\C,1,r1\C,1,r1,2,
a1\C,2,r2,1,a2,3,d1,0\C,3,r2,1,a2,2,-d1,0\C,4,r3,2,a3,1,d2,0\H,1,r4,2,
a4,4,d3,0\H,1,r5,2,a5,4,-d4,0\H,1,r5,3,a5,5,d4,0\H,2,r6,1,a6,3,-d5,0\H
,2,r7,1,a7,3,-d6,0\H,4,r8,2,a8,1,d7,0\H,4,r9,2,a9,1,d8,0\H,6,r10,4,a10
,2,d9,0\H,6,r11,4,a11,2,d10,0\H,5,r8,3,a8,1,-d7,0\H,5,r9,3,a9,1,-d8,0\
H,3,r6,1,a6,2,d5,0\H,3,r7,1,a7,2,d6,0\|r1=2.0367224\r2=1.52858521\r3=1
.53462317\r4=1.48042435\r5=1.53383544\r6=1.09423152\r7=1.09734506\r8=1
.09932879\r9=1.10205939\r10=1.09805252\r11=1.10003158\|a1=89.80872211\|a
2=115.3602832\|a3=114.37527537\|a4=106.4028692\|a5=84.0551148\|a6=103.3920
884\|a7=105.46059723\|a8=109.65012813\|a9=107.97800476\|a10=109.37423778\|a
11=109.44595342\|d1=50.27284332\|d2=-62.93976817\|d3=-56.77024968\|d4=161.
19957624\|d5=187.6991485\|d6=73.99385974\|d7=60.36143199\|d8=175.50712278\
|d9=183.88321752\|d10=-59.51867422\|Version=NEC-SX-4-SUPER-UX-G98RevA.7\
HF=-202.192026\|S2=0.758683\|S2-1=0.\|S2A=0.750058\|RMSD=9.515e-09\|RMSF=2.
379e-05\|Dipole=0.5180192,0.0577227,0.5198643\|PG=C01 [X(C5H13Si1)]\|@

```

**CCSD(T)/DZP//B3LYP/DZP**

```
CCSD(T)=-201.537168
```

**6-Sila-1-hexyl Radical SiC<sub>5</sub>H<sub>13</sub>•****SCF/6-311G\*\***

```

1\1\ MARCCENTRE-BNET1\POpt\UHF\6-311G(d,p)\C5H13Si1(2)\ROOT\05-Sep-200
0\1\1\#UHF/6-311G** SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK\|ca
lcl on the ground state of SiC5H13 radicca\0,2\Si\C,1,r1\C,2,r2,1,a1
\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,0\H,1,r6,2,a5,
3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r7,2,a6,3,-d5,0\H,2,r8,3,a7,4,-d6,0\H,2,
r8,3,a7,4,d6,0\H,3,r9,4,a8,5,d7,0\H,3,r9,4,a8,5,-d7,0\H,4,r10,5,a9,6,-
d8,0\H,4,r10,5,a9,6,d8,0\H,5,r11,4,a10,3,-d9,0\H,5,r11,4,a10,3,d9,0\H,
6,r12,5,a11,4,d10,0\H,6,r12,5,a11,4,-d10,0\|r1=1.88836963\r2=1.5363786
3\r3=1.52948647\r4=1.53795972\r5=1.50028061\r6=1.48092239\r7=1.4816405
4\r8=1.08946706\r9=1.08904548\r10=1.08856154\r11=1.08817827\r12=1.0765
1883\|a1=114.59256705\|a2=113.25334395\|a3=113.01235457\|a4=113.38151644\|a
5=110.35449075\|a6=110.63888992\|a7=109.80145112\|a8=108.9911011\|a9=109.2
2247688\|a10=108.85147994\|a11=120.50065053\|d1=180.\|d2=180.\|d3=180.\|d4=1
80.\|d5=59.95916108\|d6=58.08858815\|d7=57.73701643\|d8=58.00541424\|d9=57.
90283335\|d10=82.56679278\|Version=DEC-AXP-OSF/1-G98RevA.7\|State=2-A'\|H
F=-485.8499651\|S2=0.762691\|S2-1=0.\|S2A=0.750106\|RMSD=3.907e-09\|RMSF=2.
519e-05\|Dipole=-0.0641619,0.,0.250356\|PG=CS [SG(C5H13Si1),X(H12)]\|@

```

**SCF/DZP**

```

1\1\ MARCCENTRE-BNET1\POpt\UHF\Gen\C5H13Si1(2)\ROOT\10-Oct-2000\1\1\#UH
F/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT\|calc on the gro
und state SiC5H13\0,2\Si\C,1,r1\C,2,r2,1,a1\C,3,r3,2,a2,1,d1,0\C,4,r4
,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,0\H,1,r6,2,a5,3,d4,0\H,1,r7,2,a6,3,d5,0\
H,1,r7,2,a6,3,-d5,0\H,2,r8,3,a7,4,-d6,0\H,2,r8,3,a7,4,d6,0\H,3,r9,4,a8
,5,d7,0\H,3,r9,4,a8,5,-d7,0\H,4,r10,5,a9,6,-d8,0\H,4,r10,5,a9,6,d8,0\H
,5,r11,4,a10,3,-d9,0\H,5,r11,4,a10,3,d9,0\H,6,r12,5,a11,4,d10,0\H,6,r1
2,5,a11,4,-d10,0\|r1=1.88662294\r2=1.53692877\r3=1.53092142\r4=1.53899
777\r5=1.50340402\r6=1.47174573\r7=1.47224606\r8=1.08870514\r9=1.08875
021\r10=1.08819402\r11=1.08776624\r12=1.07719999\|a1=114.3478333\|a2=113

```

---

```
.08725223\ a3=112.80620942\ a4=113.19372446\ a5=110.46804739\ a6=110.61540
192\ a7=109.79090965\ a8=109.0492567\ a9=109.27187514\ a10=108.907169\ a11=
120.49455279\ d1=180.\ d2=180.\ d3=180.\ d4=180.\ d5=59.9224088\ d6=58.09812
251\ d7=57.80349111\ d8=58.0770231\ d9=58.00781318\ d10=82.48814919\ \Versi
on=DEC-AXP-OSF/1-G98RevA.7\ State=2-A'\ HF=-200.6814954\ S2=0.761796\ S2-1
=0.\ S2A=0.750092\ RMSD=2.787e-09\ RMSF=3.827e-05\ Dipole=-0.0792212,0.,0.
1834777\ PG=CS [SG(C5H1Si1),X(H12)]\ \@
```

## MP2/DZP

```
1\1\ MARCCENTRE-BNET3\POpt\UMP2-FC\Gen\C5H13Si1(2)\ROOT\11-Oct-2000\1\
\#MP2=DIRECT/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS
=CHECK\ \calc on the ground state SiC5H13\ \0,2\Si\C,1,r1\C,2,r2,1,a1\C,
3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,0\H,1,r6,2,a5,3,d
4,0\H,1,r7,2,a6,3,d5,0\H,1,r7,2,a6,3,-d5,0\H,2,r8,3,a7,4,-d6,0\H,2,r8,
3,a7,4,d6,0\H,3,r9,4,a8,5,d7,0\H,3,r9,4,a8,5,-d7,0\H,4,r10,5,a9,6,-d8,
0\H,4,r10,5,a9,6,d8,0\H,5,r11,4,a10,3,-d9,0\H,5,r11,4,a10,3,d9,0\H,6,r
12,5,a11,4,d10,0\H,6,r12,5,a11,4,-d10,0\ \r1=1.88664729\r2=1.53802372\r
3=1.53177881\r4=1.54364609\r5=1.4987185\r6=1.47024179\r7=1.47054273\r8
=1.09686007\r9=1.09792199\r10=1.096984\r11=1.09645977\r12=1.08363921\ a
1=112.94209613\ a2=112.72700498\ a3=112.3896607\ a4=113.027352\ a5=111.455
34634\ a6=110.00484862\ a7=109.52568855\ a8=108.87466348\ a9=109.30793854\
a10=108.39294635\ a11=120.271389\ d1=180.\ d2=180.\ d3=180.\ d4=180.\ d5=59.
53416126\ d6=58.16686672\ d7=57.92998563\ d8=58.3385308\ d9=57.98112931\ d1
0=81.56065578\ \Version=DEC-AXP-OSF/1-G98RevA.7\ State=2-A'\ HF=-200.6808
858\ MP2=-201.4644224\ PUHF=-200.6839719\ PMP2-0=-201.4663929\ S2=0.761894
\ S2-1=0.753254\ S2A=0.750094\ RMSD=7.266e-09\ RMSF=3.173e-05\ Dipole=-0.10
90617,0.,0.1587489\ PG=CS [SG(C5H1Si1),X(H12)]\ \@
```

## B3LYP/DZP

```
1\1\ MARCCENTRE-BNET4\POpt\UB3LYP\Gen\C5H13Si1(2)\ROOT\13-Oct-2000\1\
\#B3LYP/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK
\ \calc on the ground state SiC5H13\ \0,2\Si\C,1,r1\C,2,r2,1,a1\C,3,r3,2
,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,0\H,1,r6,2,a5,3,d4,0\H,
1,r7,2,a6,3,d5,0\H,1,r7,2,a6,3,-d5,0\H,2,r8,3,a7,4,-d6,0\H,2,r8,3,a7,4
,d6,0\H,3,r9,4,a8,5,d7,0\H,3,r9,4,a8,5,-d7,0\H,4,r10,5,a9,6,-d8,0\H,4,
r10,5,a9,6,d8,0\H,5,r11,4,a10,3,-d9,0\H,5,r11,4,a10,3,d9,0\H,6,r12,5,a
11,4,d10,0\H,6,r12,5,a11,4,-d10,0\ \r1=1.88892662\r2=1.54371567\r3=1.53
808957\r4=1.55341949\r5=1.49753125\r6=1.47927506\r7=1.4795879\r8=1.099
09805\r9=1.09959889\r10=1.09856964\r11=1.09942422\r12=1.08722264\ a1=11
3.83987995\ a2=113.17754779\ a3=112.51531301\ a4=113.45351129\ a5=110.9977
0999\ a6=110.58650581\ a7=109.80922723\ a8=109.04913228\ a9=109.20888546\ a
10=108.252061\ a11=120.94351578\ d1=180.\ d2=180.\ d3=180.\ d4=180.\ d5=59.8
0307548\ d6=58.04191774\ d7=57.69425819\ d8=58.03912315\ d9=57.73625408\ d1
0=85.73049933\ \Version=DEC-AXP-OSF/1-G98RevA.7\ State=2-A'\ HF=-202.2283
396\ S2=0.753677\ S2-1=0.\ S2A=0.750009\ RMSD=4.482e-09\ RMSF=1.953e-05\ Dip
ole=-0.0655586,0.,0.1908991\ PG=CS [SG(C5H1Si1),X(H12)]\ \@
```

## CCSD(T)/DZP//B3LYP/DZP

```
CCSD(T)=-201.5787874
```

## Transition State 1 (Y = Ge, Z = CH<sub>2</sub>) GeC<sub>5</sub>H<sub>13</sub>

## MP2/DZP

```
1\1\GINC-SATORI\PTS\UMP2-FC\Gen\C5H13Ge1(2)\SMHORVAT\07-Feb-2001\1\ \#M
```

---

---

```

P2=DIRECT/GEN PSEUDO=READ SCF=DIRECT OPT=(EF,TS,READFC) GEOM=CHECKPOINT
T GUESS=CHECK\calc on the 1,5 trans of GeH3 b/w c with H ax\0,2\Ge\C
,1,r1\C,1,r1x,2,a1\C,2,r2,1,a2,3,d1,0\C,3,r2x,1,a2x,2,-dlx,0\C,4,r3,2,
a3,1,d2,0\H,1,r4,2,a4,4,d3,0\H,1,r5,2,a5,4,-d4,0\H,1,r5x,3,a5x,5,d4x,0
\H,2,r6,1,a6,3,-d5,0\H,2,r7,1,a7,3,-d6,0\H,4,r8,2,a8,1,d7,0\H,4,r9,2,a
9,1,d8,0\H,6,r10,4,a10,2,d9,0\H,6,r11,4,a11,2,d10,0\H,5,r8x,3,a8x,1,-d
7x,0\H,5,r9,3,a9,1,-d8,0\H,3,r6x,1,a6x,2,d5x,0\H,3,r7x,1,a7x,2,d6x,0\
r1=2.15912924\r1x=2.16035159\r2=1.51933623\r2x=1.51929712\r3=1.5281015
5\r4=1.53877344\r5=1.56866446\r5x=1.56883648\r6=1.09274507\r6x=1.09268
445\r7=1.09499087\r7x=1.09497749\r8=1.09762643\r8x=1.09762588\r9=1.100
23044\r10=1.09612686\r11=1.09803197\al=81.16916661\ax=115.17290998\ax
=115.14218368\ax=113.66354815\ax=104.11310727\ax=84.11775295\ax=84.02
479523\ax=99.8595307\ax=99.88882699\ax=105.8798146\ax=105.82772586\ax
=109.75639954\ax=109.75957987\ax=108.06593118\ax=109.50387193\ax=1.09
30299697\dl=57.60081762\dlx=57.59972978\dl=-69.89652125\dl=-45.0148
6278\dl=151.50724823\dlx=151.1917598\dl=182.04069693\dlx=182.01720472\
dl=-67.89706698\dlx=67.85078314\dl=53.18137625\dlx=53.18640211\dl=169.0
4146575\dl=183.61156092\dl=-59.13352658\Version=NEC-SX-4-SUPER-UX-G9
8RevA.7\HF=-200.4742702\MP2=-201.2817474\PUHF=-200.4836993\PMP2-0=-201
.2887858\S2=0.82442\S2-1=0.786008\S2A=0.75223\RMSD=8.046e-09\RMSF=1.65
3e-05\Dipole=0.5334919,0.1101375,0.621139\PG=C01 [X(C5H13Ge1)]\@

```

### B3LYP/DZP

```

1\1\GINC-SATORI\PTS\UB3LYP\Gen\C5H13Ge1(2)\SMHORVAT\11-Feb-2001\1\#B3
LYP/GEN PSEUDO=READ SCF=DIRECT OPT=(EF,TS,READFC) GEOM=CHECKPOINT GUES
S=CHECK\calc on the 1,5 trans of GeH3 b/w c with H ax\0,2\Ge\C,1,r1\
C,1,r1x,2,a1\C,2,r2,1,a2,3,d1,0\C,3,r2x,1,a2x,2,-dlx,0\C,4,r3,2,a3,1,d
2,0\H,1,r4,2,a4,4,d3,0\H,1,r5,2,a5,4,-d4,0\H,1,r5x,3,a5x,5,d4x,0\H,2,r
6,1,a6,3,-d5,0\H,2,r7,1,a7,3,-d6,0\H,4,r8,2,a8,1,d7,0\H,4,r9,2,a9,1,d8
,0\H,6,r10,4,a10,2,d9,0\H,6,r11,4,a11,2,d10,0\H,5,r8x,3,a8x,1,-d7x,0\H
,5,r9,3,a9,1,-d8,0\H,3,r6x,1,a6x,2,d5x,0\H,3,r7x,1,a7x,2,d6x,0\|r1=2.1
7719441\r1x=2.17694849\r2=1.52114035\r2x=1.52115998\r3=1.5346701\r4=1.
54739634\r5=1.58549854\r5x=1.5854082\r6=1.09323392\r6x=1.09324801\r7=1
.09545568\r7x=1.09545576\r8=1.09937513\r8x=1.09937482\r9=1.10310568\r1
0=1.09793309\r11=1.09992666\al=84.20767538\ax=115.71924205\ax=115.720
92856\ax=114.5781012\ax=104.86824535\ax=83.74793258\ax=83.76833882\ax
=99.6898103\ax=99.68070557\ax=104.46447744\ax=104.47514807\ax=109.73
764412\ax=109.73723617\ax=107.92640055\ax=109.27194158\ax=109.43273
201\dl=51.99969955\dlx=51.99466607\dl=-66.11934255\dl=-51.83137191\dl=
157.33404972\dlx=157.43180519\dl=186.87973434\dlx=186.89001112\dl=73.3
7468055\dlx=73.38545909\dl=57.54333343\dlx=57.54247155\dl=172.54451526
\dl=185.06591002\dl=-58.39827144\Version=NEC-SX-4-SUPER-UX-G98RevA.7
\HF=-202.0619091\S2=0.761697\S2-1=0.\S2A=0.750083\RMSD=8.246e-09\RMSF=
5.796e-05\Dipole=0.5869502,0.1113442,0.6495002\PG=C01 [X(C5H13Ge1)]\@

```

### CCSD(T)/DZP//B3LYP/DZP

```
CCSD(T)=-201.3989715
```

## 6-Germa-1-hexyl Radical $\text{GeC}_5\text{H}_{13}^\bullet$

### MP2/DZP

```

1\1\ MARCCENTRE-BNET3\POpt\UMP2-FC\Gen\C5H13Ge1(2)\ROOT\11-Oct-2000\1\
\#MP2=DIRECT/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS
=CHECK\calc1 on the ground state of GeC5H13 radicc1\0,2\Ge\C,1,r1\C
,2,r2,1,a1\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,0\H
,1,r6,2,a5,3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r7,2,a6,3,-d5,0\H,2,r8,3,a7,4,
-d6,0\H,2,r8,3,a7,4,d6,0\H,3,r9,4,a8,5,d7,0\H,3,r9,4,a8,5,-d7,0\H,4,r1
0,5,a9,6,-d8,0\H,4,r10,5,a9,6,d8,0\H,5,r11,4,a10,3,-d9,0\H,5,r11,4,a10
,3,d9,0\H,6,r12,5,a11,4,d10,0\H,6,r12,5,a11,4,-d10,0\|r1=1.97233712\r2

```

---

---

```
=1.53638724\r3=1.53212114\r4=1.54383435\r5=1.49865649\r6=1.53647082\r7
=1.53679117\r8=1.09658407\r9=1.09793237\r10=1.09697753\r11=1.09645718\
r12=1.08364099\al=112.8653277\al=112.54344868\al=112.39866142\al=113.0
1717667\al=111.48069615\al=109.88929206\al=109.80912617\al=108.8568998
3\al=109.30228394\al=108.38971423\al=120.26914861\d1=180.\d2=180.\d3
=180.\d4=180.\d5=59.50600931\d6=58.50746201\d7=57.94057958\d8=58.33411
161\d9=57.97966647\d10=81.53981181\Version=DEC-AXP-OSF/1-G98RevA.7\St
ate=2-A'\HF=-200.5426016\MP2=-201.3242558\PUHF=-200.5456871\PM2-0=-20
1.3262259\S2=0.761893\S2-1=0.753254\S2A=0.750094\RMSD=6.481e-09\RMSF=3
.394e-05\Dipole=-0.1082012,0.,0.1774728\PG=CS [SG(C5H1Ge1),X(H12)]\@
```

### B3LYP/DZP

```
1\1\ MARCCENTRE-BNET4\POpt\UB3LYP\Gen\C5H13Ge1(2)\ROOT\13-Oct-2000\1\
#B3LYP/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK
\calc on the ground state of GeC5H13 radical\0,2\Ge\C,1,r1\C,2,r2,
1,a1\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,0\H,1,r6,2
,a5,3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r7,2,a6,3,-d5,0\H,2,r8,3,a7,4,-d6,0\
H,2,r8,3,a7,4,d6,0\H,3,r9,4,a8,5,d7,0\H,3,r9,4,a8,5,-d7,0\H,4,r10,5,a9
,6,-d8,0\H,4,r10,5,a9,6,d8,0\H,5,r11,4,a10,3,-d9,0\H,5,r11,4,a10,3,d9,
0\H,6,r12,5,a11,4,d10,0\H,6,r12,5,a11,4,-d10,0\|r1=1.9768498\r2=1.5410
1075\r3=1.53883293\r4=1.55359676\r5=1.49746006\r6=1.54554402\r7=1.5459
344\r8=1.09802743\r9=1.09950101\r10=1.09848991\r11=1.09936587\r12=1.08
722826\al=113.85502644\al=112.84617646\al=112.59942511\al=113.38769778
\al=110.88644781\al=110.41993464\al=110.11889162\al=109.02242265\al=10
9.18965236\al=108.27005032\al=120.94282386\d1=180.\d2=180.\d3=180.\d
4=180.\d5=59.77593177\d6=58.47609356\d7=57.72446943\d8=58.03654611\d9=
57.7608855\d10=85.64063349\Version=DEC-AXP-OSF/1-G98RevA.7\State=2-A'
\HF=-202.0970537\S2=0.753676\S2-1=0.\S2A=0.750009\RMSD=3.162e-09\RMSF=
1.656e-05\Dipole=-0.0660986,0.,0.2086589\PG=CS [SG(C5H1Ge1),X(H12)]\@
```

### CCSD(T)/DZP/B3LYP/DZP

```
CCSD(T)=-201.4380049
```

## Transition State 3 (Y = Sn, Z = CH<sub>2</sub>) SnC<sub>5</sub>H<sub>13</sub>

### MP2/DZP

```
1\1\GINC-SATORI\PTS\UMP2-FC\Gen\C5H13Sn1(2)\SMHORVAT\09-Feb-2001\1\#M
P2=DIRECT/GEN PSEUDO=READ SCF=DIRECT OPT=(EF,TS,READFC) GEOM=CHECKPOIN
T GUESS=CHECK\calc on the 1,5 trans of SnH3 b/w c with H ax\0,2\Sn\C
,1,r1\C,1,r1x,2,a1\C,2,r2,1,a2,3,d1,0\C,3,r2x,1,a2x,2,-d1x,0\C,4,r3,2,
a3,1,d2,0\H,1,r4,2,a4,4,d3,0\H,1,r5,2,a5,4,-d4,0\H,1,r5x,3,a5x,5,d4x,0
\H,2,r6,1,a6,3,-d5,0\H,2,r7,1,a7,3,-d6,0\H,4,r8,2,a8,1,d7,0\H,4,r9,2,a
9,1,d8,0\H,6,r10,4,a10,2,d9,0\H,6,r11,4,a11,2,d10,0\H,5,r8x,3,a8x,1,-d
7x,0\H,5,r9,3,a9,1,-d8,0\H,3,r6x,1,a6x,2,d5x,0\H,3,r7x,1,a7x,2,d6x,0\
r1=2.3485487\r1x=2.34884336\r2=1.51681571\r2x=1.51680822\r3=1.52919062
\r4=1.70854875\r5=1.72663242\r5x=1.7266756\r6=1.09333312\r6x=1.0933171
6\r7=1.09372179\r7x=1.09371693\r8=1.09774814\r8x=1.09774986\r9=1.10066
689\r10=1.09612038\r11=1.09804584\al=74.91109154\al=115.39717441\al=115.
38592028\al=113.69793243\al=102.81674189\al=84.81850213\al=84.7937
1497\al=96.49179449\al=96.49883599\al=106.62200962\al=106.6136428\al=
110.03240637\al=110.03391072\al=108.20252036\al=109.30651185\al=110
9.21069359\d1=59.4499032\d1x=59.44715079\d2=-73.32553299\d3=-40.644761
66\d4=148.40262874\d4x=148.30034853\d5=181.16889537\d5x=181.16749352\d
6=67.40200884\d6x=67.39355805\d7=50.02652478\d7x=50.02795592\d8=165.94
547601\d9=184.67734249\d10=-58.28611956\Version=NEC-SX-4-SUPER-UX-G98
RevA.7\HF=-200.0745691\MP2=-200.8682965\PUHF=-200.0847523\PM2-0=-200.
876175\S2=0.844752\S2-1=0.801264\S2A=0.752221\RMSD=8.419e-09\RMSF=5.09
1e-06\Dipole=0.5714894,0.1350808,0.7456619\PG=C01 [X(C5H13Sn1)]\@
```

---

**B3LYP/DZP**

```

1\1\GINC-SATORI\PTS\UB3LYP\Gen\C5H13Sn1(2)\SMHORVAT\20-Feb-2001\1\1\#B3
LYP/GEN PSEUDO=READ SCF=DIRECT OPT=(EF,TS,READFC) GEOM=CHECKPOINT GUES
S=CHECK OPTCYC=100\calc on the 1,5 trans of SnH3 b/w c with H ax\0,2
\Sn\C,1,r1\C,1,r1x,2,a1\C,2,r2,1,a2,3,d1,0\C,3,r2x,1,a2x,2,-d1x,0\C,4,
r3,2,a3,1,d2,0\H,1,r4,2,a4,4,d3,0\H,1,r5,2,a5,4,-d4,0\H,1,r5x,3,a5x,5,
d4x,0\H,2,r6,1,a6,3,-d5,0\H,2,r7,1,a7,3,-d6,0\H,4,r8,2,a8,1,d7,0\H,4,r
9,2,a9,1,d8,0\H,6,r10,4,a10,2,d9,0\H,6,r11,4,a11,2,d10,0\H,5,r8x,3,a8x
,1,-d7x,0\H,5,r9,3,a9,1,-d8,0\H,3,r6x,1,a6x,2,d5x,0\H,3,r7x,1,a7x,2,d6
x,0\|r1=2.3585528\r1x=2.35903962\r2=1.51800577\r2x=1.5179009\r3=1.5362
7734\r4=1.71794016\r5=1.74440869\r5x=1.74415279\r6=1.0934702\r6x=1.093
49966\r7=1.09452324\r7x=1.09451554\r8=1.09944925\r8x=1.09944695\r9=1.1
0382857\r10=1.09791406\r11=1.09986629\|a1=79.36855637\|a2=116.29345106\|a
2x=116.29609617\|a3=114.96119602\|a4=104.17969273\|a5=84.00809592\|a5x=83.
98779111\|a6=97.04596519\|a6x=97.00232302\|a7=104.11880403\|a7x=104.107383
63\|a8=109.94194216\|a8x=109.94052133\|a9=107.88833769\|a10=108.95678376\|a
11=109.36330471\|d1=51.47786812\|d1x=51.48617033\|d2=-67.90799217\|d3=-50.
38639141\|d4=156.85166105\|d4x=157.24692109\|d5=187.92284179\|d5x=187.9228
8856\|d6=74.74725135\|d6x=74.75393504\|d7=56.28225931\|d7x=56.28401525\|d8=
171.18147638\|d9=187.10204916\|d10=-56.65533169\|Version=NEC-SX-4-SUPER-
UX-G98RevA.7\|HF=-201.657055\|S2=0.764519\|S2-1=0.\|S2A=0.750091\|RMSD=3.75
6e-09\|RMSF=4.450e-05\|Dipole=0.6712788,0.1383101,0.8064971\|PG=C01 [X(C5
H13Sn1)]\|@

```

**CCSD(T)/DZP/B3LYP/DZP**

```

CCSD(T)=-200.9859325

```

**6-Stanna-1-hexyl Radical SnC<sub>5</sub>H<sub>13</sub><sup>•</sup>****MP2/DZP**

```

1\1\GINC-SATORI\POpt\UMP2-FC\Gen\C5H13Sn1(2)\SMHORVAT\18-Dec-2000\1\1\#
MP2=DIRECT/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=C
HECK\calc1 on the ground state of SnC5H13 radical\0,2\Sn\C,1,r1\C,2
,r2,1,a1\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,0\H,1,
r6,2,a5,3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r7,2,a6,3,-d5,0\H,2,r8,3,a7,4,-d
6,0\H,2,r8,3,a7,4,d6,0\H,3,r9,4,a8,5,d7,0\H,3,r9,4,a8,5,-d7,0\H,4,r10,
5,a9,6,-d8,0\H,4,r10,5,a9,6,d8,0\H,5,r11,4,a10,3,-d9,0\H,5,r11,4,a10,3
,d9,0\H,6,r12,5,a11,4,d10,0\H,6,r12,5,a11,4,-d10,0\|r1=2.15323708\r2=1
.53741119\r3=1.53260352\r4=1.54411271\r5=1.49859847\r6=1.70576272\r7=1.
70583304\r8=1.096611\r9=1.09810481\r10=1.09701479\r11=1.09648269\r12=1
.08367865\|a1=113.07777082\|a2=112.53033284\|a3=112.41363356\|a4=113.02024
637\|a5=111.52151519\|a6=109.62262089\|a7=109.77328752\|a8=108.65234389\|a9
=109.29176379\|a10=108.39462308\|a11=120.24990568\|d1=180.\|d2=180.\|d3=180
.\|d4=180.\|d5=59.43471505\|d6=58.482434\|d7=57.80493905\|d8=58.3406169\|d9=
57.98992653\|d10=81.41430545\|Version=NEC-SX-4-SUPER-UX-G98RevA.7\|State
=2-A'\|HF=-200.1248531\|MP2=-200.8997417\|PUHF=-200.1279356\|PMP2-0=-200.9
0171\|S2=0.761884\|S2-1=0.753252\|S2A=0.750094\|RMSD=2.449e-09\|RMSF=3.916e
-05\|Dipole=-0.1168728,0.,0.1815802\|PG=CS [SG(C5H1Sn1),X(H12)]\|@

```

**B3LYP/DZP**

```

1\1\GINC-SATORI\POpt\UB3LYP\Gen\C5H13Sn1(2)\SMHORVAT\14-Nov-2000\1\1\#B
3LYP/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK\

```



---

```

calcl on the ground state of SnC5H13 radical\0,2\Sn\C,1,r1\C,2,r2,1,
a1\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,0\H,1,r6,2,a
5,3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r7,2,a6,3,-d5,0\H,2,r8,3,a7,4,-d6,0\H,
2,r8,3,a7,4,d6,0\H,3,r9,4,a8,5,d7,0\H,3,r9,4,a8,5,-d7,0\H,4,r10,5,a9,6
,-d8,0\H,4,r10,5,a9,6,d8,0\H,5,r11,4,a10,3,-d9,0\H,5,r11,4,a10,3,d9,0\
H,6,r12,5,a11,4,d10,0\H,6,r12,5,a11,4,-d10,0\|r1=2.1550456\r2=1.541411
41\r3=1.539465\r4=1.55377878\r5=1.49735431\r6=1.71451686\r7=1.71463203
\r8=1.09739603\r9=1.09960588\r10=1.09848806\r11=1.09939766\r12=1.08723
579\|a1=114.0956527\|a2=112.78421863\|a3=112.60175871\|a4=113.36588217\|a5=
110.89610838\|a6=110.15740565\|a7=110.18391551\|a8=108.84572822\|a9=109.20
608271\|a10=108.28463396\|a11=120.94102252\|d1=180.\|d2=180.\|d3=180.\|d4=18
0.\|d5=59.71850894\|d6=58.51564259\|d7=57.60547773\|d8=58.05459885\|d9=57.7
7076526\|d10=85.59164117\|Version=NEC-SX-4-SUPER-UX-G98RevA.7\|State=2-A
'\|HF=-201.6798807\|S2=0.753679\|S2-1=0.\|S2A=0.750009\|RMSD=3.446e-09\|RMSF
=2.256e-05\|Dipole=-0.0713344,0.,0.2249818\|PG=CS [SG(C5H1Sn1),X(H12)]\|
@

```

### CCSD(T)/DZP// B3LYP/DZP

```
CCSD(T)=-201.0128317
```

### Transition State 3 (Y = Si, CH<sub>2</sub> = O) SiO<sub>2</sub>C<sub>3</sub>H<sub>11</sub>

#### SCF/DZP

```

1\1\ MARCCENTRE-ANET06\POpt\UHF\Gen\C3H9O2Si1(2)\SONIA\22-Dec-2000\1\|
#UHF/GEN PSEUDO=READ SCF=QC OPT=GRAD GEOM=CHECKPOINT OPTCYC=100\|Calc
on the translocation of SiH3 Between 2 O\0,2\Si\O,1,r1\O,1,r1,2,a1\C,
2,r2,1,a2,3,d1,0\C,3,r2,1,a2,2,-d1,0\C,4,r3,2,a3,1,d2,0\H,1,r4,2,a4,4,
d3,0\H,1,r5,2,a5,4,-d4,0\H,1,r5,3,a5,5,d4,0\H,4,r8,2,a8,1,d7,0\H,4,r9,
2,a9,1,d8,0\H,6,r10,4,a10,2,d9,0\H,6,r11,4,a11,2,d10,0\H,5,r8,3,a8,1,-
d7,0\H,5,r9,3,a9,1,-d8,0\|r1=1.87192534\r2=1.40218865\r3=1.53485512\r4
=1.4593711\r5=1.48926867\r8=1.08939041\r9=1.08380328\r10=1.08645852\r1
1=1.08377847\|a1=72.2048983\|a2=120.47094873\|a3=108.02847944\|a4=97.95172
096\|a5=86.8485802\|a8=110.32142433\|a9=108.1407682\|a10=108.55500338\|a11=
108.9667597\|d1=73.20936601\|d2=-78.24377259\|d3=172.89226482\|d4=80.08013
013\|d7=42.73487543\|d8=161.49904097\|d9=174.1770154\|d10=-67.66711165\|Ve
rsion=DEC-AXP-OSF/1-G98RevA.7\|HF=-272.3112516\|S2=0.767873\|S2-1=0.\|S2A=
0.750232\|RMSD=0.000e+00\|RMSF=1.031e-02\|Dipole=-0.0966634,1.1530035,1.4
999849\|PG=C01 [X(C3H9O2Si1)]\|@

```

#### MP2/DZP

```

1\|#MP2=DIRECT/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUE
SS=CHECK\|Calc on the translocation of SiH3 Between 2 O\0,2\Si\O,1,r1
\O,1,r1,2,a1\C,2,r2,1,a2,3,d1,0\C,3,r2,1,a2,2,-d1,0\C,4,r3,2,a3,1,d2,0
\H,1,r4,2,a4,4,d3,0\H,1,r5,2,a5,4,-d4,0\H,1,r5,3,a5,5,d4,0\H,4,r8,2,a8
,1,d7,0\H,4,r9,2,a9,1,d8,0\H,6,r10,4,a10,2,d9,0\H,6,r11,4,a11,2,d10,0\
H,5,r8,3,a8,1,-d7,0\H,5,r9,3,a9,1,-d8,0\|r1=1.87513887\r2=1.41761778\r
3=1.53583791\r4=1.46009713\r5=1.48863814\r8=1.1002092\r9=1.09519415\r1
0=1.09593508\r11=1.09272889\|a1=67.4573206\|a2=116.13553747\|a3=107.45834
888\|a4=100.29604724\|a5=88.22955845\|a8=111.17694246\|a9=107.64844581\|a10
=111.67301295\|a11=109.1805865\|d1=81.05667897\|d2=-83.96291227\|d3=178.01
45381\|d4=71.88259444\|d7=37.17180213\|d8=156.98936188\|d9=172.00237658\|d1
0=-66.8294011\|Version=DEC-AXP-OSF/1-G98RevA.7\|HF=-272.3073285\|MP2=-27
3.1834164\|PUHF=-272.3175129\|PMP2-0=-273.1902397\|S2=0.793882\|S2-1=0.764
628\|S2A=0.750737\|RMSD=6.924e-09\|RMSF=6.870e-05\|Dipole=0.5202449,1.1832
367,0.7803683\|PG=C01 [X(C3H9O2Si1)]\|@

```

---

**B3LYP/DZP**

```

\\#B3LYP/GEN PSEUDO=READ SCF=QC OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK\\
Calc on the translocation of SiH3 Between 2 O\\0,2\\Si\\0,1,r1\\0,1,r1,2,
a1\\C,2,r2,1,a2,3,d1,0\\C,3,r2,1,a2,2,-d1,0\\C,4,r3,2,a3,1,d2,0\\H,1,r4,2,
a4,4,d3,0\\H,1,r5,2,a5,4,-d4,0\\H,1,r5,3,a5,5,d4,0\\H,4,r8,2,a8,1,d7,0\\H,
4,r9,2,a9,1,d8,0\\H,6,r10,4,a10,2,d9,0\\H,6,r11,4,a11,2,d10,0\\H,5,r8,3,a
8,1,-d7,0\\H,5,r9,3,a9,1,-d8,0\\r1=1.86487775\\r2=1.40997841\\r3=1.544319
9\\r4=1.46844027\\r5=1.5024868\\r8=1.10306545\\r9=1.09889717\\r10=1.0977365
9\\r11=1.09500991\\a1=71.46800425\\a2=118.59971326\\a3=108.23142075\\a4=100
.22302933\\a5=87.37431171\\a8=111.2510559\\a9=108.27910291\\a10=111.580497
71\\a11=109.20393292\\d1=75.70236853\\d2=-80.51342089\\d3=173.15549746\\d4=
77.7083438\\d7=40.67271481\\d8=160.40140685\\d9=173.44426362\\d10=-65.9846
3183\\Version=DEC-AXP-OSF/1-G98RevA.7\\HF=-274.0638556\\S2=0.756313\\S2-1
=0.\\S2A=0.750023\\RMSD=0.000e+00\\RMSF=2.968e-05\\Dipole=0.6591246,1.1538
688,0.9160879\\PG=C01 [X(C3H9O2Si1)]\\@

```

**CCSD(T)/DZP//B3LYP/DZP**

```
CCSD(T)=-273.276234
```

**1,5-Dioxa-6-sila-1-hexyl Radical  $\text{SiO}_2\text{C}_5\text{H}_{11}^\bullet$** **SCF/DZP**

```

1\\1\\GINC-SATORI\\POpt\\UHF\\Gen\\C3H9O2Si1(2)\\SMHORVAT\\05-Jan-2001\\1\\#UHF
/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT\\calc on the grou
nd state of SiO2C3H9 radical\\0,2\\Si\\0,1,r1\\C,2,r2,1,a1\\C,3,r3,2,a2,1,
d1,0\\C,4,r4,3,a3,2,d2,0\\O,5,r5,4,a4,3,d3,0\\H,1,r6,2,a5,3,d4,0\\H,1,r7,2
,a6,3,d5,0\\H,1,r7,2,a6,3,-d5,0\\H,3,r9,4,a8,5,d7,0\\H,3,r9,4,a8,5,-d7,0\\
H,4,r10,5,a9,6,-d8,0\\H,4,r10,5,a9,6,d8,0\\H,5,r11,4,a10,3,-d9,0\\H,5,r11
,4,a10,3,d9,0\\r1=1.64427868\\r2=1.40353948\\r3=1.52115805\\r4=1.53141632
\\r5=1.38933249\\r6=1.46296644\\r7=1.47118319\\r9=1.08940141\\r10=1.0843792
3\\r11=1.08833379\\a1=124.29625475\\a2=108.86202417\\a3=111.28255174\\a4=10
7.60384453\\a5=107.06857794\\a6=110.48675767\\a8=110.04313082\\a9=109.6706
7097\\a10=110.07761178\\d1=180.\\d2=180.\\d3=180.\\d4=180.\\d5=59.83961376\\d
7=59.20327596\\d8=59.06214452\\d9=60.22700547\\Version=NEC-SX-4-SUPER-UX
-G98RevA.7\\State=2-A'\\HF=-272.3851833\\S2=0.758379\\S2-1=0.\\S2A=0.750054
\\RMSD=4.001e-09\\RMSF=2.153e-05\\Dipole=0.5884181,0.,-0.8205527\\PG=CS [S
G(C3H102Si1),X(H8)]\\@

```

**MP2/DZP**

```

1\\1\\GINC-SATORI\\POpt\\UMP2-FC\\Gen\\C3H9O2Si1(2)\\SMHORVAT\\08-Jan-2001\\1\\
#MP2=DIRECT/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=
CHECK\\calc on the ground state of SiO2C3H9 radical\\0,2\\Si\\0,1,r1\\C,2
,r2,1,a1\\C,3,r3,2,a2,1,d1,0\\C,4,r4,3,a3,2,d2,0\\O,5,r5,4,a4,3,d3,0\\H,1,
r6,2,a5,3,d4,0\\H,1,r7,2,a6,3,d5,0\\H,1,r7,2,a6,3,-d5,0\\H,3,r9,4,a8,5,d7
,0\\H,3,r9,4,a8,5,-d7,0\\H,4,r10,5,a9,6,-d8,0\\H,4,r10,5,a9,6,d8,0\\H,5,r1
1,4,a10,3,-d9,0\\H,5,r11,4,a10,3,d9,0\\r1=1.67723845\\r2=1.42992089\\r3=1
.5234538\\r4=1.54272527\\r5=1.39167416\\r6=1.46196031\\r7=1.47111651\\r9=1.
09943702\\r10=1.09269373\\r11=1.09845231\\a1=118.91188337\\a2=108.08699969
\\a3=110.19326646\\a4=106.47474745\\a5=106.23023965\\a6=110.62992004\\a8=11
0.02483613\\a9=109.65583251\\a10=109.10328368\\d1=180.\\d2=180.\\d3=180.\\d4
=180.\\d5=59.79739681\\d7=59.44449845\\d8=59.57124544\\d9=60.14844014\\Ver
sion=NEC-SX-4-SUPER-UX-G98RevA.7\\State=2-A'\\HF=-272.3831456\\MP2=-273.2
061235\\PUHF=-272.3864971\\PMP2-0=-273.2081629\\S2=0.758655\\S2-1=0.751851
\\S2A=0.750057\\RMSD=4.164e-09\\RMSF=9.297e-05\\Dipole=0.4918073,0.,-0.905
6839\\PG=CS [SG(C3H102Si1),X(H8)]\\@

```

**B3LYP/DZP**

```

1\1\GINC-SATORI\Popt\UB3LYP\Gen\C3H9O2Si1(2)\SMHORVAT\10-Jan-2001\1\#\#
B3LYP/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK
NOSYMM\calc on the ground state of SiO2C3H9 radical\0,2\Si\0,1,r1\C,
2,r2,1,a1\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\O,5,r5,4,a4,3,d3,0\H,1
,r6,2,a5,3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r7,2,a6,3,-d5,0\H,3,r9,4,a8,5,d
7,0\H,3,r9,4,a8,5,-d7,0\H,4,r10,5,a9,6,-d8,0\H,4,r10,5,a9,6,d8,0\H,5,r
11,4,a10,3,-d9,0\H,5,r11,4,a10,3,d9,0\|r1=1.66344589\r2=1.42309624\r3=
1.53139886\r4=1.56164285\r5=1.3735794\r6=1.47125547\r7=1.4808483\r9=1.
10210581\r10=1.09461752\r11=1.105373\|a1=122.93285998\|a2=108.25115899\|a
3=110.42873716\|a4=106.60337894\|a5=106.04108604\|a6=110.92108759\|a8=109.
91748941\|a9=109.30863691\|a10=108.00043111\|d1=179.9999999\|d2=180.000000
01\|d3=180.\|d4=180.\|d5=60.08463219\|d7=59.23301588\|d8=59.14102025\|d9=59.
583083\|Version=NEC-SX-4-SUPER-UX-G98RevA.7\|HF=-274.0834856\|S2=0.75330
5\|S2-1=0.\|S2A=0.750008\|RMSD=1.997e-09\|RMSF=8.228e-05\|Dipole=0.4801229,
0.,-0.9437593\|PG=CS [SG(C3H1O2Si1),X(H8)]\|@

```

**CCSD(T)/DZP//B3LYP/DZP**

```
CCSD(T)=-273.3027359
```

**Transition State 5 SiC<sub>5</sub>H<sub>11</sub>****SCF/DZP**

```

1\1\ MARCCENTRE-BNET1\FTS\UHF\Gen\C5H11Si1(2)\SONIA\09-Jun-2001\1\#\#UH
F/GEN PSEUDO=READ SCF=QC OPT=(EF,TS,READFC) GEOM=CHECKPOINT GUESS=CHEC
K\calc on the 1,5 translocation of SiH3 b/w C centres with a DB\0,2\
Si\C,1,r1\C,1,r2,2,a1\C,2,r3,1,a2,3,d1,0\C,4,r4,2,a3,1,d2,0\C,5,r5,4,a
4,2,d3,0\H,1,r6,2,a5,4,d4,0\H,1,r7,2,a6,4,d5,0\H,1,r8,2,a7,4,d6,0\H,2,
r9,1,a8,3,d7,0\H,2,r10,1,a9,3,d8,0\H,4,r11,2,a10,1,d9,0\H,5,r12,4,a11,
2,d10,0\H,6,r13,3,a12,1,d11,0\H,6,r14,3,a13,1,d12,0\H,3,r15,1,a14,2,d1
3,0\H,3,r16,1,a15,2,d14,0\|r1=2.2054109\r2=2.15294383\r3=1.48270138\r4
=1.3442158\r5=1.50588962\r6=1.47597706\r7=1.49206516\r8=1.48015311\r9=
1.07933168\r10=1.07937169\r11=1.07891014\r12=1.07808064\r13=1.08801766
\r14=1.09142112\r15=1.08331769\r16=1.08061594\|a1=76.47843696\|a2=110.50
346047\|a3=125.81606325\|a4=125.23604935\|a5=117.96092735\|a6=83.36551911\
|a7=128.94497576\|a8=103.11055291\|a9=102.14659737\|a10=116.30709628\|a11=1
7.39799754\|a12=109.71437652\|a13=109.03741108\|a14=96.82155076\|a15=107.
91078626\|d1=63.53216083\|d2=-46.06227231\|d3=5.17114288\|d5=-110.64353588
\|d4=149.5863756\|d6=-13.89138441\|d7=-175.27452171\|d8=-60.04915277\|d9=13
1.32217732\|d10=-179.53937951\|d11=-70.58672163\|d12=174.06424898\|d13=172
.16945559\|d14=58.23850476\|Version=DEC-AXP-OSF/1-G94RevE.2\|HF=-199.422
5467\|S2=0.953\|S2-1=0.\|S2A=0.776\|RMSD=0.000e+00\|RMSF=1.201e-05\|Dipole=0
.5538266,0.1024786,0.5592006\|PG=C01 [X(C5H11Si1)]\|@

```

**MP2/DZP**

```

1\1\ MARCCENTRE-ANET04\PTS\UMP2-FC\Gen\C5H11Si1(2)\SONIA\28-Jun-2001\1
\#\#MP2=DIRECT/GEN PSEUDO=READ SCF=QC OPT=(EF,TS)\calc on the 1,5 tran
slocation of SiH3 b/w C centres with a DB\0,2\Si\C,1,2.2054\C,1,r2,2,
a1\C,2,r3,1,a2,3,d1,0\C,4,r4,2,a3,1,d2,0\C,5,r5,4,a4,2,d3,0\H,1,r6,2,a
5,4,d4,0\H,1,r7,2,a6,4,d5,0\H,1,r8,2,128.9449,4,d6,0\H,2,r9,1,a8,3,d7,
0\H,2,r10,1,a9,3,d8,0\H,4,r11,2,a10,1,d9,0\H,5,r12,4,a11,2,d10,0\H,6,r
13,3,a12,1,d11,0\H,6,r14,3,a13,1,d12,0\H,3,r15,1,a14,2,d13,0\H,3,r16,1
,a15,2,d14,0\|r2=2.11970378\r3=1.50179252\r4=1.32124992\r5=1.50491947\
r6=1.47371826\r7=1.49653552\r8=1.48041521\r9=1.0914384\r10=1.09386186\
r11=1.09063292\r12=1.08848298\r13=1.09731326\r14=1.10060193\r15=1.0939

```

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```

5902\r16=1.09097653\a1=77.52708193\a2=113.94130938\a3=127.28882566\a4=
124.9521569\a5=116.58348821\a6=85.41401725\a8=101.82210623\a9=105.2898
3143\A10=115.3785212\A11=118.44733755\A12=110.6916989\A13=108.26966522
\A14=97.52874457\A15=108.31801179\D1=54.68658432\D2=-30.49369838\D3=-2
.16124805\D5=-118.58302698\D4=140.83422703\D6=-21.05766093\D7=-185.363
47701\D8=-70.66876644\D9=148.24550555\D10=-181.32914738\D11=-62.672485
69\D12=181.35608099\D13=169.87600983\D14=54.49311343\Version=DEC-AXP-
OSF/1-G94RevE.2\HF=-199.4201509\MP2=-200.1985774\PUHF=-199.4311147\MP
2-0=-200.2074076\S2=0.858\S2-1=0.814\S2A=0.758\RMSD=0.000e+00\RMSF=5.1
04e-03\Dipole=0.556046,0.0734731,0.3756811\PG=C01 [X(C5H11Si1)]\@

```

### B3LYP/DZP

```

1\1\ MARCCENTRE-ANET05\FTS\UB3LYP\Gen\C5H11Si1(2)\SONIA\23-Jun-2001\1\
\#B3LYP/GEN PSEUDO=READ SCF=QC OPT=(EF,TS,READFC) GEOM=CHECKPOINT GUES
S=CHECK\calc on the 1,5 translocation of SiH3 b/w C centres with a DB
\0,2\Si\C,1,r1\C,1,r2,2,a1\C,2,r3,1,a2,3,d1,0\C,4,r4,2,a3,1,d2,0\C,5,
r5,4,a4,2,d3,0\H,1,r6,2,a5,4,d4,0\H,1,r7,2,a6,4,d5,0\H,1,r8,2,a7,4,d6,
0\H,2,r9,1,a8,3,d7,0\H,2,r10,1,a9,3,d8,0\H,4,r11,2,a10,1,d9,0\H,5,r12,
4,a11,2,d10,0\H,6,r13,3,a12,1,d11,0\H,6,r14,3,a13,1,d12,0\H,3,r15,1,a1
4,2,d13,0\H,3,r16,1,a15,2,d14,0\|r1=2.13116263\r2=2.00830673\r3=1.4787
3563\r4=1.35558225\r5=1.50562336\r6=1.49328103\r7=1.54216552\r8=1.4901
4655\r9=1.08977998\r10=1.09308926\r11=1.09175619\r12=1.09078127\r13=1.
10061457\r14=1.10453383\r15=1.09638601\r16=1.09541366\A1=83.57602897\A
2=107.60446286\A3=126.43019996\A4=125.52609803\A5=125.22472463\A6=78.6
3889307\A7=121.80287249\A8=110.35405271\A9=98.55688873\A10=116.15780099
4\A11=118.15647907\A12=109.87007451\A13=109.58093257\A14=103.75255039\
A15=106.97479136\D1=62.18328176\D2=-44.80773824\D3=5.81098866\D5=-120.
47020676\D4=153.0690517\D6=-31.67295384\D7=-173.92731322\D8=-58.368255
07\D9=131.27171791\D10=-179.20233219\D11=-79.35919959\D12=166.01553667
\D13=174.79627346\D14=60.80360911\Version=DEC-AXP-OSF/1-G94RevE.2\HF=
-200.9618136\S2=0.763\S2-1=0.\S2A=0.75\RMSD=0.000e+00\RMSF=3.056e-05\D
ipole=0.5311012,0.1639269,0.5346433\PG=C01 [X(C5H11Si1)]\@

```

### CCSD(T)/DZP // B3LYP/DZP

```

CCSD(T)=-200.3148308

```

### (Z)-6-Sila-3-hexen-1-yl Radical $\text{SiO}_2\text{C}_5\text{H}_{11}^\bullet$

#### SCF/DZP

```

1\1\ MARCCENTRE-ANET06\FOpt\UHF\Gen\C5H11Si1(2)\SONIA\14-Jun-2001\1\#\
UHF/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK\c
alc on the ground state of SiC5H11 with cis DB at c3 position\0,2\Si\
C,1,r1\C,2,r2,1,a1\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3
,d3,0\H,1,r6,2,a5,3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r8,2,a7,3,d6,0\H,2,r9,
1,a8,7,d7,0\H,2,r10,1,a9,7,d8,0\H,3,r11,2,a10,1,d9,0\H,3,r12,2,a11,1,d
10,0\H,4,r13,3,a12,2,d11,0\H,5,r14,4,a13,3,d12,0\H,6,r15,5,a14,4,d13,0
\H,6,r16,5,a15,4,d14,0\|r1=1.88693105\r2=1.53679351\r3=1.51080325\r4=1
.40020325\r5=1.39398136\r6=1.47127152\r7=1.47193462\r8=1.47193156\r9=1
.08833485\r10=1.08830751\r11=1.08895784\r12=1.08877179\r13=1.07759582\
r14=1.07866848\r15=1.07543793\r16=1.07563079\A1=114.21888286\A2=112.82
960795\A3=124.63185985\A4=125.84772614\A5=110.29812243\A6=110.53885853
\A7=110.54215762\A8=108.33856955\A9=108.35767024\A10=109.58291582\A11=
109.5895683\A12=117.52377758\A13=116.81935705\A14=120.65391955\A15=122
.01599845\D1=-180.01038521\D2=-180.93672998\D3=-0.02714374\D4=-180.063
48966\D5=-59.98793772\D6=59.85604043\D7=-57.47286022\D8=57.3289059\D9=
57.93504146\D10=-57.93311232\D11=-1.08759971\D12=179.95524641\D13=180.
00025911\D14=0.01021458\Version=DEC-AXP-OSF/1-G94RevE.2\HF=-199.51629

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```
31\S2=0.964\S2-1=0.\S2A=0.758\RMSD=7.699e-09\RMSF=5.383e-05\Dipole=-0.0576333,0.0018231,0.160027\PG=C01 [X(C5H11Si1)]\ \@
```

### MP2/DZP

```
1\1\ MARCCENTRE-BNET4\FOpt\UMP2-FC\Gen\C5H11Si1(2)\SONIA\07-Aug-2001\1\
\#MP2=DIRECT/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD\calc on the ground
state of SiC5H11 with cis DB at c3 position\0,2\Si\C,1,r1\C,2,r2,1,a1
\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,0\H,1,r6,2,a5,
3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r8,2,a7,3,d6,0\H,2,r9,1,a8,7,d7,0\H,2,r1
0,1,a9,7,d8,0\H,3,r11,2,a10,1,d9,0\H,3,r12,2,a11,1,d10,0\H,4,r13,3,a12
,2,d11,0\H,5,r14,4,a13,3,d12,0\H,6,r15,5,a14,4,d13,0\H,6,r16,5,a15,4,d
14,0\|r1=1.886741|r2=1.537616|r3=1.507064|r4=1.391281|r5=1.384037|r6=1
.469658|r7=1.470291|r8=1.470287|r9=1.096365|r10=1.096326|r11=1.099085\
r12=1.098878|r13=1.086803|r14=1.087612|r15=1.082617|r16=1.08288|a1=112
.995|a2=112.741|a3=124.027|a4=125.265|a5=111.069|a6=110.027|a7=110.031
|a8=108.813|a9=108.829|a10=109.668|a11=109.665|a12=117.462|a13=117.218
|a14=120.96|a15=121.586|d1=-180.01|d2=-181.256|d3=0.009|d4=-180.008|d5
=-59.599|d6=59.576|d7=-57.934|d8=57.921|d9=57.892|d10=-57.915|d11=-1.3
57|d12=179.963|d13=179.952|d14=-0.02\Version=DEC-AXP-OSF/1-G94RevE.2\
HF=-199.5155885\MP2=-200.2585177\PUHF=-199.5322644\PMP2-0=-200.2725986
\S2=0.955\S2-1=0.89\S2A=0.757\RMSD=8.897e-09\RMSF=1.999e-05\Dipole=-0.
0963112,0.0030684,0.1454697\PG=C01 [X(C5H11Si1)]\ \@
```

### B3LYP/DZP

```
1\1\ MARCCENTRE-BNET2\FOpt\UB3LYP\Gen\C5H11Si1(2)\SONIA\27-Jun-2001\1\
\#B3LYP/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD GEOM=CHECKPOINT GUESS=CHEC
K\calc on the ground state of SiC5H11 with cis DB at c3 position\0,2
\Si\C,1,r1\C,2,r2,1,a1\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,
a4,3,d3,0\H,1,r6,2,a5,3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r8,2,a7,3,d6,0\H,2
,r9,1,a8,7,d7,0\H,2,r10,1,a9,7,d8,0\H,3,r11,2,a10,1,d9,0\H,3,r12,2,a11
,1,d10,0\H,4,r13,3,a12,2,d11,0\H,5,r14,4,a13,3,d12,0\H,6,r15,5,a14,4,d
13,0\H,6,r16,5,a15,4,d14,0\|r1=1.88930505|r2=1.54346959|r3=1.50953597\
r4=1.40068174|r5=1.39139142|r6=1.47871363|r7=1.47936554|r8=1.47935794\
r9=1.0987566|r10=1.09871944|r11=1.10125639|r12=1.10104284|r13=1.089864
93|r14=1.09150248|r15=1.08634946|r16=1.08654275|a1=114.21152746|a2=113
.12206384|a3=124.75080748|a4=126.10557295|a5=110.57057563|a6=110.60898
309|a7=110.60902218|a8=108.49003795|a9=108.50900651|a10=109.74242088|a1
1=109.76112579|a12=117.17439467|a13=116.67837787|a14=120.89643232|a15
=121.77034558|d1=-180.052768|d2=-181.01131491|d3=-0.03407499|d4=-180.0
4285057|d5=-59.91709637|d6=59.83058265|d7=-57.4590191|d8=57.34527646|d
9=57.59773148|d10=-57.66221021|d11=-1.12867038|d12=179.95277051|d13=17
9.98988177|d14=0.00322019\Version=DEC-AXP-OSF/1-G94RevE.2\HF=-201.019
0933\S2=0.779\S2-1=0.\S2A=0.75\RMSD=7.070e-09\RMSF=1.088e-04\Dipole=-0.
1072077,0.0030964,0.1776008\PG=C01 [X(C5H11Si1)]\ \@
```

### CCSD(T)/DZP // B3LYP/DZP

```
CCSD(T)=-200.3753818
```

### (Z)-6-Sila-2-hexen-1-yl Radical $\text{SiO}_2\text{C}_5\text{H}_{11}^\bullet$

### UHF/DZP

```
1\1\ MARCCENTRE-ANET06\FOpt\UHF\Gen\C5H11Si1(2)\SONIA\21-Jun-2001\1\1\#
UHF/GEN PSEUDO=READ SCF=QC OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK\calc
on the ground state of SiC5H11 with cis DB at c2 position\0,2\Si\C,1,
```

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```
r1\C,2,r2,1,a1\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,
0\H,1,r6,2,a5,3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r8,2,a7,3,d6,0\H,2,r9,1,a8
,7,d7,0\H,2,r10,1,a9,7,d8,0\H,3,r11,2,a10,1,d9,0\H,4,r12,3,a11,2,d10,0
\H,5,r13,4,a12,3,d11,0\H,5,r14,4,a13,3,d12,0\H,6,r15,5,a14,4,d13,0\H,6
,r16,5,a15,4,d14,0\|r1=1.89357113\r2=1.50874662\r3=1.32942012\r4=1.509
52253\r5=1.50740921\r6=1.47213576\r7=1.47079014\r8=1.47001514\r9=1.087
44555\r10=1.08435616\r11=1.07958626\r12=1.07938843\r13=1.0877597\r14=1
.08834349\r15=1.0770053\r16=1.07657205\|a1=112.3943974\|a2=128.40673916\
a3=127.97818191\|a4=112.48215535\|a5=110.13953395\|a6=110.20739938\|a7=110
.27517329\|a8=107.93601796\|a9=108.64583853\|a10=114.78646349\|a11=117.184
9526\|a12=110.65879922\|a13=108.81917419\|a14=120.07594794\|a15=120.176980
11\|d1=101.78856093\|d2=0.66871618\|d3=121.18026166\|d4=-185.42262263\|d5=5
4.78543846\|d6=-65.36132743\|d7=54.12952494\|d8=-61.09257613\|d9=-76.94605
208\|d10=-179.56896144\|d11=-2.15360427\|d12=-118.14034676\|d13=-201.38530
543\|d14=-36.85929915\|Version=DEC-AXP-OSF/1-G94RevE.2\|HF=-199.4900174\
S2=0.766\|S2-1=0.\|S2A=0.75\|RMSD=0.000e+00\|RMSF=1.660e-05\|Dipole=-0.1449
288,0.0417092,0.0933951\|PG=C01 [X(C5H11Si1)]\|@
```

## MP2/DZP

```
1\1\ MARCCENTRE-BNET4\FOpt\UMP2-FC\Gen\C5H11Si1(2)\SONIA\07-Aug-2001\1
\|#MP2=DIRECT/GEN PSEUDO=READ SCF=DIRECT OPT=GRAD\|calc on the ground
state of SiC5H11 with cis DB at c2 position\|0,2\Si\C,1,r1\C,2,r2,1,a1
\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,0\H,1,r6,2,a5
,3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r8,2,a7,3,d6,0\H,2,r9,1,a8,7,d7,0\H,2,r1
0,1,a9,7,d8,0\H,3,r11,2,a10,1,d9,0\H,3,r12,2,a11,1,d10,0\H,4,r13,3,a12
,2,d11,0\H,5,r14,4,a13,3,d12,0\H,6,r15,5,a14,4,d13,0\H,6,r16,5,a15,4,d
14,0\|r1=1.886741\r2=1.537616\r3=1.507064\r4=1.391281\r5=1.384037\r6=1
.469658\r7=1.470291\r8=1.470287\r9=1.096365\r10=1.096326\r11=1.099085\
r12=1.098878\r13=1.086803\r14=1.087612\r15=1.082617\r16=1.08288\|a1=112
.995\|a2=112.741\|a3=124.027\|a4=125.265\|a5=111.069\|a6=110.027\|a7=110.031
\|a8=108.813\|a9=108.829\|a10=109.668\|a11=109.665\|a12=117.462\|a13=117.218
\|a14=120.96\|a15=121.586\|d1=-180.01\|d2=-181.256\|d3=0.009\|d4=-180.008\|d5
=-59.599\|d6=59.576\|d7=-57.934\|d8=57.921\|d9=57.892\|d10=-57.915\|d11=-1.3
57\|d12=179.963\|d13=179.952\|d14=-0.02\|Version=DEC-AXP-OSF/1-G94RevE.2\
HF=-199.4900174\|MP2=-200.25851647\|PUHF=-199.5322644\|PMP2-0=-200.2725986
\|S2=0.955\|S2-1=0.89\|S2A=0.757\|RMSD=8.897e-09\|RMSF=1.999e-05\|Dipole=-0.
0963112,0.0030684,0.1454697\|PG=C01 [X(C5H11Si1)]\|@
```

## B3LYP/DZP

```
1\1\ MARCCENTRE-ANET03\FOpt\UB3LYP\Gen\C5H11Si1(2)\SONIA\28-Jun-2001\1
\|#B3LYP/GEN PSEUDO=READ SCF=QC OPT=GRAD GEOM=CHECKPOINT GUESS=CHECK\|
calc on the ground state of SiC5H11 with cis DB at c2 position\|0,2\Si
\C,1,r1\C,2,r2,1,a1\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4
,3,d3,0\H,1,r6,2,a5,3,d4,0\H,1,r7,2,a6,3,d5,0\H,1,r8,2,a7,3,d6,0\H,2,r9
,1,a8,7,d7,0\H,2,r10,1,a9,7,d8,0\H,3,r11,2,a10,1,d9,0\H,4,r12,3,a11,2,
d10,0\H,5,r13,4,a12,3,d11,0\H,5,r14,4,a13,3,d12,0\H,6,r15,5,a14,4,d13,
0\H,6,r16,5,a15,4,d14,0\|r1=1.89843087\r2=1.50917718\r3=1.34753942\r4=
1.5126883\r5=1.50302236\r6=1.47984471\r7=1.47799522\r8=1.47716201\r9=1
.0984069\r10=1.09584513\r11=1.0916184\r12=1.09121618\r13=1.10287883\r1
4=1.10132214\r15=1.08735191\r16=1.08654695\|a1=112.10301496\|a2=127.9243
0247\|a3=127.5339724\|a4=113.16768211\|a5=110.45863256\|a6=110.23223553\|a7
=110.32019687\|a8=107.65427495\|a9=108.5230463\|a10=114.99129158\|a11=117.
5681316\|a12=110.08221587\|a13=109.27290179\|a14=120.75670156\|a15=120.476
38607\|d1=102.97784142\|d2=0.85419977\|d3=124.08187889\|d4=-185.06332511\|d
5=55.15165701\|d6=-64.86491\|d7=54.13372441\|d8=-61.10812236\|d9=-75.56757
569\|d10=-179.46325001\|d11=0.56812902\|d12=-114.416429\|d13=-206.45287843
\|d14=-34.0504339\|Version=DEC-AXP-OSF/1-G94RevE.2\|HF=-200.9948317\|S2=0
.754\|S2-1=0.\|S2A=0.75\|RMSD=0.000e+00\|RMSF=1.127e-05\|Dipole=-0.1189637,
0.0194916,0.0868499\|PG=C01 [X(C5H11Si1)]\|@
```

## CCSD(T)/DZP // B3LYP/DZP

```
CCSD(T)=-200.3539535
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