Electronic Supporting Information:

A Computational Study of Multi-Component Orbital Interactions during the Cyclization of Silyl, Germyl and Stannyl Radicals onto C–N and C–O Multiple Bonds

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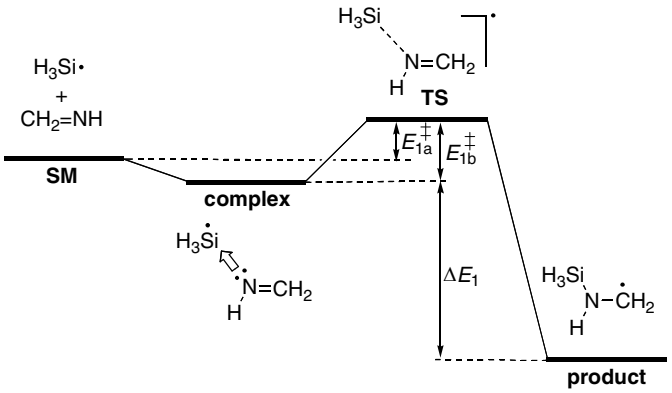
Table S1: Calculated electronic energies (in Hartrees), activation energies, $E^{\ddagger}_{1a,b}{}^{\ddagger}$, and reaction energies, ΔE_1 (in kJ mol^{-1}), and imaginary frequencies, ν_i (in cm^{-1}), for the addition of $H_3Si^{\bullet}$ to the nitrogen end in methane imine.[a,b]

Theory	imine	silyl radical	complex	TS	ν_i	product	$E_{1a}^{\ddagger}$	$E_{1b}^{\ddagger}$	ΔE
UHF/6-31G*	-94.0284617	-290.60612	-384.6369831	-384.6258819	440i	-384.686037	22.8	29.1	-128.8
	-93.985159	*-290.583251*	*-384.569310*	*-384.557724*		*-384.616099*	*28.1*	*30.4*	*-122.8*
UHF/6-311G**	-94.0567137	-290.6320187	-384.6912724	-384.6792275	440i	-384.7414195	25.0	31.6	-131.7
	-94.013872	*-290.609460*	*-384.624382*	*-384.611900*		*-384.672307*	*30.0*	*32.8*	*-125.8*
MP2/6-311G**	-94.3757595	-290.7279969	-385.1089348	-385.0952032	773i	-385.1543883	22.4	36.1	-119.3
	-94.335399	*-290.70576*	*-385.043926*	*-385.028274*		*-385.087227*	*33.8*	*41.1*	*-113.7*
B3LYP/6-311G**	-94.6581899	-291.2327714	-385.9238269	-385.9237791	73i	-385.970981	-86.2	0.1	-123.8
	-94.618384	*-291.210852*	*-385.860559*	*-385.860240*		*-385.906088*	*-81.4*	*1.0*	*-119.5*
BHandHLYP/6-311G**	-94.5934721	-291.232771	-385.8307847	-385.8286304	228i	-385.8847926	-6.3	5.7	-141.8
	-94.552091	*-291.210852*	*-385.765297*	*-385.762246*		*-385.817639*	*1.8*	*8.0*	*-137.4*
BHandHLYP/cc-pVDZ	-94.5716958	-291.2227096	-385.7998037	-385.7974866	232i	-385.8477023	-8.1	6.1	-125.8
	-94.530477	*-291.201087*	*-385.734744*	*-385.731576*		*-385.781024*	*0.0*	*8.3*	*-121.5*
BHandHLYP/aug-cc-pVDZ	-94.5821729	-291.2236789	-385.8083047	-385.8058131	216i	-385.858728	0.1	6.5	-132.4
	-94.540878	*-291.202086*	*-385.743606*	*-385.739980*		*-385.792250*	*7.8*	*9.5*	*127.7*
BHandHLYP/cc-pVTZ	-94.6048759	-291.2386301	-385.8466912	-385.8446819	191i	-385.9031517	-3.1	5.3	-148.2
	-94.563524	*-291.216813*	*-385.781612*	*-385.778416*		*-385.836351*	*5.0*	*8.4*	*-143.7*
BHandHLYP/aug-cc-pVTZ	-94.607148	-291.2388835	-385.8482459	-385.8462761	188i	-385.9057902	-0.6	5.2	-151.1
	-94.565822	*-291.217081*	*-385.783333*	*-385.780096*		*-385.839084*	*7.4*	*8.5*	*-146.4*
QCISD/cc-pVDZ	-94.3651185	-290.7462122	-385.1166348	-385.1100857	377i	-385.1529968	3.3	17.2	-95.5
	-94.325049	*-290.724847*	*-385.053094*	*-385.045444*		*-385.087197*	*11.6*	*20.1*	*-89.5*
CCSD(T)/cc-pVDZ[c]	-94.3721475	-290.7480237	-385.1260286	-385.1220462		-385.1603954	-4.9	10.5	-100.7
G3MP2	-94.4801737	-290.7862796	-385.2691166	-385.266567		-385.3170453	-0.3	6.7	-132.5

[a] For labelling see Scheme S1. [b] Data in italics include zero-point vibrational energy correction (ZPC). [c] Single-point energy calculation on BHandHLYP/aug-cc-pVTZ optimised geometry.



Scheme S1. Calculated potential energy surface for the attack of $H_3Si^{\bullet}$ at nitrogen in methane imine.

Gaussian archive entries for the reaction of $H_3Si^{\bullet}$ with imine

1) Imine

UHF/6-31G*

1\1\GINC-AC27\FOpt\UHF\6-31G(d)\C1H3N1\UXW563\29-Oct-2007\0\\# UHF/6-31G* scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,1\C,-0.5822623392,0.0281805125,0.0000135667\N,0.6561671949,-0.1440508214,-0.0000323952\H,-1.0699693052,0.9957560013,0.0000499688\H,-1.2344886662,-0.8314262917,0.000027921\H,1.1494421159,0.7323745994,-0.0000460613\\Version=IA64L-G03RevD.01\HF=-94.0284617\S2=0.\S2-1=0.\S2A=0.\RMSD=1.653e-09\RMSF=1.996e-04\Thermal=0.\Dipole=-0.5461577,0.6939526,0.0000265\PG=C01 [X(C1H3N1)]\\@

UHF/6-311G**

1\1\GINC-AC30\FOpt\UHF\6-311G(d,p)\C1H3N1\UXW563\29-Oct-2007\0\\# UHF/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,1\C,-0.5806780597,0.0274858641,0.0000136909\N,0.6554011755,-0.1444349977,-0.0000322048\H,-1.0662523321,0.9983180685,0.0000499077\H,-1.2347702442,-0.8336444338,0.0000275865\H,1.1451884605,0.733109499,-0.0000459804\\Version=IA64L-G03RevD.01\HF=-94.0567137\S2=0.\S2-1=0.\S2A=0.\RMSD=7.596e-09\RMSF=2.064e-04\Thermal=0.\Dipole=-0.5387026,0.668961,0.0000259\PG=C01 [X(C1H3N1)]\\@

MP2/6-311G**

1\1\GINC-AC30\FOpt\RMP2-FC\6-311G(d,p)\C1H3N1\UXW563\29-Oct-2007\0\\# MP2/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,1\C,-0.586929703,0.0294014506,0.0000159661\N,0.6779161749,-0.1635379875,-0.0000374688\H,-1.0749712722,1.0098175405,0.0000455887\H,-1.2441161292,-0.8404787069,0.0000312179\H,1.14698993,0.7456317041,-0.000042304\\Version=IA64L-G03RevD.01\HF=-94.0548056\MP2=-94.3757595\RMSD=6.799e-09\RMSF=3.590e-05\Thermal=0.\Dipole=-0.4690004,0.6313574,0.0000273\PG=C01 [X(C1H3N1)]\\@

B3LYP/6-311G**

1\1\GINC-AC30\FOpt\RB3LYP\6-311G(d,p)\C1H3N1\UXW563\29-Oct-2007\0\\# B3LYP/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,1\C,-0.5847572669,0.0292354987,0.0000159285\N,0.6676482817,-0.1548214298,-0.0000373701\H,-1.0827509093,1.0069334893,0.0000468421\H,-1.2438854046,-0.8416269132,0.0000309831\H,1.1626342993,0.7411133553,-0.0000433837\\Version=IA64L-G03RevD.01\HF=-94.6581899\RMSD=6.358e-09\RMSF=8.748e-05\Thermal=0.\Dipole=-0.4555873,0.6202128,0.0000271\PG=C01 [X(C1H3N1)]\\@

BHandHLYP/6-311G**

1\1\GINC-AC29\FOpt\RBHandHLYP\6-311G(d,p)\C1H3N1\UXW563\29-Oct-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,1\C,-0.5823898425,0.0286751912,0.0000141006\N,0.6590259329,-0.1489658365,-0.0000340241\H,-1.0718528634,1.0001155669,0.0000487737\H,-1.2365590176,-0.834965137,0.0000290764\H,1.1506647906,0.7359742154,-0.0000449266\\Version=IA64L-G03RevD.01\HF=-

94.5934721\RMSD=2.638e-09\RMSF=7.125e-05\Thermal=0.\Dipole=-0.4895803,0.6439376,0.0000259\PG=C01 [X(C1H3N1)]\\@

BHandHLYP/cc-pVDZ
1\1\GINC-AC29\FOpt\RBHandHLYP\CC-pVDZ\C1H3N1\UXW563\29-Oct-2007\0\\# BHandHLYP/cc-pVDZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,1\C,-0.580897,0.028623,-0.000029\N,0.664266,-0.153992,0.000022\H,-1.075897,1.007351,0.000094\H,-1.242262,-0.841549,0.000007\H,1.153679,0.740401,-0.000081\\Version=IA64L-G03RevD.01\HF=-94.5716958\RMSD=7.509e-09\RMSF=7.771e-05\Thermal=0.\Dipole=-0.4422798,0.6045619,-0.000026\Polar=24.9674846,0.6784828,16.700703,0.000121,-0.0000205,9.0389764\PG=C01 [X(C1H3N1)]\\@

BHandHLYP/aug-cc-pVDZ
1\1\GINC-AC28\FOpt\RBHandHLYP\Aug-CC-pVDZ\C1H3N1\UXW563\29-Oct-2007\0\\# BHandHLYP/aug-cc-pVDZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,1\C,-0.5861376108,0.0269580425,0.0000151315\N,0.6617741209,-0.1480427,-0.0000348486\H,-1.0713728824,1.0063011798,0.0000483448\H,-1.2412137782,-0.842880988,0.0000289944\H,1.1558391505,0.7384984658,-0.0000446221\\Version=IA64L-G03RevD.01\HF=-94.5821729\RMSD=7.092e-09\RMSF=2.256e-05\Thermal=0.\Dipole=-0.5363125,0.6322317,0.0000282\PG=C01 [X(C1H3N1)]\\@

BHandHLYP/cc-pVTZ
1\1\GINC-AC29\FOpt\RBHandHLYP\CC-pVTZ\C1H3N1\UXW563\29-Oct-2007\0\\# BHandHLYP/cc-pVTZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,1\C,-0.5831194951,0.0278907456,0.0000136609\N,0.6561452399,-0.1457531933,-0.0000331876\H,-1.0688188085,0.9978022011,0.0000493431\H,-1.2357018062,-0.8339649042,0.0000285782\H,1.1503838699,0.7348591508,-0.0000453947\\Version=IA64L-G03RevD.01\HF=-94.6048759\RMSD=2.612e-09\RMSF=1.138e-04\Thermal=0.\Dipole=-0.4979941,0.6229204,0.0000253\PG=C01 [X(C1H3N1)]\\@

BHandHLYP/aug-cc-pVTZ
1\1\GINC-AC20\FOpt\RBHandHLYP\Aug-CC-pVTZ\C1H3N1\UXW563\29-Oct-2007\0\\# BHandHLYP/aug-cc-pVTZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,1\C,-0.5847597711,0.0273850287,0.0000136694\N,0.6553171607,-0.1439902656,-0.0000330238\H,-1.0683809577,0.9979378376,0.0000495687\H,-1.2357553296,-0.8349656396,0.0000283684\H,1.1524678979,0.734467039,-0.0000455827\\Version=IA64L-G03RevD.01\HF=-94.607148\RMSD=8.437e-09\RMSF=1.191e-04\Thermal=0.\Dipole=-0.5301405,0.627802,0.0000266\PG=C01 [X(C1H3N1)]\\@

QCISD/cc-pVDZ
1\1\GINC-AC28\FOpt\RQCISD-FC\CC-pVDZ\C1H3N1\UXW563\29-Oct-2007\0\\# QCISD/cc-pVDZ scf=direct nosymm opt=(grad,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,1\C,-0.5855954487,0.0275449526,0.0002060573\N,0.683116454,-0.1658810696,-0.0000165234\H,-1.0818870804,1.0172839665,0.0000244443\H,-1.2543565042,-0.8492751041,-0.000089547\H,1.1576115793,0.7511612545,-0.0001114312\\Version=IA64L-G03RevD.01\HF=-94.0374598\MP2=-94.3412171\MP3=-94.3587395\MP4D=-94.367335\MP4DQ=-94.3610717\MP4SDQ=-94.3638557\QCISD=-94.3651185\RMSD=2.624e-09\RMSF=5.083e-05\Thermal=0.\Dipole=-0.436597,0.5953791,-0.0000689\PG=C01 [X(C1H3N1)]\\@

CCSD(T)/cc-pVDZ//BHandHLYP/aug-cc-pVTZ
1\1\GINC-AC28\SP\RCCSD(T)-FC\CC-pVDZ\C1H3N1\UXW563\30-Nov-2007\0\\# CCSD(T)/cc-pVDZ scf=direct nosymm\\freq&geom\\0,1\C,0,-0.58476,0.027385,0.000014\N,0,0.655317,-0.14399,-0.000033\H,0,-1.068381,0.997938,0.00005\H,0,-1.235755,-0.834966,0.000028\H,0,1.152468,0.734467,-0.000046\\Version=IA64L-G03RevD.01\HF=-94.0394804\MP2=-94.3385866\MP3=-94.3567508\MP4D=-94.3648323\MP4DQ=-94.3588772\MP4SDQ=-94.361371\CCSD=-94.3620001\CCSD(T)=-94.3721475\RMSD=8.647e-09\Thermal=0.\PG=C01 [X(C1H3N1)]\\@

G3MP2
1\1\GINC-AC20\Mixed\G3MP2\G3MP2\C1H3N1\UXW563\29-Oct-2007\0\\# G3MP2 scf=direct nosymm opt=(grad,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,1\C,0,0.0006037721,-0.0000000007,-0.0054040192\N,0,-0.0040000568,0.0000000015,1.2752313372\H,0,0.8941031641,0.0000000007,-0.6378838067\H,0,-0.9557496449,-0.0000000004,-0.5266192755\H,0,0.9608814916,-0.000000001,1.6254880768\\Version=IA64L-G03RevD.01\MP2/6-31G(d)=-94.3152043\QCISD(T)/6-31G(d)=-94.3468235\MP2/GTMP2Large=-94.4315204\G3MP2=-94.4801737.

2) $H_3Si•$

UHF/6-31G*

1\1\GINC-AC30\FOpt\UHF\6-31G(d)\H3Si1(2)\UXW563\29-Oct-2007\0\\# UHF/6
-31G* scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\Si,-
0.0006838964,0.0012955252,-0.0003426521\H,0.0019903975,-0.0037531377,1.4752552369\H,1.3769581799,-
0.0036951808,-0.5290804583\H,-0.7713936801,-1.1406032063,-0.5290771268\\Version=IA64L-G03RevD.01\HF=-
290.60612\S2=0.753919\S2-1=0.\S2A=0.750007\RMSD=6.178e-09\RMSF=6.062e-05\Thermal=0.\Dipole=-
0.0374418,0.0707514,-0.0256649\PG=C01[X(H3Si1)]\\@

UHF/6-311G**

1\1\GINC-AC30\FOpt\UHF\6-311G(d,p)\H3Si1(2)\UXW563\29-Oct-2007\0\\# UHF/6-311G** scf=direct nosymm
opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\Si,0.0009773656,-
0.0018436293,0.0007960212\H,0.0010080832,-0.0018972393,1.4777338158\H,1.3789153486,-0.0018382168,-
0.530888974\H,-0.7740297989,-1.1411769152,-0.5308858626\\Version=IA64L-G03RevD.01\HF=-
290.6320187\S2=0.754271\S2-1=0.\S2A=0.750008\RMSD=4.019e-09\RMSF=4.139e-05\Thermal=0.\Dipole=-
0.0627336,0.118544,-0.0430179\PG=C01 [X(H3Si1)]\\@

MP2/6-311G**

1\1\GINC-AC30\FOpt\UMP2-FC\6-311G(d,p)\H3Si1(2)\UXW563\29-Oct-2007\0\\# MP2/6-311G** scf=direct
nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\Si,0.0020669708,-
0.0039026224,0.001545143\H,0.0009184111,-0.0017275958,1.475660571\H,1.3769524526,-0.0016677032,-
0.5302269332\H,-0.7730668374,-1.1394580799,-0.53022378\\Version=IA64L-G03RevD.01\HF=-
290.6320084\MP2=-290.7279969\PUHF=-290.6329693\PMP2-0=-290.7285525\S2=0.754308\S2-
1=0.75067\S2A=0.750008\RMSD=5.239e-09\RMSF=6.550e-05\Thermal=0.\Dipole=-0.0504585,0.0953484,-
0.034596\PG=C01 [X(H3Si1)]\\@

B3LYP/6-311G**

1\1\GINC-AC30\FOpt\UBHandHLYP\6-311G(d,p)\H3Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/6-311G**
scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\Si,0.0020277741,-
0.0038262091,0.0015202323\H,0.0006846933,-0.0012802459,1.4773276234\H,1.3784306798,-0.0012183934,-
0.5310458306\H,-0.7742721501,-1.1404311529,-0.5310470242\\Version=IA64L-G03RevD.01\HF=-
291.2327714\S2=0.751629\S2-1=0.\S2A=0.750001\RMSD=3.363e-09\RMSF=4.710e-05\Thermal=0.\Dipole=-
0.040671,0.0768582,-0.027879\PG=C01 [X(H3Si1)]\\@

BHandHLYP/6-311G**

1\1\GINC-AC3\FOpt\UBHandHLYP\6-311G(d,p)\H3Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/6-311G**
scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\Si,0.0020277741,-
0.0038262091,0.0015202323\H,0.0006846933,-0.0012802459,1.4773276234\H,1.3784306798,-0.0012183934,-
0.5310458306\H,-0.7742721501,-1.1404311529,-0.5310470242\\Version=IA64L-G03RevD.01\HF=-
291.2327714\S2=0.751629\S2-1=0.\S2A=0.750001\RMSD=3.363e-09\RMSF=4.710e-05\Thermal=0.\Dipole=-
0.040671,0.0768582,-0.027879\PG=C01 [X(H3Si1)]\\@

BHandHLYP/cc-pVDZ

1\1\GINC-AC28\FOpt\UBHandHLYP\CC-pVDZ\H3Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/cc-pVDZ
scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500)
freq=noraman\\freq&geom\\0,2\Si,0.,0.,0.\H,0.,0.,1.487036\H,1.386919,0.,-0.535133\H,-0.780048,-1.146756,-
0.535148\\Version=IA64L-G03RevD.01\HF=-291.2227096\S2=0.751819\S2-1=0.\S2A=0.750001\RMSD=4.970e-
09\RMSF=6.086e-05\Thermal=0.\Dipole=-0.0179718,0.0339472,-
0.0125783\Polar=26.4716461,3.2434221,22.0590584,-1.1770034,2.2249373,27.3905896\PG=C01 [X(H3Si1)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-AC29\FOpt\UBHandHLYP\Aug-CC-pVDZ\H3Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/aug-cc-
pVDZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\Si,0.0002746817,-
0.0005155482,0.0003193484\H,0.0000592453,-0.0001018877,1.4857757279\H,1.3860653443,-0.0000527802,-
0.5346711773\H,-0.7795282719,-1.1460857842,-0.5346688989\\Version=IA64L-G03RevD.01\HF=-
291.2236789\S2=0.752085\S2-1=0.\S2A=0.750001\RMSD=3.245e-09\RMSF=9.501e-07\Thermal=0.\Dipole=-
0.0091516,0.0172965,-0.006258\PG=C01 [X(H3Si1)]\\@

BHandHLYP/cc-pVTZ

1\1\GINC-AC29\FOpt\UBHandHLYP\CC-pVTZ\H3Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/cc-pVTZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\Si,0.000579149,-0.0010926058,0.0005193687\H,0.0014094893,-0.0026344491,1.4760978904\H,1.3775566132,-0.0025605 419,-0.5299242649\H,-0.7726742525,-1.1404684036,-0.5299379941\\Version=IA64L-G03RevD.01\HF=-291.2386301\S2=0.752244\S2-1=0.\S2A=0.750002\RMSD=6.863e-09\RMSF=5.384e-05\Thermal=0.\Dipole=-0.0108329,0.0204743,-0.0074258\PG=C01 [X(H3Si1)]\\@

BHandHLYP/aug-cc-pVTZ
1\1\GINC-AC29\FOpt\UBHandHLYP\Aug-CC-pVTZ\H3Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/aug-cc-pVTZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\Si,0.0007889352,-0.0014889569,0.0006633885\H,0.0013165598,-0.0024592256,1.4762022178\H,1.3776204269,-0.0023853318,-0.5300485745\H,-0.7728549231,-1.1404224862,-0.5300620315\\Version=IA64L-G03RevD.01\HF=-291.2388835\S2=0.752324\S2-1=0.\S2A=0.750002\RMSD=2.237e-09\RMSF=5.355e-05\Thermal=0.\Dipole=-0.006562,0.0124065,-0.004496\PG=C01 [X(H3Si1)]\\@

QCISD/cc-pVDZ
1\1\GINC-AC29\FOpt\UQCISD-FC\CC-pVDZ\H3Si1(2)\UXW563\29-Oct-2007\0\\# QCISD/cc-pVDZ scf=direct nosymm opt=(grad,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\Si,0.0001608745,0.000227393,-0.0000605775\H,-0.0011039429,0.0011655244,1.4920211097\H,1.3919700733,0.001672539,-0.5378961148\H,-0.784156005,-1.1498214564,-0.5373094174\\Version=IA64L-G03RevD.01\HF=-290.6250259\MP2=-290.7194346\MP3=-290.7404739\MP4D=-290.7461385\MP4DQ=-290.7444664\PUHF=-290.6259903\PMP2-0=-290.7199771\PMP3-0=-290.7407781\MP4SDQ=-290.744919\QCISD=-290.7462122\S2=0.75431\S2-1=0.750535\S2A=0.750007\RMSD=5.403e-09\RMSF=1.012e-04\Thermal=0.\Dipole=-0.0217159,0.0418672,-0.0153615\PG=C01 [X(H3Si1)]\\@

CCSD(T)/cc-pVDZ//BHandHLYP/aug-cc-pVTZ
1\1\GINC-AC25\SP\UCCSD(T)-FC\CC-pVDZ\H3Si1(2)\UXW563\30-Nov-2007\0\\# CCSD(T)/cc-pVDZ scf=direct nosymm\\freq&geom\\0,2\Si,0,0.000789,-0.001489,0.000663\H,0,0.001317,-0.002459,1.476202\H,0,1.37762,-0.002385,-0.530049\H,0,-0.772855,-1.140422,-0.530062\\Version=IA64L-G03RevD.01\HF=-290.6249366\MP2=-290.7193021\MP3=-290.7402897\MP4D=-290.7459066\MP4DQ=-290.7442497\PUHF=-290.6259052\PMP2-0=-290.7198478\PMP3-0=-290.7405959\MP4SDQ=-290.7446916\CCSD=-290.7458694\CCSD(T)=-290.7480237\S2=0.754333\S2-1=0.750546\S2A=0.750007\RMSD=4.962e-09\Thermal=0.\PG=C01 [X(H3Si1)]\\@

G3MP2
1\1\GINC-AC20\Mixed\G3MP2\G3MP2\H3Si1(2)\UXW563\29-Oct-2007\0\\# G3MP2 scf=direct nosymm opt=(grad,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\Si,0,0.0005556286,-0.0010458821,0.0003559763\H,0,-0.0013447524,0.0025135563,1.4830734683\H,0,1.3835720987,0.0025283079,-0.5341718156\H,0,-0.7781856288,-1.1439763988,-0.5341897733\\Version=IA64L-G03RevD.01\MP2/6-31G(d)=-290.6745256\QCISD(T)/6-31G(d)=-290.6985724\MP2/GTMP2Large=-290.7503368\G3MP2=-290.7862796.

3) Complex
UHF/6-31G*
1\1\GINC-AC20\FOpt\UHF\6-31G(d)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# UHF/6-31G* scf=direct geom=checkpoint guess=check nosymm opt=(readfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,2.2983742872,0.3860665671,0.036723941\N,1.4726187849,-0.5429472915,-0.1000078277\Si,-1.8514688223,0.0547677391,-0.0670550914\H,3.3727809453,0.2512949131,0.0725804781\H,1.9408814016,1.4000351808,0.1275374656\H,1.9244953777,-1.4385456747,-0.1732309817\H,-1.1408518126,1.2881713163,0.3235021351\H,-1.6415421525,-1.0253257849,0.914965231\H,-3.3008860093,0.3422380348,-0.1842523504\\Version=IA64L-G03RevD.01\HF=-384.6369831\S2=0.753904\S2-1=0.\S2A=0.750008\RMSD=5.566e-09\RMSF=1.322e-05\Thermal=0.\Dipole=1.1778451,-0.0061534,-0.0430283\PG=C01 [X(C1H6N1Si1)]\\@

UHF/6-311G**
1\1\GINC-AC28\FOpt\UHF\6-311G(d,p)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# UHF/6-311G** scf=direct geom=checkpoint guess=check nosymm opt=(readfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,2.3255870076,0.383336581,0.0427079569\N,1.4847049035,-0.5258186008,-0.1130664133\Si,-1.8824668524,0.0512242089,-0.0616802866\H,3.3983488876,0.2237316793,0.0823328888\H,1.987468882,1.4049631965,0.147745844\H,1.9234252946,-1.4263086613,-0.196858286\H,-1.1797611871,1.3003386857,0.2947517198\H,-1.6462837692,-1.0105747131,0.9358309507\H,-3.3366211664,0.3148626242,-0.1810013746\\Version=IA64L-G03RevD.01\HF=-384.6912724\S2=0.754144\S2-1=0.\S2A=0.750008\RMSD=6.182e-09\RMSF=4.637e-07\Thermal=0.\Dipole=1.1724311,-0.0276838,-0.0861109\PG=C01 [X(C1H6N1Si1)]\\@

MP2/6-311G**
1\1\GINC-AC30\FOpt\UMP2-FC\6-311G(d,p)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# MP2/6-311G** scf=direct geom=checkpoint guess=check nosymm opt=(readfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,2.1304149712,0.4007105021,0.0336590568\N,1.311123859,-0.5780625654,-0.0508533391\Si,-1.6328635937,0.0359706634,-0.0599076169\H,3.219823591,0.306490529,-0.0024721777\H,1.7241822494,1.4052802228,0.1506068668\H,1.8297662738,-1.4526801866,-0.1577430843\H,-0.9047467978,1.246691286,0.3665697122\H,-1.5459900391,-1.0391190571,0.9439580305\H,-3.0573085137,0.3904736052,-0.273054448\\Version=IA64L-G03RevD.01\HF=-384.6885427\MP2=-385.1089348\PUHF=-384.6894729\PMP2-0=-385.1094655\S2=0.754087\S2-1=0.750572\S2A=0.750008\RMSD=7.819e-09\RMSF=2.953e-06\Thermal=0.\Dipole=1.2483014,-0.0551246,-0.1256582\PG=C01 [X(C1H6N1Si1)]\\@

B3LYP/6-311G**
1\1\GINC-AC27\FOpt\UB3LYP\6-311G(d,p)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# B3LYP/6-311G** scf=direct geom=checkpoint guess=check nosymm opt=(readfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,2.1423583659,0.4117268727,0.0197883134\N,1.2338672419,-0.4695000856,0.0478402562\Si,-1.5069108173,0.0182320183,-0.0317674034\H,3.1988387934,0.2096960043,-0.1843349016\H,1.8696236841,1.4510080912,0.2081134486\H,1.5932523227,-1.405989589,-0.1483115584\H,-1.0139164358,1.3041069147,0.5323244241\H,-1.5282248116,-1.0407150986,1.0111830101\H,-2.9144863434,0.2371898729,-0.5040725893\\Version=IA64L-G03RevD.01\HF=-385.9238269\S2=0.751709\S2-1=0.\S2A=0.750002\RMSD=5.961e-09\RMSF=6.265e-06\Thermal=0.\Dipole=1.4492526,-0.1097359,-0.195492\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/6-311G**
1\1\GINC-AC28\FOpt\UBHandHLYP\6-311G(d,p)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/6-311G** scf=direct geom=checkpoint guess=check nosymm opt=(readfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,2.1325243441,0.3982143034,0.0383380959\N,1.289669602,-0.5249419326,-0.0568057846\Si,-1.5906170062,0.0263404064,-0.0525822141\H,3.2086247665,0.2560235648,-0.0132125815\H,1.7828332012,1.4131211731,0.1821320866\H,1.7260141586,-1.4278269058,-0.1898370689\H,-0.9456487301,1.2809206365,0.3865594412\H,-1.505697173,-1.0153257422,0.9886124552\H,-3.0233011632,0.3092294963,-0.3324414293\\Version=IA64L-G03RevD.01\HF=-385.8307847\S2=0.751706\S2-1=0.\S2A=0.750001\RMSD=5.460e-09\RMSF=3.402e-05\Thermal=0.\Dipole=1.3469635,-0.0681324,-0.1187596\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/cc-pVDZ
1\1\GINC-AC27\FOpt\UBHandHLYP\CC-pVDZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/cc-pVDZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,2.1494610687,0.3974198457,0.0371932488\N,1.2916651802,-0.5189131244,-0.0488177834\Si,-1.6024817293,0.0268141941,-0.0540652077\H,3.2319016056,0.2446864737,-0.0286632262\H,1.8087071917,1.4238978833,0.1880216384\H,1.7271890387,-1.4283387107,-0.1904778598\H,-0.9696279778,1.294451875,0.4001212361\H,-1.5160822953,-1.0221892038,0.99481766\H,-3.0463300825,0.2979257669,-0.3473667059\\Version=IA64L-G03RevD.01\HF=-385.7998037\S2=0.751856\S2-1=0.\S2A=0.750001\RMSD=7.615e-09\RMSF=6.551e-06\Thermal=0.\Dipole=1.291557,-0.0696976,-0.0801852\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/aug-cc-pVDZ
1\1\GINC-AC30\FOpt\UBHandHLYP\Aug-CC-pVDZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/aug-cc-pVDZ scf=direct geom=checkpoint guess=check nosymm opt=(readfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,2.1611075171,0.3927712776,0.0400704833\N,1.3697579319,-0.5825142546,-0.0589421383\Si,-1.6800700038,0.0360656905,-0.0561696866\H,3.2487735707,0.3088874859,-0.0112248617\H,1.7506590483,1.3905069619,0.186451181\H,1.8672408032,-1.4563518318,-0.1933098156\H,-0.9457850647,1.2635136133,0.3457933895\H,-1.5821362726,-1.0173064345,0.9842178726\H,-3.1151455303,0.3801824915,-0.2861234239\\Version=IA64L-G03RevD.01\HF=-385.8083047\S2=0.752091\S2-1=0.\S2A=0.750002\RMSD=7.864e-09\RMSF=9.577e-07\Thermal=0.\Dipole=1.1696026,0.0313402,-0.0506433\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/cc-pVTZ
1\1\GINC-AC27\FOpt\UBHandHLYP\CC-pVTZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/cc-pVTZ scf=direct geom=checkpoint guess=check nosymm opt=(readfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,2.1642438833,0.3928905489,0.0440020412\N,1.3450535794,-0.5472872355,-0.0585320664\Si,-1.6589042488,0.0313747982,-0.0566855423\H,3.2405971049,0.274613762,-0.0109339366\H,1.7938491826,1.3967671354,0.1976698554\H,1.8012047986,-1.4364909449,-0.2008495601\H,-

0.9719286852,1.2751922455,0.3442374252\H,-1.5466663399,-1.0041406438,0.9868306604\H,-3.0930472749,0.332835334,-0.2949758769\\Version=IA64L-G03RevD.01\HF=-385.8466912\S2=0.752227\S2-1=0.\S2A=0.750002\RMSD=5.177e-09\RMSF=1.398e-05\Thermal=0.\Dipole=1.2153907,-0.0125943,-0.0557192\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/aug-cc-pVTZ

1\1\GINC-AC27\FOpt\UBHandHLYP\Aug-CC-pVTZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/aug-cc-pVTZ scf=direct geom=checkpoint guess=check nosymm opt=(readfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,2.1649770773,0.3904050705,0.0422558013\N,1.3744615652,-0.5748186232,-0.0585882254\Si,-1.682907068,0.0380305495,-0.0564697156\H,3.2442554254,0.3029412856,-0.0093171594\H,1.7646579207,1.383340985,0.1906386184\H,1.8572531041,-1.4504853402,-0.1955315475\H,-0.9627368039,1.2649983578,0.3376349514\H,-1.5729982519,-1.0062210775,0.9781874213\H,-3.112560969,0.3675637922,-0.2780471442\\Version=IA64L-G03RevD.01\HF=-385.8482459\S2=0.752314\S2-1=0.\S2A=0.750002\RMSD=5.513e-09\RMSF=5.599e-06\Thermal=0.\Dipole=1.1621098,0.0281858,-0.0442449\PG=C01 [X(C1H6N1Si1)]\\@

QCISD/cc-pVDZ

1\1\GINC-AC23\FOpt\UQCISD-FC\CC-pVDZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# QCISD/cc-pVDZ scf=direct nosymm opt=(grad,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.0086342005,-0.0015670974,-0.0125116367\N,0.0351784527,0.0261116379,1.2691285376\Si,2.7581962178,0.0056229621,2.7162173216\H,-0.9367940232,0.0201541384,-0.6136412239\H,0.9400619873,-0.0506098602,-0.5713876654\H,-0.9220617612,0.0717369839,1.6497842586\H,3.0118519635,-0.2567326032,1.2691841656\H,2.0315632782,-1.126760791,3.3578972518\H,4.072180573,0.2083327972,3.410988865\\Version=IA64L-G03RevD.01\HF=-384.6653531\MP2=-385.0667971\MP3=-385.104506\MP4D=-385.1187453\MP4DQ=-385.1106901\PUHF=-384.6662865\PMP2-0=-385.0673229\PMP3-0=-385.1048046\MP4SDQ=-385.114125\QCISD=-385.1166348\S2=0.754158\S2-1=0.750523\S2A=0.750008\RMSD=1.519e-09\RMSF=4.037e-05\Thermal=0.\Dipole=-0.9492165,0.070338,-0.7026547\PG=C01 [X(C1H6N1Si1)]\\@

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

1\1\GINC-AC27\SP\UCCSD(T)-FC\CC-pVDZ\C1H6N1Si1(2)\UXW563\30-Nov-2007\0\\# CCSD(T)/cc-pVDZ scf=direct nosymm\\freq&geom\\0,2\C,0,2.164977,0.390405,0.042256\N,0,1.374462,-0.574819,-0.058588\Si,0,-1.682907,0.038031,-0.05647\H,0,3.244255,0.302941,-0.009317\H,0,1.764658,1.383341,0.190639\H,0,1.857253,-1.450485,-0.195532\H,0,-0.962737,1.264998,0.337635\H,0,-1.572998,-1.006221,0.978187\H,0,-3.112561,0.367564,-0.278047\\Version=IA64L-G03RevD.01\HF=-384.6672799\MP2=-385.0641424\MP3=-385.1024967\MP4D=-385.1161914\MP4DQ=-385.1084439\PUHF=-384.6682197\PMP2-0=-385.0646688\PMP3-0=-385.1027941\MP4SDQ=-385.1115743\CCSD=-385.1132867\CCSD(T)=-385.1260286\S2=0.754154\S2-1=0.750496\S2A=0.750007\RMSD=5.735e-09\Thermal=0.\PG=C01 [X(C1H6N1Si1)]\\@

G3MP2

1\1\GINC-AC15\Mixed\G3MP2\G3MP2\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# G3MP2/6-311G** scf=direct geom=checkpoint guess=check nosymm opt=(readfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,0,2.1370429313,0.4019736159,0.031543095\N,0,1.3044841814,-0.5683899192,-0.0387518758\Si,0,-1.618231566,0.0371603657,-0.0596345882\H,0,3.2246873587,0.3012653768,-0.0194953676\H,0,1.7444790925,1.4101482282,0.1511532991\H,0,1.7953674466,-1.4618182939,-0.1519212495\H,0,-0.920156404,1.2682468522,0.3879984519\H,0,-1.5398418133,-1.0428629756,0.952449381\H,0,-3.0534292276,0.3700317489,-0.3025781444\\Version=IA64L-G03RevD.01\MP2/6-31G(d)=-384.9943921\QCISD(T)/6-31G(d)=-385.0496276\MP2/GTMP2Large=-385.1863244\G3MP2=-385.2691166

4) Transition state

UHF/6-31G*

1\1\GINC-AC12\FTS\UHF\6-31G(d)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# UHF/6-31G* scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.8968937532,0.3398486439,-0.0477484409\N,0.9000613597,-0.4551052673,0.1892640702\Si,-1.249440473,0.0510149891,-0.0081516879\H,2.7649573233,0.0404989097,-0.6117875029\H,1.8362644559,1.3575866444,0.2932556323\H,1.0486502864,-1.3792049277,-0.1772846673\H,-1.0210408793,1.3056087953,0.7398295502\H,-1.6166819447,-1.0545645354,0.8994234842\H,-2.4487638815,0.3067107479,-0.8699514381\\Version=IA64L-G03RevD.01\HF=-384.6258819\S2=0.947119\S2-1=0.\S2A=0.753967\RMSD=6.504e-09\RMSF=4.091e-05\Thermal=0.\Dipole=1.4298986,-0.2047578,-0.3694714\PG=C01 [X(C1H6N1Si1)]\\@

UHF/6-311G**

1\1\GINC-AC12\FTS\UHF\6-311G(d,p)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# UHF/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.9034312083,0.3387414166,-0.0493178339\N,0.9097979403,-0.4536783833,0.2000604326\Si,-1.2588282886,0.0502266722,0.0021530186\H,2.7576717503,0.0405662359,-0.636768243\H,1.8574956533,1.3541882423,0.3060213514\H,1.0517168207,-1.3718106167,-0.1818725665\H,-1.0395410983,1.3085796721,0.7484839926\H,-1.6348886169,-1.0523743973,0.911323481\H,-2.435955369,0.297955158,-0.893234633\\Version=IA64L-G03RevD.01\HF=-384.6792275\S2=0.943968\S2-1=0.\S2A=0.754021\RMSD=7.373e-09\RMSF=2.913e-05\Thermal=0.\Dipole=1.3866188,-0.1898091,-0.4059729\PG=C01 [X(C1H6N1Si1)]\\@

MP2/6-311G**

1\1\GINC-AC20\FTS\UMP2-FC\6-311G(d,p)\C1H6N1Si1(2)\UXW563\30-Oct-2007\0\\# MP2/6-311G** opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman nosymm scf=direct\\freq&geom\\0,2\C,1.8230416301,0.3296259741,-0.0258935014\N,0.8392008515,-0.4565819858,0.0361725166\Si,-1.2044391126,0.0301660498,-0.0395386367\H,2.8076763068,0.0333303647,-0.3851198817\H,1.675099998,1.367061932,0.2681767192\H,1.05529058,-1.4043935503,-0.271293502\H,-0.859478449,1.3125638265,0.6230095756\H,-1.5234569637,-1.0258089567,0.9452660858\H,-2.5020348411,0.326430346,-0.7439303754\\Version=IA64L-G03RevD.01\HF=-384.6764331\MP2=-385.0952032\PUHF=-384.6859337\PMP2-0=-385.1032695\S2=0.87661\S2-1=0.837987\S2A=0.752195\RMSD=3.984e-09\RMSF=2.787e-05\Thermal=0.\Dipole=1.7972367,-0.2088011,-0.2589003\PG=C01 [X(C1H6N1Si1)]\\@

B3LYP/6-311G**

1\1\GINC-AC29\FTS\UB3LYP\6-311G(d,p)\C1H6N1Si1(2)\UXW563\30-Oct-2007\0\\# B3LYP/6-311G** opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman nosymm scf=direct\\freq&geom\\0,2\C,2.0032361176,0.308824404,-0.0268943447\N,1.0294214239,-0.5020102796,0.0340720486\Si,-1.4944714488,0.0776440834,-0.0737844739\H,3.0081238248,0.0420898001,-0.3662015498\H,1.8397091317,1.3453537051,0.2687224853\H,1.2778207361,-1.4436361539,-0.2751142647\H,-1.0414780487,1.3322593625,0.5876676062\H,-1.6642107554,-1.0073779207,0.9285078601\H,-2.8472509812,0.3592469987,-0.6701263673\\Version=IA64L-G03RevD.01\HF=-385.9237791\S2=0.752691\S2-1=0.\S2A=0.750005\RMSD=7.521e-09\RMSF=1.378e-05\Thermal=0.\Dipole=1.5145791,-0.1909373,-0.2601566\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/6-311G**

1\1\GINC-AC12\FTS\UBHandHLYP\6-311G(d,p)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.90391,0.323323,-0.029933\N,0.927582,-0.472983,0.074383\Si,-1.322765,0.05453,-0.054114\H,2.870172,0.037822,-0.42656\H,1.769651,1.351684,0.274511\H,1.134385,-1.408442,-0.247765\H,-0.957456,1.312678,0.634291\H,-1.586906,-1.020129,0.924368\H,-2.627673,0.333911,-0.742332\\Version=IA64L-G03RevD.01\HF=-385.8286304\S2=0.763192\S2-1=0.\S2A=0.750054\RMSD=7.924e-09\RMSF=1.204e-05\Thermal=0.\Dipole=1.6489896,-0.2069313,-0.2881558\Polar=88.3658991,4.6935348,46.2942844,5.9680918,-0.120205,33.8831851\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/cc-pVDZ

1\1\GINC-AC27\FTS\UBHandHLYP\CC-pVDZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/cc-pVDZ scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.9120555353,0.3225941602,-0.0292992123\N,0.9284893158,-0.4712602361,0.095965997\Si,-1.3198754742,0.0530997216,-0.049626645\H,2.8702797856,0.0340965569,-0.464346743\H,1.7925260785,1.356451776,0.2930815766\H,1.1277485556,-1.4062109713,-0.2517900932\H,-0.9774733702,1.3235326721,0.6505462169\H,-1.602833207,-1.022059343,0.9394029139\H,-2.6200172195,0.3221496636,-0.7770850107\\Version=IA64L-G03RevD.01\HF=-385.7974866\S2=0.765847\S2-1=0.\S2A=0.750071\RMSD=9.438e-09\RMSF=4.786e-06\Thermal=0.\Dipole=1.5498196,-0.2047229,-0.2488398\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-AC19\FTS\UBHandHLYP\Aug-CC-pVDZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/aug-cc-pVDZ scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.9168041772,0.3219548651,-0.0251702\N,0.9445586895,-0.485715582,0.0941143953\Si,-1.3390493197,0.0503087011,-0.0508746311\H,2.8722315616,0.0504799967,-0.4704128932\H,1.7888940157,1.3458538877,0.3154765614\H,1.1499834732,-1.4104595851,-0.2655247212\H,-0.9666210456,1.3244192016,0.6230244561\H,-1.6158893889,-1.0090515869,0.9537355782\H,-2.6400121629,0.3246041015,-0.7675195451\\Version=IA64L-G03RevD.01\HF=-385.8058131\S2=0.764548\S2-

1=0.\S2A=0.750069\RMSD=6.648e-09\RMSF=6.832e-06\Thermal=0.\Dipole=1.5016802,-0.1455673,-0.2302833\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/cc-pVTZ

1\1\GINC-AC30\FTS\UBHandHLYP\CC-pVTZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/cc-pVTZ scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.9057479784,0.3193572492,-0.020890733\N,0.9389610296,-0.48273621,0.060072904\Si,-1.3393189712,0.0522150225,-0.0691679627\H,2.8793111146,0.0457982279,-0.4023463059\H,1.7592744966,1.3420797641,0.2902417537\H,1.1548122686,-1.411877004,-0.2671495539\H,-0.94061803,1.3154382872,0.5906537199\H,-1.5798320922,-1.0049308111,0.9336996724\H,-2.6674377945,0.3370494741,-0.7082644944\\Version=IA64L-G03RevD.01\HF=-385.8446819\S2=0.760993\S2-1=0.\S2A=0.75005\RMSD=4.290e-09\RMSF=1.814e-05\Thermal=0.\Dipole=1.6168248,-0.1783084,-0.2038718\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/aug-cc-pVTZ

1\1\GINC-AC3\FTS\UBHandHLYP\Aug-CC-pVTZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/aug-cc-pVTZ scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.9092461457,0.3185762368,-0.0195826886\N,0.9455051678,-0.4871163298,0.0605162927\Si,-1.3478622476,0.0521883468,-0.0674639281\H,2.8817149877,0.0502913138,-0.4072687446\H,1.7613871305,1.3388012634,0.2989270979\H,1.1628019673,-1.4136639519,-0.2727522395\H,-0.941963357,1.3171801111,0.58388412\H,-1.5866556392,-0.9999134365,0.9405617724\H,-2.6732741551,0.3360504463,-0.7099726822\\Version=IA64L-G03RevD.01\HF=-385.8462761\S2=0.760754\S2-1=0.\S2A=0.75005\RMSD=8.407e-09\RMSF=3.554e-06\Thermal=0.\Dipole=1.5795968,-0.1529196,-0.1898602\PG=C01 [X(C1H6N1Si1)]\\@

QCISD/cc-pVDZ

1\1\GINC-AC26\FTS\UQCISD-FC\CC-pVDZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# QCISD/cc-pVDZ scf=direct nosymm opt=(ts,noeigentest,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.894075592,0.336508932,-0.032737792\N,0.8830071622,-0.4668816444,0.1326627273\Si,-1.2614592734,0.039994669,-0.0253034141\H,2.832853468,0.0333384859,-0.5200510947\H,1.789416154,1.3799894504,0.2957584779\H,1.0767293129,-1.4085396147,-0.2352112069\H,-0.9729270623,1.3256681645,0.6837417491\H,-1.6172695937,-1.0314759769,0.9526135337\H,-2.5135257598,0.3037915338,-0.8446239794\\Version=IA64L-G03RevD.01\HF=-384.6543518\MP2=-385.0498752\MP3=-385.0894527\MP4D=-385.1028785\MP4DQ=-385.0954102\PUHF=-384.6674367\PMP2-0=-385.061258\PMP3-0=-385.097947\MP4SDQ=-385.1008177\QCISD=-385.1100857\S2=0.946237\S2-1=0.894535\S2A=0.754178\RMSD=7.200e-09\RMSF=1.758e-05\Thermal=0.\Dipole=1.4705184,-0.2222073,-0.270616\PG=C01 [X(C1H6N1Si1)]\\@

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

1\1\GINC-AC27\SP\UCCSD(T)-FC\CC-pVDZ\C1H6N1Si1(2)\UXW563\30-Nov-2007\0\\# CCSD(T)/cc-pVDZ scf=direct nosymm\\freq&geom\\0,2\C,0,1.909246,0.318576,-0.019583\N,0,0.945505,-0.487116,0.060516\Si,0,-1.347862,0.052188,-0.067464\H,0,2.881715,0.050291,-0.407269\H,0,1.761387,1.338801,0.29 8927\H,0,1.162802,-1.413664,-0.272752\H,0,-0.941963,1.31718,0.583884\H,0,-1.586656,-0.999913,0.940562\H,0,-2.673274,0.33605,-0.709973\\Version=IA64L-G03RevD.01\HF=-384.6575678\MP2=-385.0555871\MP3=-385.0939238\MP4D=-385.1073537\MP4DQ=-385.0996945\PUHF=-384.6632752\PMP2-0=-385.0604673\PMP3-0=-385.0974235\MP4SDQ=-385.1039234\CCSD=-385.1084216\CCSD(T)=-385.1220462\S2=0.830392\S2-1=0.806909\S2A=0.751038\RMSD=2.859e-09\Thermal=0.\PG=C01 [X(C1H6N1Si1)]\\@

G3MP2

1\1\GINC-AC10\Mixed\G3MP2\G3MP2\C1H6N1Si1(2)\UXW563\30-Oct-2007\0\\# G3MP2 opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman nosymm scf=direct\\freq&geom\\0,2\C,0,1.8282622931,0.3312615021,-0.0272648691\N,0,0.8373443689,-0.4500859421,0.0323564691\Si,0,-1.197109248,0.0336433061,-0.0429935743\H,0,2.8143250399,0.0297857404,-0.3758005276\H,0,1.6846821488,1.3711979265,0.2542296603\H,0,1.0377697697,-1.4088072421,-0.2621119494\H,0,-0.8696208463,1.319699119,0.6397515377\H,0,-1.5163811697,-1.0419100201,0.9345041345\H,0,-2.5083723565,0.3276096101,-0.7458218815\\Version=IA64L-G03RevD.01\MP2/6-31G(d)=-384.9804325\QCISD(T)/6-31G(d)=-385.0426089\MP2/GTMP2Large=-385.177264\G3MP2=-385.266567.

5) Product

UHF/6-31G*

1\1\GINC-AC12\FOpt\UHF\6-31G(d)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# UHF/6-31G* scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.7194153204,-

0.3085809761,0.0727917445\N,0.5776237872,0.4932743587,-0.0363204866\Si,-1.0543623017,-0.0847321746,0.0081402883\H,2.6697588603,0.1778046347,-0.0525543772\H,1.6301166133,-1.3190871862,-0.2847492519\H,0.7370274128,1.4605538309,0.1481296487\H,-1.1968494379,-1.1979757211,-0.9486729933\H,-1.9230157279,1.0446880605,-0.3712941642\H,-1.4889115264,-0.5792248268,1.332764592\\Version=IA64L-G03RevD.01\HF=-384.686037\S2=0.75973\S2-1=0.\S2A=0.750068\RMSD=3.731e-09\RMSF=3.130e-05\Thermal=0.\Dipole=0.1322613,0.3071578,-0.0088328\PG=C01 [X(C1H6N1Si1)]\\@

UHF/6-311G**
1\1\GINC-AC12\FOpt\UHF\6-311G(d,p)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# UHF/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.7196844799,-0.3003071635,0.0813496577\N,0.573530757,0.4914234982,-0.0383891103\Si,-1.0524824286,-0.0860644098,0.0037447312\H,2.6699040236,0.1816320941,-0.061185607\H,1.6308219707,-1.3331761985,-0.2069147814\H,0.7345512968,1.4656507627,0.0852112093\H,-1.2208138172,-1.1666096122,-0.9901247015\H,-1.9220776941,1.0612132483,-0.3253060008\H,-1.4623155881,-0.6270422193,1.3198496033\\Version=IA64L-G03RevD.01\HF=-384.7414195\S2=0.760684\S2-1=0.\S2A=0.75008\RMSD=8.021e-09\RMSF=1.536e-06\Thermal=0.\Dipole=0.1193106,0.3045364,-0.0466692\PG=C01 [X(C1H6N1Si1)]\\@

MP2/6-311G**
1\1\GINC-AC30\FOpt\UMP2-FC\6-311G(d,p)\C1H6N1Si1(2)\UXW563\30-Oct-2007\0\\# MP2/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.7070192796,-0.3056053235,0.0730648519\N,0.5782369507,0.5063371814,-0.0697484082\Si,-1.0563922745,-0.0882665985,0.0064511069\H,2.6740722425,0.1702962981,-0.0277031319\H,1.6041313269,-1.3316442549,-0.2600934106\H,0.744813092,1.4826418759,0.12461142\H,-1.1941337496,-1.1898975361,-0.9647993788\H,-1.9304538575,1.0452016165,-0.3480884056\H,-1.4564900101,-0.602343259,1.3345403565\\Version=IA64L-G03RevD.01\HF=-384.7409553\MP2=-385.1543883\PUHF=-384.7438803\PMP2-0=-385.1561762\S2=0.760814\S2-1=0.752367\S2A=0.750082\RMSD=6.618e-09\RMSF=3.710e-06\Thermal=0.\Dipole=0.0048496,0.3512086,-0.0207152\PG=C01 [X(C1H6N1Si1)]\\@

B3LYP/6-311G**
1\1\GINC-AC22\FOpt\UB3LYP\6-311G(d,p)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# B3LYP/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.7258120068,-0.2924899808,0.0657732196\N,0.5792205885,0.4910367552,-0.0466487584\Si,-1.0641607366,-0.0915685171,0.0016397972\H,2.687457213,0.1871121238,-0.0498652318\H,1.6327985774,-1.3523004986,-0.1297545232\H,0.7362898969,1.4856445644,0.02389543\H,-1.2520368537,-1.1433901295,-1.030891508\H,-1.9255101103,1.0825403073,-0.2803428035\H,-1.4490675819,-0.6798646247,1.3144293784\\Version=IA64L-G03RevD.01\HF=-385.970981\S2=0.753198\S2-1=0.\S2A=0.750007\RMSD=3.312e-09\RMSF=2.070e-06\Thermal=0.\Dipole=-0.0090457,0.3673942,-0.0688831\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/6-311G**
1\1\GINC-AC28\FOpt\UBHandHLYP\6-311G(d,p)\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.7132113502,-0.2931977193,0.064197806\N,0.5749232303,0.4914942904,-0.0403223751\Si,-1.0527589849,-0.0899099691,0.0032536108\H,2.6693685701,0.1817690855,-0.0500188412\H,1.6187159125,-1.340750862,-0.1570334401\H,0.734514234,1.4753956857,0.0435950022\H,-1.2278868417,-1.1471276499,-1.0114462104\H,-1.9158856633,1.0671465109,-0.295316269\H,-1.4433988073,-0.6580993722,1.3113257168\\Version=IA64L-G03RevD.01\HF=-385.8847926\S2=0.755025\S2-1=0.\S2A=0.750017\RMSD=6.979e-09\RMSF=9.015e-07\Thermal=0.\Dipole=0.0205987,0.3491869,-0.0631851\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/cc-pVDZ
1\1\GINC-AC15\FOpt\UBHandHLYP\CC-pVDZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/cc-pVDZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.7163075277,-0.2967118027,0.0615154512\N,0.5834123437,0.4969010864,-0.0555105734\Si,-1.0626480369,-0.0897447773,0.0033474998\H,2.6824485594,0.1817374215,-0.0449350691\H,1.6180641706,-1.3429344114,-0.206718617\H,0.7404442208,1.4785150154,0.1017995762\H,-1.2164575639,-1.1788733712,-0.994449682\H,-1.9322610906,1.0649590486,-0.3318000235\H,-1.4585071307,-0.6271282094,1.3349864375\\Version=IA64L-G03RevD.01\HF=-385.8477023\S2=0.754858\S2-1=0.\S2A=0.750016\RMSD=9.551e-09\RMSF=5.922e-06\Thermal=0.\Dipole=-0.0111051,0.3575169,-0.0368011\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/aug-cc-pVDZ
1\1\GINC-AC15\FOpt\UBHandHLYP\Aug-CC-pVDZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/aug-cc-pVDZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.7094565114,-0.2927069045,0.0470511095\N,0.5826338674,0.5045423274,-0.0636410555\Si,-1.065545311,-0.089903459,-0.0005623416\H,2.6810818721,0.1726779973,-0.0172939954\H,1.6068248811,-1.3479199493,-

0.1606718814\H,0.7423376457,1.4877217088,0.0525151864\H,-1.2259606272,-1.1578207003,-1.0179901729\H,-1.9405716273,1.0679851179,-0.2988412035\H,-1.4194542123,-0.6578561384,1.3276693544\\Version=IA64L-G03RevD.01\HF=-385.858728\S2=0.75609\S2-1=0.\S2A=0.750024\RMSD=6.318e-09\RMSF=5.166e-06\Thermal=0.\Dipole=-0.0708894,0.341646,-0.039853\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/cc-pVTZ
1\1\GINC-AC28\FOpt\UBHandHLYP\CC-pVTZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/cc-pVTZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.7088342351,-0.2885103917,0.0564955286\N,0.5742660687,0.4917124868,-0.0439453324\Si,-1.0510656517,-0.0885443115,-0.0019514819\H,2.6663698723,0.1787009778,-0.0498513349\H,1.6115474978,-1.343286561,-0.1073836018\H,0.7319323173,1.475358395,0.0162025152\H,-1.2357577798,-1.1289899121,-1.0318423343\H,-1.9174976479,1.0725249621,-0.2705973404\H,-1.4178259118,-0.6822456455,1.301108382\\Version=IA64L-G03RevD.01\HF=-385.9031517\S2=0.755726\S2-1=0.\S2A=0.750022\RMSD=5.353e-09\RMSF=1.846e-05\Thermal=0.\Dipole=0.0323978,0.3608054,-0.0670106\PG=C01 [X(C1H6N1Si1)]\\@

BHandHLYP/aug-cc-pVTZ
1\1\GINC-AC30\FOpt\UBHandHLYP\Aug-CC-pVTZ\C1H6N1Si1(2)\UXW563\29-Oct-2007\0\\# BHandHLYP/aug-cc-pVTZ scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.7067864731,-0.2867640578,0.0524425801\N,0.5744351825,0.4937997214,-0.0466545011\Si,-1.0519430557,-0.0882148302,-0.0043510555\H,2.6669307508,0.1765024352,-0.0417392352\H,1.6080041732,-1.3453365116,-0.0802063888\H,0.732996123,1.4781654259,-0.009043223\H,-1.2438006743,-1.1173401148,-1.0439243853\H,-1.92097482,1.0743650767,-0.2533820727\H,-1.4016311527,-0.6984571447,1.2950932815\\Version=IA64L-G03RevD.01\HF=-385.9057902\S2=0.75618\S2-1=0.\S2A=0.750025\RMSD=4.256e-09\RMSF=1.868e-05\Thermal=0.\Dipole=-0.0138409,0.3538245,-0.0704897\PG=C01 [X(C1H6N1Si1)]\\@

QCISD/cc-pVDZ
1\1\GINC-AC24\FOpt\UQCISD-FC\CC-pVDZ\C1H6N1Si1(2)\UXW563\30-Oct-2007\0\\# QCISD/cc-pVDZ scf=direct nosymm opt=(grad,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,0.0139702502,0.0054095804,-0.0171527149\N,-0.0347367673,-0.0495965138,1.3886484432\Si,1.4122521155,0.0071103783,2.4012810787\H,-0.941938033,-0.0269450504,-0.551955226\H,0.8864461336,-0.461245893,-0.4910466723\H,-0.8990575263,0.3148244411,1.7836331214\H,2.3325755703,-1.0703154912,1.942712476\H,0.9658715105,-0.2304385417,3.8017930219\H,2.1538857834,1.3037659084,2.3446840288\\Version=IA64L-G03RevD.01\HF=-384.7092929\MP2=-385.1042654\MP3=-385.1420183\MP4D=-385.1541713\MP4DQ=-385.1473802\PUHF=-384.7122323\PMP2-0=-385.1060497\PMP3-0=-385.1430366\MP4SDQ=-385.1503028\QCISD=-385.1529968\S2=0.760681\S2-1=0.752248\S2A=0.75008\RMSD=9.910e-09\RMSF=2.722e-05\Thermal=0.\Dipole=-0.2857176,0.049301,0.1934496\PG=C01 [X(C1H6N1Si1)]\\@

CCSD(T)/cc-pVDZ//BHandHLYP/aug-cc-pVTZ
1\1\GINC-AC25\SP\UCCSD(T)-FC\CC-pVDZ\C1H6N1Si1(2)\UXW563\30-Nov-2007\0\\# CCSD(T)/cc-pVDZ scf=direct nosymm\\freq&geom\\0,2\C,0,1.706786,-0.286764,0.052443\N,0,0.574435,0.4938,-0.046655\Si,0,-1.051943,-0.088215,-0.004351\H,0,2.666931,0.176502,-0.041739\H,0,1.608004,-1.345337,-0.080206\H,0,0.732996,1.478165,-0.009043\H,0,-1.243801,-1.11734,-1.043924\H,0,-1.920975,1.074365,-0.253382\H,0,-1.401631,-0.698457,1.295093\\Version=IA64L-G03RevD.01\HF=-384.708682\MP2=-385.1017754\MP3=-385.1395959\MP4D=-385.1514138\MP4DQ=-385.1447845\PUHF=-384.7117899\PMP2-0=-385.1036447\PMP3-0=-385.1406431\MP4SDQ=-385.1475035\CCSD=-385.1493267\CCSD(T)=-385.1603954\S2=0.761058\S2-1=0.752204\S2A=0.750084\RMSD=6.768e-09\Thermal=0.\PG=C01 [X(C1H6N1Si1)]\\@

G3MP2
1\1\GINC-AC30\Mixed\G3MP2\G3MP2\C1H6N1Si1(2)\UXW563\30-Oct-2007\0\\# G3MP2 scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,0,1.7095235372,-0.3131849452,0.0611036228\N,0,0.5829193799,0.508179874,-0.0573526517\Si,0,-1.056754458,-0.0863037897,0.0124804021\H,0,2.6767413245,0.1658218833,-0.0243837308\H,0,1.607775193,-1.3183965109,-0.3298018869\H,0,0.7470767934,1.4801843621,0.1785765107\H,0,-1.1688502579,-1.2231698628,-0.9331922149\H,0,-1.935236124,1.0378030477,-0.392764245\H,0,-1.4923923882,-0.5642140584,1.3535691937\\Version=IA64L-G03RevD.01\MP2/6-31G(d)=-385.0364857\QCISD(T)/6-31G(d)=-385.0881357\MP2/GTMP2Large=-385.2398577\G3MP2=-385.3170453.

Extended Tables 1 – 5:

Table 1. Activation energies $E_{1\text{-}2}^{\ddagger}$, reaction energies $\Delta E_{1\text{-}2}$ (in kJ mol^{-1}), imaginary frequencies ν_i (in cm^{-1}) and contribution of orbital interactions in the *endo* transition state for cyclization of *Si*-, *Ge*- and *Sn*-radicals onto C=N double bonds.[a]

entry	radical	*exo* pathway			*endo* pathway			orbital interactions in *endo* transition state / kJ mol^{-1}		
		$E_1^{\ddagger}$	ν_i	ΔE_1	$E_2^{\ddagger}$	ν_i	ΔE_2	SOMO → π*	LP_N → SOMO	LP_N → σ*
1[b]	***E*-1a**	65.7 *62.0*	486i	30.1 *28.5*	10.2 *10.3*	319i	-117.7 *-114.8*	89.0 (18%)	354.6 (71%)	55.6 (11%)
2[b]	***Z*-1a**	65.4 *61.2*	483i	28.6 *26.7*	66.1 *64.2*	497i	-122.0 *-119.7*	166.8 (87%)	19.8 (10%)	4.8 (3%)
3[b]	***E*-1b**	32.7 *32.6*	360i	-39.2 *-37.0*	14.2 *16.3*	208i	-133.3 *-128.3*	15.6 (7%)	172.8 (76%)	39.8 (17%)
4[b]	***Z*-1b**	35.1 *34.2*	364i	-38.0 *-36.5*	38.6 *38.8*	413i	-138.8 *-134.2*	161.6 (71%)	58.6 (26%)	6.3 (3%)
5[b]	***E*-1c**	42.2 *40.0*	303i	-54.6 *-51.9*	28.9 *30.2*	229i	-127.4 *-123.1*	105.7 (39%)	145.8 (54%)	17.7 (7%)
6[b]	***Z*-1c**	42.6 *40.6*	287i	-56.2 *-53.1*	39.5 *40.0*	313i	-109.4 *-105.1*	130.7 (60%)	77.7 (36%)	8.5 (4%)
7[b]	***E*-2b**	29.4 *29.0*	352i	-48.3 *-45.2*	19.6 *21.3*	393i	-119.6 *-113.5*	135.6 (25%)	353.9 (65%)	51.8 (10%)
8[b]	***E*-3b**	29.8 *28.6*	263i	-48.3 *-48.6*	24.0 *24.0*	168i	-148.2 *-146.5*	82.0 (32%)	143.9 (56%)	30.2 (12%)
9[b]	***E*-4b**	42.4 *42.5*	415i	-17.4 *-19.1*	10.0 *12.8*	142i	-128.7 *-123.5*	47.3 (11%)	307.6 (74%)	63.6 (15%)
10[b]	***E*-5b**	37.5 *27.7*	267i	-56.1 *-55.3*	31.2 *31.3*	267i	-131.5 *-128.6*	137.8 (32%)	265.0 (60%)	35.7 (8%)
11[b]	***E*-6b**	21.8 *21.9*	302i	-83.2 *-77.9*	40.9 *39.5*	403i	-82.1 *-77.8*	196.1 (38%)	288.8 (57%)	25.5 (5%)
12[b]	***E*-7b**	58.3 *56.6*	485i	18.6 *18.3*	33.3 *34.6*	296i	-91.6 *-86.9*	167.7 (26%)	412.6 (64%)	60.1 (9%)
13[b]	***E*-8b**	34.8 *31.5*	326i	-23.7 *-24.6*	22.2 *21.0*	255i	-84.8 *-84.2*	146.9 (29%)	342.7 (67%)	23.2 (4%)
14[b]	***E*-9b**	35.4 *34.0*	458i	-22.5 *-20.8*	4.6 *5.8*	397i	-136.8 *-124.0*	145.9 (25%)	376.6 (65%)	55.4 (10%)
15[b]	***E*-10a**	71.2 *66.7*	394i	59.6 *57.1*	23.3 *21.3*	409i	-50.9 *-49.8*	192.1 (33%)	366.8 (62%)	30.3 (5%)
16[b]	***E*-10b**	33.8 *32.8*	317i	-9.9 *-8.7*	23.7 *23.3*	288i	-63.0 *-59.9*	155.3 (31%)	327.9 (65%)	23.0 (4%)
17[b]	***E*-10c**	49.0 *47.0*	272i	-14.1 *-11.4*	34.1 *33.9*	275i	-52.3 *-50.4*	171.7 (48%)	167.1 (47%)	15.4 (5%)
18[c]	***E*-11a**	pathway not possible			18.6 *15.5*	494i	-18.0 *-18.5*	456.3 (67%)	202.5 (29%)	27.7 (4%)
19[c]	***E*-11b**	42.1 *40.4*	330i	24.3 *24.2*	17.7 *16.1*	401i	-29.0 *-28.3*	339.1 (66%)	143.2 (28%)	28.3 (6%)
20[c]	***E*-11c**	58.4 *55.5*	306i	24.1 *24.3*	19.5 *19.5*	370i	-24.5 *-24.3*	217.9 (50%)	181.1 (42%)	34.6 (8%)

[a]Data in italics include zero-point vibrational energy correction (ZPC). [b]BHandHLYP/6-311G**. [c]BHandHLYP/DZP.

Table 2. Activation energies $E_{3\text{-}4}^{\ddagger}$, reaction energies $\Delta E_{3\text{-}4}$ (in kJ mol^{-1}), imaginary frequencies ν_i (in cm^{-1}) and contribution of orbital interactions in the *exo* transition state for cyclization of *Si*-, *Ge*- and *Sn*-radicals onto N=C double bonds.[a]

entry	radical	*exo* pathway			*endo* pathway			orbital interactions in *exo* transition state / kJ mol^{-1}		
		$E_3^{\ddagger}$	ν_i		$E_4^{\ddagger}$	ν_i	ΔE_4	SOMO → π*	LP_N → SOMO	LP_N → σ*
1[b]	**12a**	38.9 *35.9*	505i	-56.4 *-57.8*	38.5 *36.5*	347i	-60.0 *-57.7*	222.9 (37%)	339.7 (56%)	43.7 (7%)
2[b]	**12b**	12.9 *13.1*	426i	-122.0 *-120.0*	36.8 *36.4*	274i	-70.7 *-66.4*	109.8 (22%)	340.6 (67%)	55.6 (11%)
3[b]	**12c**	13.0 *15.5*	329i	-131.6 *-127.3*	31.2 *31.1*	260i	-73.6 *-65.2*	6.0 (2%)	317.1 (86%)	45.7 (12%)
4[b]	**13b**	6.4 *7.7*	309i	-104.4 *-98.0*	37.4 *39.2*	403i	-42.6 *-36.2*	113.0 (22%)	350.9 (68%)	52.4 (10%)
5[b]	**13c**	20.1 *22.5*	331i	-103.6 *-96.7*	47.7 *48.1*	371i	-34.7 *-28.2*	131.7 (27%)	314.2 (66%)	34.1 (7%)
6[b]	**14a**	59.0 *54.0*	517i	16.6 *13.7*	39.8 *38.2*	314i	-25.4 *-23.7*	530.6 (58%)	365.8 (40%)	24.2 (2%)
7[b]	**14b**	31.3 *28.6*	500i	-51.9 *-51.1*	38.1 *37.0*	247i	-34.7 *-31.1*	244.6 (39%)	350.2 (56%)	31.7 (5%)
8[b]	**14c**	31.7 *30.3*	457i	-60.2 *-58.0*	32.8 *32.1*	241i	-37.3 *-32.2*	5.7 (2%)	323.5 (89%)	35.9 (9%)
9[c]	**15a**	59.9 *53.6*	542i	42.5 *38.0*	42.1 *39.9*	317i	12.4 *12.8*	3929.1 (94%)	209.7 (5%)	26.6 (1%)
10[c]	**15b**	30.3 *26.7*	604i	-17.3 *-18.1*	39.8 *38.5*	272i	1.1 2.8	554.0 (72%)	186.2 (24%)	31.7 (4%)
11[c]	**15c**	20.9 *18.4*	578i	-34.3 *-34.0*	25.8 *24.8*	255i	-14.2 *-11.3*	559.7 (72%)	183.9 (24%)	32.5 (4%)

[a]Data in italics include zero-point vibrational energy correction (ZPC). [b]BHandHLYP/6-311G**. [c]BHandHLYP/DZP.

Table 3. Activation energies $E_{5\text{-}6}^{\ddagger}$, reaction energies $\Delta E_{5\text{-}6}$ (in kJ mol^{-1}), imaginary frequencies ν_i (in cm^{-1}) and contribution of orbital interactions in the *N*-philic transition state for addition of $H_3Si^{\bullet}$, $H_3Ge^{\bullet}$ and $H_3Sn^{\bullet}$ to the C≡N triple bond in acetonitrile.[a,b]

Entry	X	*C*-philic pathway			*N*-philic pathway			orbital interactions in *N*-philic transition state / kJ mol^{-1}		
		$E_5^{\ddagger}$	ν_i	ΔE_5	$E_6^{\ddagger}$	ν_i	ΔE_6	SOMO → π*	LP_N → SOMO	LP_N → σ*
1[c]	Si	42.6 *43.6*	453i	-44.0 *-36.1*	40.4 *41.9*	447i	-60.8 *-51.8*	203.9 (35%)	338.7 (58%)	46.3 (7%)
2[c]	Ge	46.3 *46.7*	418i	-9.8 *-3.5*	53.3 *53.1*	397i	4.2 *11.1*	286.9 (54%)	217.9 (41%)	26.1 (5%)
3[d]	Sn	55.2 *54.5*	408i	25.7 *29.3*	82.8 *80.2*	613i	30.9 *35.1*	370.7 (64%)	165.1 (29%)	40.3 (7%)

[a]Via association complex (see text). [b]Data in italics include zero-point vibrational energy correction (ZPC). [c]BHandHLYP/6-311G**. [d]BHandHLYP/DZP.

Table 4. Activation energies $E_{7\text{-}8}^{\ddagger}$, reaction energies $\Delta E_{7\text{-}8}$ (in kJ mol^{-1}), imaginary frequencies ν_i (in cm^{-1}) and contribution of orbital interactions in the *endo* transition state for cyclization of *Si*-radicals onto C≡N triple bonds (BHandHLYP/6-311G**).[a]

entry	radical	*exo* pathway			*endo* pathway			orbital interactions in *endo* transition state / kJ mol^{-1}		
		$E_7^{\ddagger}$	ν_i	ΔE_7	$E_8^{\ddagger}$	ν_i	ΔE_8	SOMO → π*	LP_N → SOMO	LP_N → σ*
1	**16a**	47.2 *44.8*	442i	-29.1 *-26.2*	62.4 *59.9*	506i	-44.2 *-38.0*	197.2 (68%)	93.1 (32%)	0.0 (0%)
2	**16b**	50.1 *49.0*	451i	-44.4 *-39.5*	66.8 *64.9*	500i	-41.7 *-35.1*	202.5 (61%)	123.4 (37%)	5.1 (2%)
3	**16c**	64.4 *64.0*	421i	-26.4 *-20.3*	70.8 *70.1*	485i	-34.8 *-27.4*	197.4 (57%)	140.4 (41%)	6.9 (2%)
4	**16d**	65.6 *67.4*	400i	-24.3 *-16.9*	81.5 *81.0*	433i	-16.6 *-8.0*	238.7 (58%)	167.9 (40%)	10.1 (2%)

[a]Data in italics include zero-point vibrational energy correction (ZPC).

Table 5. Activation energies $E_{9\text{-}10}^{\ddagger}$, reaction energies $\Delta E_{9\text{-}10}$ (in kJ mol^{-1}), imaginary frequencies ν_i (in cm^{-1}) and contribution of orbital interactions in the *endo* transition state for cyclization of *Si*-, *Ge*- and *Sn*-radicals onto C=O double bonds.[a]

entry	radical	*exo* pathway			*endo* pathway			orbital interactions in *endo* transition state / kJ mol^{-1}		
		$E_9^{\ddagger}$	ν_i	ΔE_9	$E_{10}^{\ddagger}$	ν_i	ΔE_{10}	SOMO → π*	LP_O → SOMO	LP_O → σ*
1[b]	**17a**	53.1 *54.5*	395i	53.1 *54.5*	44.0 *42.9*	728i	-108.1 *-102.7*	213.8 (37%)	318.2 (56%)	39.4 (7%)
2[b]	**17b**	33.2 *34.1*	318i	-15.5 *-9.5*	46.4 *46.5*	616i	-126.9 *-119.6*	195.8 (41%)	221.5 (46%)	64.7 (13%)
3[b]	**17c**	41.0 *40.6*	245i	-26.9 *-20.2*	46.9 *49.2*	522i	-116.7 *-108.7*	142.2 (34%)	232.6 (56%)	42.6 (10%)
4[b]	**18a**	87.7 *86.1*	413i	74.4 *75.6*	40.5 *39.1*	733i	-102.3 *-96.6*	242.8 (37%)	352.1 (54%)	61.3 (9%)
5[b]	**18b**	44.5 *45.7*	366i	6.4 *11.7*	43.6 *43.8*	619i	-119.1 *-111.8*	215.6 (44%)	226.9 (46%)	46.6 (10%)
6[b]	**18c**	57.6 *58.5*	296i	-0.1 *6.8*	43.9 *46.1*	518i	-106.7 *-98.1*	156.1 (34%)	247.2 (54%)	51.9 (12%)
7[b]	**19a**	81.4 *79.3*	224i	--[c]	57.9 *55.8*	672i	-29.0 -24.9	304.1 (46%)	328.7 (50%)	21.4 (4%)
8[b]	**19b**	36.7 *37.0*	270i	12.8 *17.3*	58.9 56.8	592i	-40.5 -35.5	287.5 (57%)	193.5 (39%)	20.3 (4%)
9[b]	**19c**	44.8 *44.0*	215i	6.5 *11.8*	60.1 *60.0*	569i	-31.8 *-26.1*	253.4 (50%)	242.0 (48%)	31.0 (2%)
10[d]	**20a**	pathway not possible			51.8 *48.7*	713i	-5.4 *-3.2*	721.2 (81%)	147.4 (17%)	16.6 (2%)
11[d]	**20b**	45.7 *45.9*	257i	38.2 *41.1*	51.5 *49. 4*	655i	-17.9 *-14.9*	576.6 (80%)	126.3 (17%)	24.2 (3%)
12[d]	**20c**	56.5 55.6	233i	37.6 *41.0*	49.2 *48.7*	563i	-13.9 *-9.9*	412.0 (70%)	145.4 (25%)	32.4 (5%)

[a]Data in italics include zero-point vibrational energy correction (ZPC). [b]BHandHLYP/6-311G**. [c]Could not be located (see text). [d]BHandHLYP/DZP.

Figures 6 – 10:

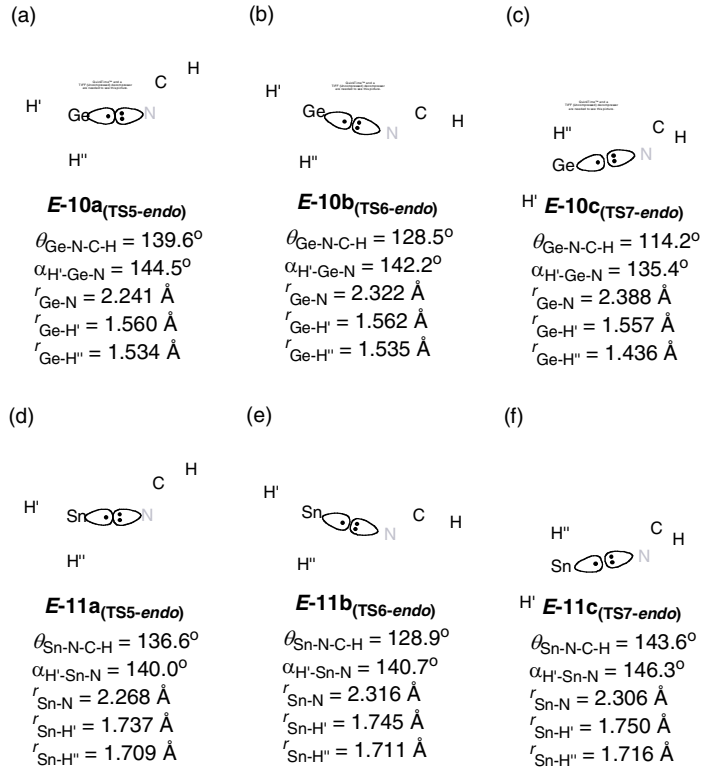
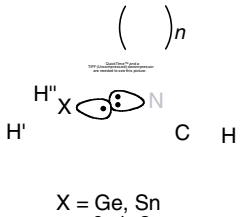
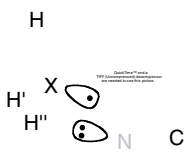


Figure 7. Optimized geometries of the transition states, selected dihedral angles (θ), angles (α), distances (r) and motion vectors (blue arrows) for the *endo* cyclization of (a-c) ***E*-10a-c** (BHandHLYP/6-311G**) and (d-f) ***E*-11a-c** (BHandHLYP/DZP). For clarity, only the SOMO and LP_N are shown.



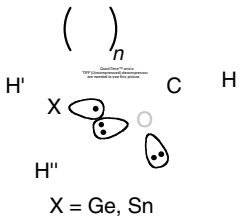
Radical	Transition state	$\theta_{X\text{-}N\text{-}C\text{-}H}$ /°	$\alpha_{H'\text{-}X\text{-}N}$ /°	$r_{X\text{-}N}$ /Å	$r_{X\text{-}H'}$ /Å	$r_{X\text{-}H''}$ /Å
14a	4-*exo*	117.9	137.4	2.161	1.550	1.529
15a	4-*exo*	125.8	136.0	2.203	1.729	1.706
14b	5-*exo*	138.0	143.7	2.235	1.560	1.533
15b	5-*exo*	142.5	142.4	2.268	1.701	1.708
14c	6-*exo*	144.0	143.7	2.232	1.569	1.537
15c	6-*exo*	146.2	148.5	2.270	1.750	1.714

Figure 8. Optimized geometries of the transition states: selected dihedral angles (θ), angles (α) and distances (r) for the *exo* cyclization of **14a-c** (BHandHLYP/6-311G**) and **15a-c** (BHandHLYP/DZP).



Radical	$\alpha_{H\text{-}X\text{-}N}$ /°	$r_{X\text{-}N}$ /Å	$r_{X\text{-}H}$ /Å	$r_{X\text{-}H'}$ /Å	$r_{X\text{-}H''}$ /Å
•SiH_3	140.9	2.156	1.496	1.474	1.474
•GeH_3	128.5	2.220	1.546	1.527	1.527
•SnH_3	134.0	2.274	1.734	1.706	1.706

Figure 9. Optimized geometries of the *N*-philic transition states: selected angles (α), distances (r) and motion vectors (blue) for the addition of SiH_3•, GeH_3• and SnH_3• to acetonitrile (for Si, Ge: BHandHLYP/6-311G**; for Sn: BHandHLYP/DZP).



Radical	Transition state	$\theta_{X\text{-}O\text{-}C\text{-}H}$ /°	$\alpha_{H'\text{-}X\text{-}O}$ /°	$r_{X\text{-}O}$ /Å	$r_{X\text{-}H'}$ /Å	$r_{X\text{-}H''}$ /Å
19a	5-*endo*	136.2	136.1	2.195	1.545	1.529
20a	5-*endo*	135.9	137.8	2.242	1.727	1.706
19b	6-*endo*	121.9	133.8	2.223	1.549	1.529
20b	6-*endo*	124.9	146.5	2.254	1.734	1.706
19c	7-*endo*	135.2	138.7	2.201	1.553	1.529
20c	7-*endo*	140.1	142.6	2.254	1.739	1.706

Figure 10. Optimized geometries of the transition states: selected dihedral angles (θ), angles (α), distances (r) and motion vectors (blue arrows) for the *endo* cyclization of **19a-c** (BHandHLYP/6-311G**) and **20a-c** (BHandHLYP/DZP). For clarity, only the SOMO and LP_O are shown.

Gaussian archive entries for Table 1

I. Cyclization of *E*-1a:

***E*-1a**

1\1\GINC-AC11\FOpt\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\20-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\N,4,B6,1,A5,2,D4,0\H,4,B7,1,A6,2,D5,0\H,7,B8,4,A7,1,D6,0\H,2,B9,1,A8,4,D7,0\H,2,B10,1,A9,4,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\\B1=1.5519983\B2=1.88019367\B3=1.54975989\B4=1.08592423\B5=1.08563215\B6=1.40123321\B7=1.09424359\B8=1.01488279\B9=1.08194809\B10=1.08568591\B11=1.47936428\B12=1.47494864\A1=87.43462654\A2=101.61622785\A3=113.95907877\A4=107.59570798\A5=115.99337097\A6=110.75553406\A7=108.24743524\A8=115.5433598\A9=111.66307367\A10=120.55924794\A11=114.64856008\D1=22.88787068\D2=-146.36873864\D3=94.04999221\D4=-142.97426811\D5=83.95514239\D6=-166.04742378\D7=145.5952476\D8=-89.72885308\D9=-134.64386875\D10=91.68360937\\Version=IA64L-G03RevD.01\State=2-A\HF=-463.2325668\S2=0.757193\S2-1=0.\S2A=0.750034\RMSD=5.286e-09\RMSF=5.436e-05\Thermal=0.\Dipole=-0.0292036,-0.5704418,0.533021\PG=C01 [X(C3H8N1Si1)]\\@

4-*exo* transition state

1\1\GINC-AC43\FTS\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\04-Jul-2006\0\\# BHandHLYP/6-311G** scf=(qc,direct) opt=(TS,NoEigentest,Z-matrix,calcFC,MaxCycle=500) freq=noraman\\single-point\\0,2\C,0.0001091612,0.0044224638,0.0014996525\C,-0.000188078,-0.0078106275,1.5385815201\Si,1.8703310794,-0.0106636018,1.7196722843\C,1.2494879202,-0.7500857735,-0.427050114\H,-0.8928652323,-0.4345864092,-0.438989013\H,0.0901203538,1.0169219952,-0.3783093795\N,1.9797122499,-0.2908929676,-1.4125761735\H,1.2497218439,-1.8111150713,-0.1745926521\H,2.6892099137,-0.9680740691,-1.6626500976\H,-0.5540410761,0.8066699168,1.9901844254\H,-0.4057551117,-0.9410665392,1.9205354969\H,2.4517676486,-0.7816355861,2.8429493495\H,2.4840170504,1.3290399462,1.6457844428\\Version=IA64L-G03RevD.01\State=2-A\HF=-463.219032\S2=0.80369\S2-1=0.\S2A=0.750304\RMSD=0.000e+00\RMSF=7.084e-06\Thermal=0.\Dipole=-0.2434331,-0.5936915,0.5162398\PG=C01 [X(C3H8N1Si1)]\\@

4-*exo* product

1\1\GINC-AC11\FOpt\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\20-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\N,4,B6,1,A5,2,D4,0\H,4,B7,1,A6,2,D5,0\H,7,B8,4,A7,1,D6,0\H,2,B9,1,A8,4,D7,0\H,2,B10,1,A9,4,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\\B1=1.5519983\B2=1.88019367\B3=1.54975989\B4=1.08592423\B5=1.08563215\B6=1.40123321\B7=1.09424359\B8=1.01488279\B9=1.08194809\B10=1.08568591\B11=1.47936428\B12=1.47494864\A1=87.43462654\A2=101.61622785\A3=113.95907877\A4=107.59570798\A5=115.99337097\A6=110.75553406\A7=108.24743524\A8=115.5433598\A9=111.66307367\A10=120.55924794\A11=114.64856008\D1=22.88787068\D2=-146.36873864\D3=94.04999221\D4=-142.97426811\D5=83.95514239\D6=-166.04742378\D7=145.5952476\D8=-89.72885308\D9=-134.64386875\D10=91.68360937\\Version=IA64L-G03RevD.01\State=2-A\HF=-463.2325668\S2=0.757193\S2-1=0.\S2A=0.750034\RMSD=5.286e-09\RMSF=5.436e-05\Thermal=0.\Dipole=-0.0292036,-0.5704418,0.533021\PG=C01 [X(C3H8N1Si1)]\\@

5-*endo* transition state

1\1\GINC-AC31\FTS\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\13-Jun-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.1187693569,-0.3736760127,-1.004645567\C,-1.2007151055,0.1481480279,0.4380987429\Si,0.5020149,0.2534774838,1.2988854979\N,1.2007637662,-0.1249352812,-0.705661581\C,0.251687528,-0.1261730796,-1.5498565335\H,-1.6119583644,1.1556525808,0.4425016787\H,-1.8831674475,-0.4569522023,1.0259570224\H,-1.2847167348,-1.4511846206,-1.0274456833\H,-1.8693523543,0.0640665312,-1.6561882403\H,0.4074921084,0.0681863784,-2.6044569381\H,2.1245928915,0.0629456203,-1.0600261054\H,0.1806741913,1.0493385915,2.5423489385\H,0.9817539781,-1.0588940173,1.7904887677\\Version=IA64L-G03RevD.01\HF=-463.2401676\S2=0.762852\S2-1=0.\S2A=0.750053\RMSD=8.597e-09\RMSF=4.951e-06\Thermal=0.\Dipole=-0.0392113,-0.1082247,-1.6825722\PG=C01 [X(C3H8N1Si1)]\\@

5-*endo* product

1\1\GINC-AC38\FOpt\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\19-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,2,B5,1,A4,5,D3,H,

2,B6,1,A5,5,D4,0\H,1,B7,5,A6,4,D5,0\H,1,B8,5,A7,4,D6,0\H,5,B9,4,A8,3,D7,0\H,4,B10,3,A9,2,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\\B1=1.54502919\B2=1.8798842\B3=1.73435739\B4=1.40069077\B5=1.08384474\B6=1.08708871\B7=1.08620105\B8=1.09491737\B9=1.07731351\B10=0.99813169\B11=1.4790635\B12=1.47984214\A1=103.33692932\A2=93.39077968\A3=113.18359511\A4=112.13898861\A5=110.17050567\A6=111.27722687\A7=110.24418007\A8=117.76887048\A9=128.28845259\A10=114.50471458\A11=114.95269534\D1=-18.20040483\D2=0.99561525\D3=154.65425648\D4=-85.59654083\D5=-155.51307255\D6=86.62927026\D7=-193.97774318\D8=192.19581993\D9=-136.08840268\D10=99.48355874\\Version=IA64L-G03RevD.01\State=2-A\HF=-463.288877\S2=0.755362\S2-1=0.\S2A=0.75002\RMSD=0.000e+00\RMSF=1.248e-05\Thermal=0.\Dipole=0.1207388,0.0270159,-0.0673346\PG=C01 [X(C3H8N1Si1)]\\@

Cyclization of *Z*-1a:

<u>*Z*-1a</u>

1\1\GINC-AC29\FOpt\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\16-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.0804285541,1.5996790982,-0.0183222752\C,1.4985646855,0.9740511431,0.0460624596\Si,0.6649191258,-0.7113493091,-0.0595575053\C,-0.784059639,0.4231130959,0.5216203724\H,-0.0393308802,2.5267733638,0.5341249365\H,-0.1932949867,1.7939755602,-1.053384947\N,-2.0910011232,0.1857375592,0.0798186428\H,-0.7489846015,0.4051142563,1.611698338\H,2.1893817244,1.2986818422,-0.7206225658\H,1.9574318106,1.1368097871,1.0162697573\H,1.1018463135,-1.8343177812,0.7942351129\H,0.4777942801,-1.1893031814,-1.4444966738\H,-2.1732549741,0.5503704161,-0.8650631756\\Version=IA64L-G03RevD.01\HF=-463.2315171\S2=0.757317\S2-1=0.\S2A=0.750035\RMSD=3.956e-09\RMSF=3.532e-05\Thermal=0.\Dipole=0.8245603,0.3636481,-0.2435065\PG=C01 [X(C3H8N1Si1)]\\@

<u>4-*exo* transition state</u>

1\1\GINC-AC12\FTS\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\20-Sep-2006\1\\# BHandHLYP/6-311G** opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\N,4,B6,1,A5,2,D4,0\H,4,B7,1,A6,2,D5,0\H,7,B8,4,A7,1,D6,0\H,2,B9,1,A8,4,D7,0\H,2,B10,1,A9,4,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\\B1=1.53675461\B2=1.88131059\B3=1.52660918\B4=1.08824674\B5=1.08790768\B6=1.30877405\B7=1.08707732\B8=1.01419709\B9=1.08345602\B10=1.08657694\B11=1.47958019\B12=1.47733932\A1=95.31990142\A2=105.62035104\A3=111.06023415\A4=108.6424501\A5=126.3302289\A6=114.12143669\A7=109.702089\A8=114.34220289\A9=110.68554037\A10=118.08595325\A11=112.96684497\D1=32.61628606\D2=-149.82570486\D3=92.31606132\D4=-141.52438773\D5=63.60454354\D6=14.54786308\D7=156.91271837\D8=-80.85056873\D9=-146.43467473\D10=82.52429417\\Version=IA64L-G03RevD.01\State=2-A\HF=-463.2175133\S2=0.804244\S2-1=0.\S2A=0.750304\RMSD=0.000e+00\RMSF=7.407e-05\Thermal=0.\Dipole=-0.7907407,0.350948,0.551912\PG=C01 [X(C3H8N1Si1)]\\@

<u>4-*exo* product</u>

1\1\GINC-AC11\FOpt\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\20-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\N,4,B6,1,A5,2,D4,0\H,4,B7,1,A6,2,D5,0\H,7,B8,4,A7,1,D6,0\H,2,B9,1,A8,4,D7,0\H,2,B10,1,A9,4,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\\B1=1.5519983\B2=1.88019367\B3=1.54975989\B4=1.08592423\B5=1.08563215\B6=1.40123321\B7=1.09424359\B8=1.01488279\B9=1.08194809\B10=1.08568591\B11=1.47936428\B12=1.47494864\A1=87.43462654\A2=101.61622785\A3=113.95907877\A4=107.59570798\A5=115.99337097\A6=110.75553406\A7=108.24743524\A8=115.5433598\A9=111.66307367\A10=120.55924794\A11=114.64856008\D1=22.88787068\D2=-146.36873864\D3=94.04999221\D4=-142.97426811\D5=83.95514239\D6=-166.04742378\D7=145.5952476\D8=-89.72885308\D9=-134.64386875\D10=91.68360937\\Version=IA64L-G03RevD.01\State=2-A\HF=-463.2325668\S2=0.757193\S2-1=0.\S2A=0.750034\RMSD=5.286e-09\RMSF=5.436e-05\Thermal=0.\Dipole=-0.0292036,-0.5704418,0.533021\PG=C01 [X(C3H8N1Si1)]\\@

<u>5-*endo* transition state</u>

1\1\GINC-AC14\FTS\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\07-Jul-2006\1\\# BHandHLYP/6-311G** scf=(qc,direct) opt=(TS,Noeigentest,Z-matrix,calcfc,maxcycle=500) freq=noraman\\single-point\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,2,B5,1,A4,5,D3,0\H,2,B6,1,A5,5,D4,0\H,1,B7,5,A6,4,D5,0\H,1,B8,5,A7,4,D6,0\H,5,B9,4,A8,3,D7,0\H,4,B10,3,A9,2,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\\B1=1.56240846\B2=1.9042578\B3=2.39636862\B4=1.30290673\B5=1.0855303\B6=1.08603941\B7=1.08421851\B8=1.0870804\B9=1.08276692\B10=1.01231072\B11=1.47387426\B12=1.48636186\A1=109.41977485\A2=85.85326972\A3=89.18654202\A4=111.26009777\A5=109.40950691\A6=112.85997094\A7=110.11586914\A8=116.88420642\A9=85.92550001\A10=111.8917198\A11=111.18222741\D1=-2.23140168\D2=-

25.85569933\D3=149.97274354\D4=-92.37887784\D5=172.43902682\D6=51.764685\D7=-102.09815045\D8=84.77241948\D9=-101.09528899\D10=135.90758673\\Version=IA64L-G03RevD.01\State=2-A\HF=-463.2172146\S2=0.797004\S2-1=0.\S2A=0.750254\RMSD=0.000e+00\RMSF=3.275e-05\Thermal=0.\Dipole=-0.9041107,0.2407463,-0.1202971\PG=C01 [X(C3H8N1Si1)]\\@

5-*endo* product

1\1\GINC-AC38\FOpt\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\19-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,2,B5,1,A4,5,D3,0\H,2,B6,1,A5,5,D4,0\H,1,B7,5,A6,4,D5,0\H,1,B8,5,A7,4,D6,0\H,5,B9,4,A8,3,D7,0\H,4,B10,3,A9,2,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\\B1=1.54502919\B2=1.8798842\B3=1.73435739\B4=1.40069077\B5=1.08384474\B6=1.08708871\B7=1.08620105\B8=1.09491737\B9=1.07731351\B10=0.99813169\B11=1.4790635\B12=1.47984214\A1=103.33692932\A2=93.39077968\A3=113.18359511\A4=112.13898861\A5=110.17050567\A6=111.27722687\A7=110.24418007\A8=117.76887048\A9=128.28845259\A10=114.50471458\A11=114.95269534\D1=-18.20040483\D2=0.99561525\D3=154.65425648\D4=-85.59654083\D5=-155.51307255\D6=86.62927026\D7=-193.97774318\D8=192.19581993\D9=-136.08840268\D10=99.48355874\\Version=IA64L-G03RevD.01\State=2-A\HF=-463.288877\S2=0.755362\S2-1=0.\S2A=0.75002\RMSD=0.000e+00\RMSF=1.248e-05\Thermal=0.\Dipole=0.1207388,0.0270159,-0.0673346\PG=C01 [X(C3H8N1Si1)]\\@

Cyclization of *E*-1b:

***E*-1b**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\FOpt\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\EVA\30-Apr-2006\0\\#BHANDHLYP/6-311G** OPT=(Z-MATRIX,READFC) OPTCYC=500 FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\geom and freq\\0,2\Si,-2.3099926059,-0.6705947843,-1.3378579766\C,-0.6388196748,0.1946301668,-1.2106301041\C,0.0963674034,-0.0381942101,0.1084580431\C,1.4197011788,0.706307255,0.1749091742\C,2.1849906016,0.511085668,1.4459418802\H,3.1345280421,1.0463657517,1.4976607771\H,2.0648118336,0.4090783317,-0.6535342125\H,1.2608338295,1.7775747802,0.0407743993\H,-0.5222545423,0.2693854791,0.9468157025\H,0.2811597504,-1.0981049167,0.2570980183\H,-0.0238479385,-0.128358813,-2.0491463865\H,-0.8151373773,1.2613305438,-1.3592494233\H,-3.2187892305,-0.2631196512,-0.241011664\H,-2.9566870699,-0.4013313347,-2.6433010869\N,1.7640705031,-0.2146195276,2.380946909\H,2.4133486102,-0.2251297756,3.1552032249\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-502.5410521\S2=0.751607\S2-1=0.\S2A=0.750001\RMSD=9.169e-09\RMSF=1.662e-05\Dipole=0.8989245,0.5288669,-0.1486539\PG=C01 [X(C4H10N1Si1)]\\@

5-*exo* transition state

1\1\GINC-AC29\FTS\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UXW563\16-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.0709649752,1.4426176199,0.1505298287\C,-1.9304686589,0.2250512093,-0.2076538976\Si,-0.9431291209,-1.3726859145,-0.038078671\C,0.3242740932,1.304739388,-0.4496127075\H,-1.5406718301,2.3572773564,-0.2011202164\H,-0.9697523817,1.5244031998,1.2274152689\H,0.2602532089,1.161583684,-1.5262518933\H,0.8996142064,2.2133742068,-0.2820691775\N,1.1953662174,0.1073520087,1.4582011143\H,-1.3019322895,-2.355809434,-1.0906168076\H,-1.0341948538,-2.0195478715,1.2854431744\H,-2.8333517572,0.1908837579,0.3963758204\H,-2.2499991965,0.2920677874,-1.2460581743\H,1.8366661327,-0.6231782287,1.7356077548\C,1.0950944854,0.1596283811,0.1690451425\H,1.7749079597,-0.3801823805,-0.4839906502\\Version=IA64L-G03RevD.01\HF=-502.5285866\S2=0.797158\S2-1=0.\S2A=0.750239\RMSD=4.158e-09\RMSF=1.158e-05\Thermal=0.\Dipole=0.1740453,0.0034899,-0.5921808\PG=C01 [X(C4H10N1Si1)]\\@

5-*exo* product

1\1\GINC-AC7\FOpt\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UXW563\16-Nov007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.7905327061,1.2364931946,-0.4141466022\C,1.6077786048,-0.0646071045,-0.3008696486\Si,0.3073742184,-1.3876915409,0.0401660563\C,-1.1585676617,-0.1514560966,0.2976802574\C,-0.393217085,1.1587519897,0.5501922215\H,1.4022659466,2.1119211041,-0.2160648972\H,0.4026537714,1.3346509707,-1.4234322363\H,-0.0315838831,1.167248947,1.5781090257\H,-1.0603680278,2.0079329563,0.4331799053\N,-1.8688741301,-0.0926891691,-0.9287661067\H,-1.7701027536,-0.4396262258,1.1534843471\H,0.5733133582,-2.1678005814,1.2694707378\H,0.0544818337,-2.3350035005,-1.0631471974\H,2.2047866822,-0.2532497749,-1.1864313076\H,2.2927908923,-0.0108643514,0.5420691569\H,-2.5808651224,-0.8156202773,-0.9193396921\\Version=IA64L-G03RevD.01\HF=-502.5559799\S2=0.756416\S2-1=0.\S2A=0.750029\RMSD=6.887e-09\RMSF=4.649e-05\Thermal=0.\Dipole=0.1163398,-0.2208948,0.5019393\PG=C01 [X(C4H10N1Si1)]\\@

6-*endo* transition state

1\1\GINC-AC21\FTS\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UXW563\13-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.6348586942,1.4037559596,-0.3280263044\C,0.6907822076,1.171084097,0.4068772039\Si,1.6301210945,-0.4014169791,-0.1070072782\N,-0.3523375534,-1.4709318561,0.1243154365\C,-1.5076880911,-0.9801367606,-0.0512960301\C,-1.7768646703,0.4824443989,0.1000034503\H,1.3465390786,2.0180171559,0.2234241754\H,0.5113019098,1.1515387257,1.4805369673\H,-0.9719743528,2.4254407305,-0.1675362047\H,-0.4871424161,1.3023844092,-1.4019991751\H,-2.6768332955,0.7270171539,-0.4580760671\H,-2.0185771288,0.6599820418,1.1497739883\H,-2.347775559,-1.6160825875,-0.3155983627\H,2.1264362534,-1.1628063689,1.0618675612\H,2.8744832221,0.0932913674,-0.8043535038\H,-0.3075080049,-2.4691954879,-0.0152628564\\Version=IA64L-G03RevD.01\HF=-502.5356229\S2=0.760245\S2-1=0.\S2A=0.75004\RMSD=7.216e-09\RMSF=2.117e-05\Thermal=0.\Dipole=-1.7291751,-0.2859438,-0.0246171\PG=C01 [X(C4H10N1Si1)]\\@

6-*endo* product

1\1\GINC-AC13\FOpt\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UXW563\19-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11,3,D10,0\H,3,B13,2,A12,1,D11,0\H,3,B14,2,A13,1,D12,0\H,4,B15,3,A14,2,D13,0\\B1=1.53559804\B2=1.8694935\B3=1.73613836\B4=1.39839318\B5=1.49244822\B6=1.08717171\B7=1.08862154\B8=1.08731444\B9=1.08891479\B10=1.08650572\B11=1.09762018\B12=1.07690073\B13=1.47735791\B14=1.48388112\B15=1.00087518\A1=110.14155801\A2=103.82816694\A3=122.5770416\A4=118.97776964\A5=110.71549882\A6=109.55826673\A7=109.76082503\A8=109.87161688\A9=108.38867432\A10=110.22068314\A11=115.46243782\A12=114.17631726\A13=109.78912777\A14=119.9072874\D1=-38.97565182\D2=28.84470221\D3=-35.00247807\D4=180.13809693\D5=-62.34497653\D6=179.32432484\D7=-63.80538938\D8=-188.56362764\D9=-72.7800995\D10=174.73301815\D11=202.43416194\D12=81.94115937\D13=-173.8368467\\Version=IA64L-G03RevD.01\State=2-A\HF=-502.5918154\S2=0.755465\S2-1=0.\S2A=0.750021\RMSD=0.000e+00\RMSF=2.194e-05\Thermal=0.\Dipole=0.0337331,-0.1404593,-0.0066856\PG=C01 [X(C4H10N1Si1)]\\@

Cyclization of *Z*-1b:

***Z*-1b**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\FOpt\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UWILLE\06-Jul-2006\1\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) OPT=(Z-MATRIX,READFC) OPTCYC=500 FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\geom and freq\\0,2\Si\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,4,B7,3,A6,2,D5,0\3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\H,2,B10,1,A9,3,D8,0\H,2,B11,1,A13,D9,0\H,1,B12,2,A11,3,D10,0\H,1,B13,2,A12,3,D11,0\N,5,B14,4,A13,3,D12,0\H,5,B15,4,A14,3,D13,0\\B1=1.88766668\B2=1.52815773\B3=1.52044804\B4=1.50326317\B5=1.08743561\B6=1.09042832\B7=1.0904458\B8=1.08864413\B9=1.08848448\B10=1.08836072\B11=1.09078665\B12=1.48140797\B13=1.48013393\B14=1.2557867\B15=1.88052558\A1=114.6664498\A2=112.60543104\A3=115.8538459\A4=114.45120635\A5=110.0221912\A6=110.06229116\A7=109.52952875\A8=109.51117746\A9=108.34118278\A10=107.3805044\A11=111.29255898\A12=111.18680476\A13=128.88444187\A14=98.82842399\D1=-178.71538592\D2=-179.92364608\D3=-179.97605895\D4=-57.6583438\D5=57.78552442\D6=-56.8707006\D7=59.42366905\D8=123.41963236\D9=-122.40181632\D10=57.12000575\D11=-180.064662\D12=0.03001201\D13=0.02495164\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-502.5389451\S2=0.751603\S2-1=0.\S2A=0.750001\RMSD=0.000e+00\RMSF=7.688e-06\Dipole=-0.9410364,0.050171,-0.05457\PG=C01 [X(C4H10N1Si1)]\\@

5-*exo* transition state

1\1\GINC-AC57\FTS\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UXW563\03-Jul-2006\1\\# BHandHLYP/6-311G** scf=verytight opt=(TS,NoEigentest,Z-matrix,calcFC,MaxCycle=100) freq=noraman\\single-point\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\H,1,B5,5,A4,4,D3,0\H,1,B6,5,A5,4,D4,0\H,5,B7,4,A6,1,D5,0\H,5,B8,4,A7,1,D6,0\N,4,B9,1,A8,5,D7,0\H,4,B10,1,A9,5,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\H,2,B13,1,A12,5,D11,0\H,2,B14,1,A13,5,D12,0\H,4,B15,1,A14,5,D13,0\\B1=1.53099915\B2=1.88900171\B3=2.54088246\B4=1.51873437\B5=1.08664237\B6=1.08827344\B7=1.08753517\B8=1.08872929\B9=1.29443676\B10=1.08235832\B11=1.4824785\B12=1.47567975\B13=1.08695697\B14=1.0883387\B15=1.90452815\A1=110.63971725\A2=94.11578909\A3=33.57973268\A4=109.91542662\A5=109.44369312\A6=109.19986996\A7=107.8118355\A8=104.61093785\A9=138.32594656\A10=111.64420663\A11=113.43321713\A12=111.12479204\A13=109.55792963\A14=76.11899918\D1=15.08678092\D2=122.21392439\D3=172.87570844\D4=56.77427955\D5=-122.06152364\D6=122.24010002\D7=131.6815127\D8=-61.90600195\D9=-146.4638171\D10=88.75351551\D11=169.02117653\D12=-73.25039355\D13=122.50214872\\Version=IA64L-

G03RevD.01\State=2-A\HF=-502.5255815\S2=0.799105\S2-1=0.\S2A=0.750251\RMSD=3.860e-09\RMSF=2.551e-05\Thermal=0.\Dipole=-1.051112,-0.3557215,-0.1188315\PG=C01 [X(C4H10N1Si1)]\\@

5-*exo* product
1\1\GINC-AC6\FOpt\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UXW563\19-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\H,1,B5,5,A4,4,D3,0\H,1,B6,5,A5,4,D4,0\H,5,B7,4,A6,1,D5,0\H,5,B8,4,A7,1,D6,0\N,4,B9,1,A8,5,D7,0\H,4,B10,1,A9,5,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\H,2,B13,1,A12,5,D11,0\H,2,B14,1,A13,5,D12,0\H,10,B15,4,A14,1,D13,0\\B1=1.53802432\B2=1.88980662\B3=2.51432637\B4=1.54337039\B5=1.08615681\B6=1.08917405\B7=1.08897848\B8=1.08743072\B9=1.42007257\B10=1.08682979\B11=1.47802513\B12=1.47504922\B13=1.08469518\B14=1.08765834\B15=1.0169007\A1=103.62310066\A2=85.09019231\A3=34.93188739\A4=111.18725146\A5=109.54016077\A6=108.74927154\A7=110.47855543\A8=106.81833682\A9=140.83691529\A10=113.71119711\A11=113.76336272\A12=112.4431905\A13=110.02944703\A14=108.23803715\D1=11.18802656\D2=131.87267365\D3=-174.87802314\D4=67.95399771\D5=-119.09276118\D6=123.97381922\D7=112.04060408\D8=-42.33799174\D9=-131.80849468\D10=102.68014663\D11=161.82517183\D12=-78.81667803\D13=-5.67347023\\Version=IA64L-G03RevD.01\State=2-A\HF=-502.5534299\S2=0.756201\S2-1=0.\S2A=0.750027\RMSD=0.000e+00\RMSF=3.547e-05\Thermal=0.\Dipole=-0.9495989,-0.2546303,0.0476918\PG=C01 [X(C4H10N1Si1)]\\@

6-*endo* transition state
1\1\GINC-AC41\FTS\UHF\6-311G(d,p)\C4H10N1Si1(2)\UXW563\03-Jul-2006\1\\# UHF/6-311G** scf=(qc,direct) opt=(TS,NoEigentest,Z-matrix,calcFC,MaxCycle=100) freq=noraman\\single-point\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,6,A7,5,D6,0\H,1,B9,6,A8,5,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11,3,D10,0\H,3,B13,2,A12,1,D11,0\H,3,B14,2,A13,1,D12,0\H,4,B15,3,A14,2,D13,0\\B1=1.54074762\B2=1.90813741\B3=2.3722826\B4=1.31996301\B5=1.50266778\B6=1.0885923\B7=1.09060313\B8=1.08738002\B9=1.08803807\B10=1.08595518\B11=1.08867144\B12=1.08035495\B13=1.48874235\B14=1.47975713\B15=1.00499122\A1=117.13741344\A2=94.7785327\A3=97.49831745\A4=123.98690752\A5=108.9148743\A6=109.40531265\A7=108.78007485\A8=108.59635891\A9=110.39381339\A10=110.0267888\A11=116.07637302\A12=108.06560319\A13=111.06558168\A14=92.7460868\D1=-42.92419658\D2=44.90785954\D3=-72.31805759\D4=178.55066404\D5=-66.51966566\D6=178.01492192\D7=62.64560228\D8=-154.88738261\D9=-36.53652403\D10=89.82876446\D11=177.23309088\D12=57.6179398\D13=-66.33950416\\Version=IA64L-G03RevD.01\State=2-A\HF=-500.6495847\S2=0.962654\S2-1=0.\S2A=0.754985\RMSD=0.000e+00\RMSF=1.060e-05\Thermal=0.\Dipole=-0.8303987,-0.1364687,-0.5355721\PG=C01 [X(C4H10N1Si1)]\\@

6-*endo* product
1\1\GINC-AC13\FOpt\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UXW563\19-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11,3,D10,0\H,3,B13,2,A12,1,D11,0\H,3,B14,2,A13,1,D12,0\H,4,B15,3,A14,2,D13,0\\B1=1.53559804\B2=1.8694935\B3=1.73613836\B4=1.39839318\B5=1.49244822\B6=1.08717171\B7=1.08862154\B8=1.08731444\B9=1.08891479\B10=1.08650572\B11=1.09762018\B12=1.07690073\B13=1.47735791\B14=1.48388112\B15=1.00087518\A1=110.14155801\A2=103.82816694\A3=122.5770416\A4=118.97776964\A5=110.71549882\A6=109.55826673\A7=109.76082503\A8=109.87161688\A9=108.38867432\A10=110.22068314\A11=115.46243782\A12=114.17631726\A13=109.78912777\A14=119.9072874\D1=-38.97565182\D2=28.84470221\D3=-35.00247807\D4=180.13809693\D5=-62.34497653\D6=179.32432484\D7=-63.80538938\D8=-188.56362764\D9=-72.7800995\D10=174.73301815\D11=202.43416194\D12=81.94115937\D13=-173.8368467\\Version=IA64L-G03RevD.01\State=2-A\HF=-502.5918154\S2=0.755465\S2-1=0.\S2A=0.750021\RMSD=0.000e+00\RMSF=2.194e-05\Thermal=0.\Dipole=0.0337331,-0.1404593,-0.0066856\PG=C01 [X(C4H10N1Si1)]\\@

Cyclization of *E*-1c:

***E*-1c**
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET6\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UWILLE\06-May-2006\0\\#BHANDHLYP/6-311G** OPT=(Z-MATRIX,CALCFC) OPTCYC=500 FREQ=NORAMAN\\geom and freq\\0,2\C,-2.1688422171,0.2060712745,0.0170587937\C,-0.8952111956,0.9092314472,-0.4723696412\C,0.3379650934,0.0167741578,-0.4831282248\C,1.5622785887,0.7301286299,-1.028637469\C,2.8045597454,-0.1025771295,-1.0760485256\H,3.6867623735,0.4107532403,-1.4620434088\H,1.7805914683,1.6209101075,-0.4371683211\H,1.3714290003,1.0998681886,-2.0376572187\H,0.1472932244,-0.8714998968,-1.0800378451\H,0.5571622283,-0.3455361695,0.5173906591\H,-0.705335489,1.7870432701,0.1440294471\H,-1.0718888503,1.2822236587,-1.4812045964\H,-3.0230225022,0.8622467592,-0.137690894\H,-2.3582993387,-0.6789139947,-0.5880096718\N,2.8282461763,-

1.3010025172,-0.7004879518\Si,-2.1887045524,-0.3062770584,1.8344365336\H,-1.8219902835,0.8292787901,2.71373263\H,-1.3145270285,-1.4613298137,2.135268524\H,3.7514656076,-1.6979179819,-0.8065547109\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-541.8370247\S2=0.751681\S2-1=0.\S2A=0.750001\RMSD=7.519e-09\RMSF=1.831e-06\Dipole=0.5755306,0.7528974,-0.2554942\Polar=94.1405061,-0.4637692,90.0561767,-6.7708915,-1.7395048,74.5050452\PG=C01 [X(C5H12N1Si1)]\\@

6-*exo* transition state
1\1\GINC-AC19\Freq\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\16-Nov-2007\0\\#N Geom=AllCheck Guess=Read SCRF=Check GenChk UBHandHLYP/6-311G(d,p) Freq\\freq&geom\\0,2\C,-1.3267528805,-0.1874379221,-2.1969594479\C,-0.3221103012,0.0575658448,-3.3257343589\Si,1.3966255214,-0.6290226671,-2.9809981988\C,1.5835397484,0.1575974133,-0.43838982\C,0.166710407,-0.2086307935,-0.0643156457\C,-0.9654885132,0.4496260844,-0.8553231683\H,1.721435001,1.170890035,-0.8148269193\H,0.0675190552,0.0913672147,0.9788761618\H,0.0713315113,-1.2909948655,-0.0677945729\H,-1.8539901933,0.4253418789,-0.2300440358\H,-0.7396436905,1.5060745999,-1.005044351\H,-2.2962155014,0.1980320118,-2.5054323448\H,-1.4635104637,-1.2584891401,-2.052328294\H,-0.6945164208,-0.3770748323,-4.2525799132\H,-0.2295279179,1.1272066,-3.508042814\H,2.3897171503,-0.1653181579,-3.9782565606\H,1.4002507487,-2.1065223582,-2.9206764721\N,2.557925387,-0.5398310535,0.0272178174\H,3.4412208236,-0.0906397717,-0.1736571717\\Version=IA64L-G03RevD.01\HF=-541.8209535\S2=0.795269\S2-1=0.\S2A=0.750231\RMSD=2.246e-09\RMSF=5.502e-06\ZeroPoint=0.1641685\Thermal=0.1724184\Dipole=-0.5249403,0.7654263,-0.3332316

6-*exo* product
1\1\GINC-AC26\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\16-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.9222197162,0.2198023123,0.2937884806\C,-1.4305010013,-1.1243096358,-0.2610759738\Si,0.4082204193,-1.3418511275,0.0499869559\C,1.1692304856,0.3366449557,-0.4697554842\C,0.3259094785,1.4626072704,0.1403302797\C,-1.1518644914,1.4239816772,-0.2471782817\H,1.0717787525,0.3618884031,-1.5619081579\H,0.7561944656,2.4124041431,-0.1685058561\H,0.4270809918,1.4236777114,1.2237698927\H,-1.6264624316,2.3327668792,0.1136991697\H,-1.241605869,1.447535311,-1.3339067244\H,-2.9784308292,0.3415423532,0.0648472403\H,-1.8469220278,0.2139745399,1.3807338754\H,-1.9914538888,-1.9470702604,0.1755281015\H,-1.6098729418,-1.1647277753,-1.3348019938\H,1.0002868773,-2.4428925755,-0.7408560281\H,0.6762419269,-1.5814422266,1.4822731824\N,2.5188803144,0.4004589589,-0.0347542728\H,3.0885183451,-0.1106377544,-0.7019296155\\Version=IA64L-G03RevD.01\HF=-541.8578188\S2=0.756184\S2-1=0.\S2A=0.750027\RMSD=4.581e-09\RMSF=1.351e-05\Thermal=0.\Dipole=-0.6392068,-0.1877289,-0.5881539\PG=C01 [X(C5H12N1Si1)]\\@

7-*endo* transition state
1\1\GINC-AC57\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\13-Jun-2007\1\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C\C,1,r1\Si,2,r2,1,a1\N,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,5,r5,4,a4,3,d3,0\C,1,r6,2,a5,3,d4,0\H,4,r7,3,a6,2,d5,0\H,5,r8,4,a7,3,d6,0\H,6,r9,5,a8,4,d7,0\H,6,r10,5,a9,4,d8,0\H,7,r11,1,a10,2,d9,0\H,7,r12,1,a11,2,d10,0\H,1,r13,7,a12,6,d11,0\H,1,r14,7,a13,6,d12,0\H,2,r15,1,a14,7,d13,0\H,2,r16,1,a15,7,d14,0\H,3,r17,2,a16,1,d15,0\H,3,r18,2,a17,1,d16,0\\r1=1.53516736\r2=1.90111716\r3=2.42222609\r4=1.27489102\r5=1.49081334\r6=1.52646439\r7=1.00917176\r8=1.08783229\r9=1.08867684\r10=1.08622869\r11=1.0873338\r12=1.08985753\r13=1.08833178\r14=1.08896575\r15=1.08862226\r16=1.09048652\r17=1.49787478\r18=1.47961125\a1=119.62789429\a2=95.62755285\a3=114.82309779\a4=121.60494152\a5=116.50526932\a6=104.99314304\a7=121.78159447\a8=107.7148553\a9=108.71582984\a10=107.99251023\a11=109.558706\a12=106.87874376\a13=108.84363611\a14=108.25275797\a15=109.63784869\a16=106.14732598\a17=110.15978187\d1=-66.9579317\d2=10.1923125\d3=60.07562972\d4=84.92659004\d5=-113.94766559\d6=-118.19685542\d7=135.58721142\d8=19.36292303\d9=172.86482139\d10=57.76048264\d11=172.31056093\d12=58.42555561\d13=-156.27626081\d14=-42.02290789\d15=-215.9959346\d16=28.93285651\\Version=IA64L-G03RevD.01\HF=-541.8274449\S2=0.768309\S2-1=0.\S2A=0.750073\RMSD=8.586e-09\RMSF=1.595e-05\Thermal=0.\Dipole=-0.5501021,-0.960589,-0.5156031\PG=C01 [X(C5H12N1Si1)]\\@

7-*endo* product
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UWILLE\27-May-2006\0\\#BHANDHLYP/6-311G** SCF=VERYTIGHT OPT=(Z-MATRIX,CALCFC)OPTCYC=700 FREQ=NORAMAN\\geom and freq\\0,2\C,-1.1070855717,-1.4870011674,0.1148961134\C,0.3339374257,-1.5949846292,-0.3953561084\Si,1.5343785596,-0.3119721971,0.2479033801\N,1.0512705037,1.2623244662,-0.2856918089\C,-0.2148006624,1.8268511088,-0.1792898218\C,-1.3321956673,1.0822921454,0.4616779805\C,-1.844917843,-0.1970867003,-

0.2403582335\H,1.7423064099,1.8665007205,-0.6831384768\H,-0.4265399764,2.6558381476,-0.8320798462\H,-2.1641555286,1.7753949997,0.545099786\H,-1.0661596776,0.8194113788,1.4895802775\H,-2.8877376101,-0.3324341372,0.0388924007\H,-1.8329762005,-0.0466791466,-1.3184993704\H,-1.6788001112,-2.324330237,-0.2801523112\H,-1.1166964364,-1.6042349345,1.1984429316\H,0.7321823653,-2.5759523585,-0.136577233\H,0.3444288585,-1.5399892995,-1.4835508951\H,2.8908355649,-0.5133033319,-0.3023165711\H,1.6134928935,-0.4293068504,1.7240750671\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-541.8869609\S2=0.755534\S2-1=0.\S2A=0.750022\RMSD=5.036e-09\RMSF=7.698e-06\Dipole=-0.0606654,-0.0135901,-0.2854713\PG=C01 [X(C5H12N1Si1)]\\@

Cyclization of *Z*-1c:

<u>*Z*-1c</u>

1\1\GINC-AC31\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\02-Jul-2006\1\\# BHandHLYP/6-311G** scf=(qc,direct) freq=noraman opt=(Z-matrix,readFC,MaxCycle=500) geom=checkpoint guess=check\\single-point\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,4,B7,3,A6,2,D5,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\H,2,B10,1,A9,3,D8,0\H,2,B11,1,A10,3,D9,0\H,1,B12,2,A11,3,D10,0\N,5,B13,4,A12,3,D11,0\H,5,B14,4,A13,3,D12,0\Si,1,B15,2,A14,3,D13,0\H,16,B16,1,A15,2,D14,0\H,16,B17,1,A16,2,D15,0\H,1,B18,2,A17,3,D16,0\\B1=1.52765817\B2=1.52394745\B3=1.51892527\B4=1.50307829\B5=1.08738751\B6=1.09061053\B7=1.09062944\B8=1.08912002\B9=1.08916422\B10=1.08892204\B11=1.0891132\B12=1.09097023\B13=1.25579161\B14=1.8794667\B15=1.88682211\B16=1.48172896\B17=1.48045722\B18=1.08850083\A1=113.00855093\A2=112.79911001\A3=115.84110835\A4=114.48197936\A5=110.18312515\A6=110.1951364\A7=109.02899627\A8=109.01010956\A9=109.63102209\A10=109.69807099\A11=109.86361814\A12=128.84804495\A13=98.7479189\A14=114.72855042\A15=111.37788201\A16=111.35123738\A17=110.10636531\D1=-179.63043019\D2=-180.00346366\D3=179.98776462\D4=57.78159473\D5=-57.76972463\D6=58.29866999\D7=-57.57073401\D8=-121.93285382\D9=121.93460444\D10=-57.37055159\D11=-0.0201033\D12=-0.01324643\D13=-178.38546418\D14=57.12871883\D15=179.97128986\D16=59.10208766\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8365847\S2=0.751608\S2-1=0.\S2A=0.750001\RMSD=0.000e+00\RMSF=2.357e-05\Thermal=0.\Dipole=-0.7190478,-0.0627517,-0.1692212\PG=C01 [X(C5H12N1Si1)]\\@

<u>6-*exo* transition state</u>

1\1\GINC-AC50\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\13-Jul-2006\1\\# BHandHLYP/6-311G** scf=(qc,direct) opt=(TS,NoEigentest,calcFC,MaxCycle=500,Z-matrix) freq=noraman\\geom%freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,5,B7,4,A6,3,D5,0\H,5,B8,4,A7,3,D6,0\H,6,B9,5,A8,4,D7,0\H,6,B10,5,A9,4,D8,0\H,1,B11,6,A10,5,D9,0\H,1,B12,6,A11,5,D10,0\H,2,B13,1,A12,6,D11,0\H,2,B14,1,A13,6,D12,0\H,3,B15,2,A14,1,D13,0\H,3,B16,2,A15,1,D14,0\N,4,B17,3,A16,2,D15,0\H,18,B18,4,A17,3,D16,0\\B1=1.53094221\B2=1.88419164\B3=2.67739062\B4=1.51488379\B5=1.53091832\B6=1.08557696\B7=1.09044268\B8=1.08878954\B9=1.08668879\B10=1.0900901\B11=1.08786052\B12=1.08964075\B13=1.08931628\B14=1.08902615\B15=1.47946685\B16=1.48116819\B17=1.28332994\B18=1.0142483\A1=114.12886616\A2=97.55394585\A3=95.66137189\A4=117.37683664\A5=86.60571918\A6=105.04843485\A7=109.51698058\A8=107.37575699\A9=109.28956541\A10=108.01048795\A11=108.83495823\A12=109.72555699\A13=109.60012395\A14=112.21686892\A15=111.60507992\A16=103.32917774\A17=110.28963977\D1=-42.38135292\D2=41.36384669\D3=-58.23931501\D4=-74.02136814\D5=-178.03259929\D6=68.69697181\D7=-156.33716457\D8=-42.07905897\D9=164.38858934\D10=49.93353194\D11=-176.42239203\D12=-60.25891515\D13=-170.26552128\D14=65.98079559\D15=169.6544399\D16=-93.41491225\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8203629\S2=0.793128\S2-1=0.\S2A=0.750216\RMSD=0.000e+00\RMSF=1.950e-05\Thermal=0.\Dipole=-0.892688,0.2681059,-0.7838435\PG=C01 [X(C5H12N1Si1)]\\@

<u>6-*exo* product</u>

1\1\GINC-AC19\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\01-Jul-2006\0\\# BHandHLYP/6-311G** scf=(qc,direct) freq=noraman opt=(Z-matrix,readFC,MaxCycle=500) geom=checkpoint guess=check\\single-point\\0,2\C,0.0580390654,0.0138128512,-0.0177830002\C,0.0587399502,0.0361425255,1.5165802497\Si,1.8028022596,-0.0903999421,2.2049049019\C,2.6164998674,-1.4708090983,1.1586595039\C,2.2672951502,-1.2634956547,-0.3224086813\C,0.7681051945,-1.2010734393,-0.6142492478\H,2.1479367564,-2.3898267183,1.5185101428\H,2.7126394792,-2.0731308866,-0.8974753075\H,2.7390534043,-0.3436863987,-0.6723289674\H,0.6253194482,-1.1969845798,-1.691763652\H,0.2927120946,-2.1116490732,-0.2490633539\H,-0.9669990671,0.0375240163,-0.380356456\H,0.5328719812,0.9188738373,-0.3959371975\H,-0.4323920647,0.933310769,1.8856679525\H,-0.5199528585,-0.806461053,1.8936137134\H,1.8239656277,-0.4221519752,3.641848383\H,2.5468364227,1.169735861,1.9844939897\N,3.9946248671,-1.5106820134,1.4883496364\H,4.4855927003,-0.9004908273,0.8400041035\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8579985\S2=0.756294\S2-1=0.\S2A=0.750028\RMSD=0.000e+00\RMSF=3.965e-06\Thermal=0.\Dipole=-0.7389325,0.3020377,-0.6546212\PG=C01 [X(C5H12N1Si1)]\\@

7-*endo* transition state

1\1\GINC-AC18\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\01-Jul-2006\0\\# BHandHLYP/6-311G** scf=(qc,direct) freq=noraman opt=(TS,NoEigentest,Z-matrix,calcFC,MaxCycle=500)\\single-point\\0,2\C,0.5580146934,-1.5544006545,-0.3753557975\C,-0.7094585201,-1.2871258932,0.46347464\Si,-1.9382519375,0.0223182449,-0.1501710762\N,-0.3216687597,1.8698811771,-0.1398757599\C,0.7176897054,1.4019266022,0.4503638661\C,1.8564793684,0.6952800229,-0.2049688317\C,1.8200065173,-0.8139127548,0.0766408124\H,-0.1958954275,1.8733861308,-1.1436375294\H,0.6953823194,1.3871379016,1.5342964002\H,2.8013910747,1.0934858784,0.1602149853\H,1.8236170978,0.8719867254,-1.2785040233\H,2.6819513018,-1.2612647931,-0.4133805283\H,1.9596224174,-0.9796170754,1.1440407555\H,0.7835524194,-2.6166907717,-0.3263293931\H,0.3754239557,-1.345032291,-1.4292915499\H,-1.2900868738,-2.2059533834,0.5258387172\H,-0.4300146654,-1.0571887496,1.4893534313\H,-2.8035807722,0.4525160189,0.968512629\H,-2.8047019144,-0.6056543355,-1.1915087486\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8215443\S2=0.780642\S2-1=0.\S2A=0.750135\RMSD=0.000e+00\RMSF=6.957e-06\Thermal=0.\Dipole=1.1146127,-0.4040545,-0.1177343\PG=C01 [X(C5H12N1Si1)]\\@

7-*endo* product

1\1\GINC-AC43\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\19-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\C,1,B6,2,A5,3,D4,0\H,4,B7,3,A6,2,D5,0\H,5,B8,4,A7,3,D6,0\H,6,B9,5,A8,4,D7,0\H,6,B10,5,A9,4,D8,0\H,7,B11,1,A10,2,D9,0\H,7,B12,1,A11,2,D10,0\H,1,B13,7,A12,6,D11,0\H,1,B14,7,A13,6,D12,0\H,2,B15,1,A14,7,D13,0\H,2,B16,1,A15,7,D14,0\H,3,B17,2,A16,1,D15,0\H,3,B18,2,A17,1,D16,0\\B1=1.54077897\B2=1.88374594\B3=1.73833011\B4=1.40188327\B5=1.49124021\B6=1.53312267\B7=1.00406965\B8=1.08016811\B9=1.08801873\B10=1.09082735\B11=1.08872616\B12=1.08947998\B13=1.08768799\B14=1.09024085\B15=1.08947246\B16=1.08888064\B17=1.47782439\B18=1.47966898\A1=115.3125774\A2=108.96724305\A3=116.80950509\A4=119.35308771\A5=115.78418608\A6=116.00504765\A7=115.14192983\A8=110.04084172\A9=109.23391927\A10=108.13787445\A11=108.62311732\A12=107.10685974\A13=109.43351161\A14=109.32282125\A15=109.17888456\A16=109.75701434\A17=111.26327126\D1=-30.55574099\D2=-39.37041298\D3=90.93306573\D4=78.92320169\D5=97.8184457\D6=-59.53102224\D7=159.36467425\D8=42.63064018\D9=161.62030048\D10=46.95172374\D11=162.6999242\D12=48.81293444\D13=-159.73113265\D14=-44.75856954\D15=-152.41144648\D16=86.82090474\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8782656\S2=0.755381\S2-1=0.\S2A=0.750021\RMSD=0.000e+00\RMSF=5.675e-05\Thermal=0.\Dipole=-0.3950364,0.2125467,-0.4275087\PG=C01 [X(C5H12N1Si1)]\\@

Cyclization of *E*-2b:

***E*-2b**

1\1\GINC-AC22\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\14-Jul-2006\1\\# BHandHLYP/6-311G** opt=(Z-matrix,readFC,MaxCycle=500) freq=noraman scf=(qc,direct) geom=checkpoint guess=check\\geom & freq\\0,2\Si\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,4,B7,3,A6,2,D5,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\H,2,B10,1,A9,3,D8,0\H,2,B11,1,A10,3,D9,0\H,1,B12,2,A11,3,D10,0\H,1,B13,2,A12,3,D11,0\N,5,B14,4,A13,3,D12,0\C,15,B15,5,A14,4,D13,0\H,16,B16,15,A15,5,D14,0\H,16,B17,15,A16,5,D15,0\H,16,B18,15,A17,5,D16,0\\B1=1.88599099\B2=1.52804722\B3=1.51995977\B4=1.49647619\B5=1.09462259\B6=1.09125475\B7=1.09117438\B8=1.08647632\B9=1.08612204\B10=1.0888093\B11=1.09135595\B12=1.48162656\B13=1.48155724\B14=1.25148242\B15=1.44069877\B16=1.08609263\B17=1.09244998\B18=1.08607909\A1=114.48675752\A2=112.48285592\A3=114.83196782\A4=115.57568252\A5=110.28039207\A6=110.24094301\A7=110.41907543\A8=110.37628606\A9=108.25296179\A10=107.17507396\A11=111.53664757\A12=111.33311401\A13=123.08982564\A14=118.49517123\A15=109.23443113\A16=113.45178693\A17=109.22968524\D1=-177.70278164\D2=-179.9024337\D3=-179.92018942\D4=-57.67838522\D5=57.91770019\D6=-55.90757994\D7=60.40008954\D8=123.57398334\D9=-122.43810666\D10=57.56917395\D11=-179.75456237\D12=0.07176866\D13=-179.97816613\D14=-121.60665128\D15=0.05928229\D16=121.71678642\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8338993\S2=0.751609\S2-1=0.\S2A=0.750001\RMSD=0.000e+00\RMSF=9.939e-06\Thermal=0.\Dipole=-0.0773119,0.0321723,0.8740211\PG=C01 [X(C5H12N1Si1)]\\@

5-*exo* transition state

1\1\GINC-AC24\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\14-Jul-2006\1\\# BHandHLYP/6-311G** opt=(TS,NoEigentest,Z-matrix,calcFC,MaxCycle=500) freq=noraman scf=(qc,direct)\\geom & freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\H,1,B5,5,A4,4,D3,0\H,1,B6,5,A5,4,D4,0\H,5,B7,4,A6,1,D5,0\H,5,B8,4,A7,1,D6,0\N,4,B9,1,A8,5,D7,0\H,4,B10,1,A9,5,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\H,2,B13,1,A12,5,D11,0\H,2,B14,1,A13,5,D12,0\C,10,B15,4,A14,1,D13,0\H,16,B16,10,A15,4,D14,0\H,16,B17,10,A16,4,D15,0\H,16,B18,10,A17,4,D16,0\\B1=1.53214712\B2=1.8860618\B3=2.5210483\B4=1.51178735\B5=1.08689171\B6=1.08501636\B7=1.08803348\B8=1.08825448\B9=1.2880211\B10=1.0894823\B11=1.48416464\B12=1.47702638\B13=1.08702223\B14=1.08860989\B15=1.43640132\B16=1.08617853\B17=1.08866609\B18=1.09218585\A1

=111.03571223\A2=94.51829714\A3=34.06072776\A4=110.05146134\A5=108.17437213\A6=109.29808212\A7=107
.69537722\A8=96.74529001\A9=141.96425629\A10=111.78940906\A11=114.18099047\A12=111.12525033\A13=10
9.78986403\A14=117.56785767\A15=109.20407645\A16=109.39393148\A17=113.70776732\D1=12.93969256\D2=1
21.12056858\D3=171.89903608\D4=54.9607394\D5=-122.56881873\D6=121.54677542\D7=134.71069596\D8=-
55.77093791\D9=-146.51554994\D10=89.02424141\D11=167.3356178\D12=-
74.85496694\D13=160.56855637\D14=131.09468076\D15=-112.33381459\D16=9.20533825\\Version=IA64L-
G03RevD.01\State=2-A\HF=-541.822715\S2=0.798863\S2-1=0.\S2A=0.750271\RMSD=0.000e+00\RMSF=4.034e-
05\Thermal=0.\Dipole=0.0336695,-0.4429271,-0.0778049\PG=C01 [X(C5H12N1Si1)]\\@

5-*exo* product
1\1\GINC-AC11\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\18-Sep-2006\1\\# BHandHLYP/6-
311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) scf=(qc,direct)
freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\H,1,B5,5,A4,4,D3,0\
H,1,B6,5,A5,4,D4,0\H,5,B7,4,A6,1,D5,0\H,5,B8,4,A7,1,D6,0\N,4,B9,1,A8,5,D7,0\H,4,B10,1,A9,5,D8,0\H,3,B11,2,A1
0,1,D9,0\H,3,B12,2,A11,1,D10,0\H,2,B13,1,A12,5,D11,0\H,2,B14,1,A13,5,D12,0\C,10,B15,4,A14,1,D13,0\H,16,B16,
10,A15,4,D14,0\H,16,B17,10,A16,4,D15,0\H,16,B18,10,A17,4,D16,0\\B1=1.54060752\B2=1.886627\B3=2.50036781\
B4=1.53973503\B5=1.08635696\B6=1.08571784\B7=1.08976857\B8=1.08612859\B9=1.419968\B10=1.09273067\B1
1=1.48023491\B12=1.47630532\B13=1.08457403\B14=1.08753332\B15=1.43255111\B16=1.08365576\B17=1.09316
596\B18=1.09301244\A1=103.79409372\A2
=85.52062635\A3=35.28056388\A4=111.18573117\A5=108.32951907\A6=108.8338805\A7=110.13018907\A8=97.6
3577437\A9=143.55931201\A10=113.16996306\A11=115.39082555\A12=112.26182845\A13=110.42433778\A14=11
3.57068737\A15=110.36042062\A16=111.56767586\A17=110.87556066\D1=6.93325251\D2=131.4382658\D3=-
175.35785214\D4=66.89699838\D5=-119.68010772\D6=122.85411522\D7=115.2404433\D8=-33.02207618\D9=-
125.54955072\D10=109.0302845\D11=
157.77697329\D12=-82.75866646\D13=170.69417663\D14=180.97140487\D15=-
58.46407009\D16=60.43942184\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8523123\S2=0.756827\S2-
1=0.\S2A=0.750035\RMSD=0.000e+00\RMSF=1.318e-05\Thermal=0.\Dipole=0.1509409,-
0.3684658,0.1614789\PG=C01 [X(C5H12N1Si1)]\\@

6-*endo* transition state
1\1\GINC-AC39\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\24-Jul-2006\1\\# BHandHLYP/6-
311G** opt=(TS,NoEigentest,calcFC,MaxCycle=500,z-matrix) freq=noraman scf=(qc,direct)\\geom &
freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2
,B7,1,A6,6,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11
,3,D10,0\H,3,B13,2,A12,1,D11,0\H,3,B14,2,A13,1,D12,0\C,4,B15,3,A14,2,D13,0\H,16,B16,4,A15,3,D14,0\H,16,B17,
4,A16,3,D15,0\H,16,B18,4,A17,3,D16,0\\B1=1.53151902\B2=1.89697903\B3=2.13750549\B4=1.27551399\B5=1.494
75287\B6=1.08628419\B7=1.08859708\B8=1.08786349\B9=1.08883359\B10=1.08679584\B11=1.09242674\B12=1.0
8654173\B13=1.4820287\B14=1.51487187\B15=1.45355295\B16=1.08560758\B17=1.08670678\B18=1.08238722\A1
=112.88976364\A2=89.8412174\A3=124.51602826\A4=123.70166803\A5=109.40267399\A6=109.51026112\A7=110
.37445241\A8=109.97374452\A9=108.22379791\A10=107.1455912\A11=119.17814681\A12=112.69478884\A13=10
4.41845086\A14=114.61361941\A15=108.77078327\A16=111.85820082\A17=109.73286918\D1=-
49.47820025\D2=31.78916688\D3=-26.10703695\D4=-168.7453009\D5=-52.39702477\D6=-168.5283711\D7=-
51.91293913\D8=-202.83998712\D9=-89.17418016\D10=154.41736072\D11=-
139.95503616\D12=107.26991377\D13=191.76771581\D14=91.34439682\D15=-148.03334741\D16=-
26.76729042\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8264191\S2=0.767517\S2-
1=0.\S2A=0.750083\RMSD=0.000e+00\RMSF=2.506e-05\Thermal=0.\Dipole=0.1238799,-1.0358693,-
1.2173628\PG=C01 [X(C5H12N1Si1)]\\@

6-*endo* product
1\1\GINC-AC45\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\21-Jul-2006\1\\# BHandHLYP/6-
311G** opt=(Z-matrix,readFC,MaxCycle=500) geom=checkpoint guess=check freq=noraman scf=(qc,direct)\\geom &
freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2
,B7,1,A6,6,D5,0\H,1,B8,6,A7,5,D6,0\H,1,B9,6,A8,5,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11
,3,D10,0\H,3,B13,2,A12,1,D11,0\H,3,B14,2,A13,1,D12,0\C,4,B15,3,A14,2,D13,0\H,16,B16,4,A15,3,D14,0\H,16,B17,
4,A16,3,D15,0\H,16,B18,4,A17,3,D16,0\\B1=1.5337853\B2=1.86819951\B3=1.74078626\B4=1.39343016\B5=1.4935
593
3\B6=1.08726714\B7=1.08859891\B8=1.087338\B9=1.0887815\B10=1.08648315\B11=1.09745899\B12=1.07837421\
B13=1.47775874\B14=1.48501198\B15=1.44919648\B16=1.08730789\B17=1.09030653\B18=1.08540197\A1=110.18
305384\A2=105.26340691\A3=120.49132602\A4=120.29252789\A5=110.87874898\A6=109.58396819\A7=109.2822
4552\A8=108.98372204\A9=108.12207867\A10=110.32482088\A11=114.84495978\A12=114.00377463\A13=110.21
908754\A14=119.77932754\A15=110.26454247\A16=112.18365679\A17=110.14975105\D1=-
38.37524881\D2=27.89632364\D3=-34.83177158\D4=-181.00529163\D5=-
63.39952931\D6=175.52948537\D7=59.31937172\D8=172.44658131\D9=-71.93232735\D10=174.58036291\D11=-

157.02712088\D12=82.46289146\D13=184.55097904\D14=147.90783615\D15=-91.40237484\D16=29.19148912\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8793669\S2=0.75565\S2-1=0.\S2A=0.750023\RMSD=0.000e+00\RMSF=3.741e-05\Thermal=0.\Dipole=-0.020401,-0.132641,0.0159976\PG=C01 [X(C5H12N1Si1)]\\@

Cyclization of *E*-3b:

***E*-3b**

1\1\GINC-AC45\FOpt\UBHandHLYP\6-311G(d,p)\C6H14N1Si1(2)\UXW563\26-Jul-2006\1\\# BHandHLYP/6-311G** opt=(Z-matrix,readFC,MaxCycle=500) geom=checkpoint guess=check freq=noraman scf=verytight\\geom & freq\\0,2\Si\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,4,B7,3,A6,2,D5,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\H,2,B10,1,A9,3,D8,0\H,2,B11,1,A10,3,D9,0\N,5,B12,4,A11,3,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\H,14,B16,1,A15,2,D14,0\C,1,B17,14,A16,2,D15,0\H,18,B18,1,A17,14,D16,0\H,18,B19,1,A18,14,D17,0\H,18,B20,1,A19,14,D18,0\H,13,B21,5,A20,4,D19,0\\B1=1.89111422\B2=1.52777189\B3=1.51994806\B4=1.49628194\B5=1.09143378\B6=1.09125519\B7=1.09144922\B8=1.08616986\B9=1.08646899\B10=1.08969176\B11=1.09332776\B12=1.25644041\B13=1.88305894\B14=1.08600385\B15=1.08541801\B16=1.08983605\B17=1.88381778\B18=1.08596454\B19=1.08596386\B20=1.08967288\B21=1.01053424\A1=115.31992113\A2=112.68299453\A3=114.88860572\A4=114.91001942\A5=110.35048918\A6=110.39030116\A7=110.5113949\A8=110.35573513\A9=108.04435122\A10=107.29534105\A11=122.51795587\A12=110.9617967\A13=111.02306365\A14=111.65647871\A15=110.55683947\A16=110.19336236\A17=111.43007343\A18=111.30021015\A19=110.59927543\A20=111.10991324\D1=179.48849094\D2=179.18394538\D3=179.36153492\D4=-58.60157941\D5=57.04161656\D6=-58.69091667\D7=57.58933797\D8=123.61497777\D9=-122.7436336\D10=-0.69842038\D11=57.23343056\D12=178.692101\D13=-60.98186236\D14=59.10752729\D15=-121.70787931\D16=-179.38882912\D17=-59.0206738\D18=60.70503011\D19=-179.94914472\\Version=IA64L-G03RevD.01\State=2-A\HF=-581.16224\S2=0.751504\S2-1=0.\S2A=0.750001\RMSD=6.411e-09\RMSF=1.003e-05\Thermal=0.\Dipole=-0.3695972,-0.1509332,0.763391\PG=C01 [X(C6H14N1Si1)]\\@

5-*exo* transition state

1\1\GINC-AC30\FTS\UBHandHLYP\6-311G(d,p)\C6H14N1Si1(2)\UXW563\25-Jul-2006\1\\# BHandHLYP/6-311G** opt=(ts,noeigentest,Z-matrix,calcFC,MaxCycle=500) freq=noraman scf=(qc,direct)\\geom & freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\H,1,B5,5,A4,4,D3,0\H,1,B6,5,A5,4,D4,0\H,5,B7,4,A6,1,D5,0\H,5,B8,4,A7,1,D6,0\N,4,B9,1,A8,5,D7,0\H,4,B10,1,A9,5,D8,0\H,2,B11,1,A10,5,D9,0\H,2,B12,1,A11,5,D10,0\C,3,B13,2,A12,1,D11,0\H,14,B14,3,A13,2,D12,0\H,14,B15,3,A14,2,D13,0\H,14,B16,3,A15,2,D14,0\C,3,B17,2,A16,1,D15,0\H,18,B18,3,A17,2,D16,0\H,18,B19,3,A18,2,D17,0\H,18,B20,3,A19,2,D18,0\H,10,B21,4,A20,1,D19,0\\B1=1.53231569\B2=1.88824072\B3=2.52349932\B4=1.51252721\B5=1.08705601\B6=1.0851993\B7=1.08819642\B8=1.08864917\B9=1.29245364\B10=1.08612859\B11=1.08869244\B12=1.08949157\B13=1.87454029\B14=1.08850915\B15=1.08662214\B16=1.08485143\B17=1.88408708\B18=1.08606976\B19=1.08965114\B20=1.08586351\B21=1.01086457\A1=111.45896175\A2=95.21301102\A3=33.99071712\A4=109.98954573\A5=108.15104166\A6=109.52505801\A7=107.42170356\A8=96.52619836\A9=140.7258463\A10=110.88503974\A11=109.5119279\A12=113.6359788\A13=110.83078486\A14=111.33473985\A15=110.25289322\A16=111.5679449\A17=111.37915376\A18=110.51150857\A19=111.49427516\A20=110.41859239\D1=13.61373775\D2=119.88181272\D3=170.33657918\D4=53.63899941\D5=-122.71710553\D6=121.37561917\D7=134.09069129\D8=-56.43939935\D9=168.49229533\D10=-74.23150942\D11=89.4252809\D12=62.08078233\D13=-178.16177996\D14=-58.02319953\D15=-144.57583465\D16=176.53914744\D17=-63.92191867\D18=55.84123797\D19=161.10098531\\Version=IA64L-G03RevD.01\State=2-A\HF=-581.150884\S2=0.79219\S2-1=0.\S2A=0.750188\RMSD=0.000e+00\RMSF=2.762e-05\Thermal=0.\Dipole=0.0825741,-0.516161,0.4965997\PG=C01 [X(C6H14N1Si1)]\\@

5-*exo* product

1\1\GINC-AC58\FOpt\UBHandHLYP\6-311G(d,p)\C6H14N1Si1(2)\UXW563\18-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\H,1,B5,5,A4,4,D3,0\H,1,B6,5,A5,4,D4,0\H,5,B7,4,A6,1,D5,0\H,5,B8,4,A7,1,D6,0\N,4,B9,1,A8,5,D7,0\H,4,B10,1,A9,5,D8,0\H,2,B11,1,A10,5,D9,0\H,2,B12,1,A11,5,D10,0\C,3,B13,2,A12,1,D11,0\H,14,B14,3,A13,2,D12,0\H,14,B15,3,A14,2,D13,0\H,14,B16,3,A15,2,D14,0\C,3,B17,2,A16,1,D15,0\H,18,B18,3,A17,2,D16,0\H,18,B19,3,A18,2,D17,0\H,18,B20,3,A19,2,D18,0\H,10,B21,4,A20,1,D19,0\\B1=1.5402252\B2=1.88998365\B3=2.49377627\B4=1.53777302\B5=1.08655857\B6=1.08596806\B7=1.09002209\B8=1.08648459\B9=1.4168853\B10=1.09196925\B11=1.08572299\B12=1.08857759\B13=1.87197218\B14=1.08720997\B15=1.08719139\B16=1.08534257\B17=1.87659778\B18=1.08691135\B19=1.08764151\B20=1.08660507\B21=1.01452894\A1=104.53099361\A2=85.41777014\A3=35.47166427\A4=111.26312971\A5=108.24553247\A6=109.12012451\A7=110.27665817\A8=97.27195398\A9=143.78725805\A10=111.99571151\A11=110.26720222\A12=114.95986538\A13=110.68879624\A14=111.4140115\A15=110.95980948\A16=112.65801746\A17=111.48591957\A18=110.73065075\A19=111.36032199\A20=108.25669067\D1=6.18522745\D2=131.22117396\D3=-175.84719695\D4=66.62975655\D5=-119.62800888\D6=122.77256907\D7=115.99392014\D8=-33.80984455\D9=157.43079113\D10=-

83.71951762\D11=110.29222323\D12=67.27872388\D13=186.77429047\D14=-52.89037285\D15=-122.63541465\D16=-185.91854319\D17=-66.19017076\D18=53.51993211\D19=165.09155703\\Version=IA64L-G03RevD.01\State=2-A\HF=-581.1806429\S2=0.756506\S2-1=0.\S2A=0.75003\RMSD=0.000e+00\RMSF=4.115e-05\Thermal=0.\Dipole=0.2529062,-0.4301048,0.6037473\PG=C01 [X(C6H14N1Si1)]\\@

6-*endo* transition state

1\1\GINC-AC6\FTS\UBHandHLYP\6-311G(d,p)\C6H14N1Si1(2)\UXW563\21-Jul-2006\1\\# BHandHLYP/6-311G** opt=(TS,NoEigentest,Z-matrix,calcFC,MaxCycle=500) freq=noraman scf=(qc,direct)\\geom freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,6,A7,5,D6,0\H,1,B9,6,A8,5,D7,0\H,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11,3,D10,0\H,4,B13,12,2,D11,0\C,3,B14,2,A13,1,D12,0\H,15,B15,3,A14,2,D13,0\H,15,B16,3,2,D14,0\H,15,B17,3,A16,2,D15,0\C,3,B18,2,A17,1,D16,0\H,19,B19,3,A18,2,D17,0\H,19,B20,3,A19,2,D18,0\H,19,B21,3,A20,2,D19,0\\B1=1.53287668\B2=1.90438378\B3=2.40783246\B4=1.26977876\B5=1.49755104\B6=1.08915341\B7=1.08961934\B8=1.08790383\B9=1.08936399\B10=1.08620655\B11=1.09017918\B12=1.08660584\B13=1.00949865\B14=1.8842048\B15=1.08680663\B16=1.08928608\B17=1.08488753\B18=1.90599082\B19=1.09116872\B20=1.08644628\B21=1.08688736\A1=116.76277728\A2=84.44240844\A3=121.67783579\A4=120.94254783\A5=108.65774471\A6=109.03817996\A7=107.03617289\A8=108.99360069\A9=108.93612286\A10=108.29877556\A11=121.41974123\A12=112.38213882\A13=110.04335173\A14=111.49853569\A15=110.46642174\A16=111.05381102\A17=106.4141247\A18=110.83404146\A19=111.32231647\A20=111.37189781\D1=-48.35181144\D2=36.43799367\D3=-39.65664342\D4=-164.21978855\D5=-49.0712855\D6=174.95812554\D7=60.79184242\D8=-188.60423073\D9=-73.05723022\D10=138.34967093\D11=174.84669804\D12=-139.4379307\D13=-174.41482642\D14=-55.19663322\D15=64.73314963\D16=105.09858425\D17=59.89584439\D18=179.90299685\D19=-60.01841504\\Version=IA64L-G03RevD.01\State=2-A\HF=-581.1531172\S2=0.765152\S2-1=0.\S2A=0.750051\RMSD=8.770e-09\RMSF=1.657e-05\Thermal=0.\Dipole=0.0640924,-0.5125673,-0.9618837\PG=C01 [X(C6H14N1Si1)]\\@

6-*endo* product

1\1\GINC-AC56\FOpt\UBHandHLYP\6-311G(d,p)\C6H14N1Si1(2)\UXW563\20-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,6,A7,5,D6,0\H,1,B9,6,A8,5,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11,3,D10,0\H,4,B13,3,A12,2,D11,0\C,3,B14,2,A13,1,D12,0\H,15,B15,3,A14,2,D13,0\H,15,B16,3,A15,2,D14,0\H,15,B17,3,A16,2,D15,0\C,3,B18,2,A17,1,D16,0\H,19,B19,3,A18,2,D17,0\H,19,B20,3,A19,2,D18,0\H,19,B21,3,A20,2,D19,0\\B1=1.53494496\B2=1.87462716\B3=1.745131\B4=1.39743543\B5=1.49208314\B6=1.08817885\B7=1.08955389\B8=1.08767474\B9=1.08890337\B10=1.08674917\B11=1.09798107\B12=1.07737574\B13=1.00140537\B14=1.87013278\B15=1.08775717\B16=1.08744452\B17=1.08591036\B18=1.87613132\B19=1.08788183\B20=1.08752172\B21=1.08661994\A1=111.35602666\A2=102.78904867\A3=123.70510988\A4=118.9801718\A5=110.43690694\A6=109.19520638\A7=109.14246297\A8=108.8888266\A9=108.42963919\A10=110.35012579\A11=115.52856192\A12=119.43867259\A13=113.48154474\A14=111.29564706\A15=111.0178209\A16=111.20493561\A17=110.7114232\A18=111.20242131\A19=111.40909695\A20=111.07023629\D1=-37.29741412\D2=26.77362964\D3=-33.90615729\D4=-179.67331548\D5=-62.9950457\D6=175.18365398\D7=59.34136299\D8=171.34814633\D9=-72.82120496\D10=176.02119446\D11=185.02930615\D12=-154.95619948\D13=-185.98403024\D14=-66.63147877\D15=53.77765546\D16=82.2361207\D17=64.43554373\D18=184.31004325\D19=-55.78038776\\Version=IA64L-G03RevD.01\State=2-A\HF=-581.2186758\S2=0.755472\S2-1=0.\S2A=0.750022\RMSD=0.000e+00\RMSF=1.254e-05\Thermal=0.\Dipole=0.1514645,-0.0044938,0.2414314\PG=C01 [X(C6H14N1Si1)]\\@

Cyclization of *E*-4b:

***E*-4b**

1\1\GINC-AC28\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\31-Jul-2006\1\\# BHandHLYP/6-311G** scf=(qc,direct) opt=(calcFC,Z-matrix,MaxCycle=500) freq=noraman\\geom & freq\\0,2\Si\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,4,B5,3,A4,2,D3,0\H,4,B6,3,A5,2,D4,0\H,3,B7,2,A6,1,D5,0\H,3,B8,2,A7,1,D6,0\H,2,B9,1,A8,3,D7,0\H,2,B10,1,A9,3,D8,0\H,1,B11,2,A10,3,D9,0\H,1,B12,2,A11,3,D10,0\N,5,B13,4,A12,3,D11,0\C,5,B14,4,A13,3,D12,0\H,15,B15,5,A14,4,D13,0\H,15,B16,5,A15,4,D14,0\H,15,B17,5,A16,4,D15,0\H,14,B18,5,A17,4,D16,0\\B1=1.88547047\B2=1.52816588\B3=1.51936385\B4=1.50633913\B5=1.09100984\B6=1.09095442\B7=1.08606167\B8=1.08577094\B9=1.08893562\B10=1.09139252\B11=1.48157977\B12=1.48171627\B13=1.25916653\B14=1.50484826\B15=1.08706782\B16=1.0844082\B17=1.08705222\B18=1.0114251\A1=114.43738265\A2=112.39956749\A3=114.97387954\A4=110.0398562\A5=110.08197458\A6=110.45548361\A7=110.44304705\A8=108.19277839\A9=107.23381591\A10=111.59909416\A11=111.3223644\A12=119.62354283\A13=115.31659377\A14=110.47302348\A15=111.40062385\A16=110.49121434\A17=111.13201439\D1=-178.54988905\D2=-179.79598446\D3=-57.53468077\D4=57.85697144\D5=-56.73079197\D6=59.58963816\D7=123.51003559\D8=-122.52024143\D9=57.41230437\D10=-179.92066395\D11=0.35580682\D12=-179.6609152\D13=59.35611625\D14=-

179.77128739\D15=-58.87667685\D16=-180.03794232\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8460297\S2=0.751609\S2-1=0.\S2A=0.750001\RMSD=0.000e+00\RMSF=3.379e-05\Thermal=0.\Dipole=-0.2268923,0.0263154,1.1969093\PG=C01 [X(C5H12N1Si1)]\\@

5-*exo* transition state

1\1\GINC-AC33\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\28-Jul-2006\1\\# BHandHLYP/6-311G** opt=(ts,noeigentest,Z-matrix,calcFC,MaxCycle=500) freq=noraman scf=verytight\\geom & freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\H,1,B5,5,A4,4,D3,0\H,1,B6,5,A5,4,D4,0\H,5,B7,4,A6,1,D5,0\H,5,B8,4,A7,1,D6,0\N,4,B9,1,A8,5,D7,0\H,3,B10,2,A9,1,D8,0\H,3,B11,2,A10,1,D9,0\H,2,B12,1,A11,5,D10,0\H,2,B13,1,A12,5,D11,0\H,10,B14,4,A13,1,D12,0\C,4,B15,1,A14,5,D13,0\H,16,B16,4,A15,1,D14,0\H,16,B17,4,A16,1,D15,0\H,16,B18,4,A17,1,D16,0\\B1=1.53416491\B2=1.88605306\B3=2.52658225\B4=1.52084223\B5=1.0868003\B6=1.08384202\B7=1.08818345\B8=1.08956136\B9=1.30132767\B10=1.48676682\B11=1.47549016\B12=1.08646544\B13=1.08848525\B14=1.0119873\B15=1.51077997\B16=1.08973002\B17=1.08454696\B18=1.08392751\A1=110.52391447\A2=93.97778919\A3=33.89724464\A4=110.08272573\A5=108.24227583\A6=109.75957104\A7=106.99630994\A8=90.91794385\A9=111.20738441\A10=115.41227534\A11=111.26135692\A12=109.82578411\A13=110.48863583\A14=146.15751254\A15=108.7084931\A16=111.3029689\A17=112.25149916\D1=9.14381466\D2=121.45168792\D3=172.50881825\D4=55.25254472\D5=-123.13680186\D6=121.33529349\D7=139.85504006\D8=-139.39456052\D9=96.0371172\D10=164.06510511\D11=-77.97914133\D12=165.72677432\D13=-37.37777319\D14=91.94193205\D15=-149.20206553\D16=-27.07394536\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8298699\S2=0.794629\S2-1=0.\S2A=0.750227\RMSD=4.301e-09\RMSF=2.027e-05\Thermal=0.\Dipole=0.1797005,-0.6772461,-0.1374576\PG=C01 [X(C5H12N1Si1)]\\@

5-*exo* product

1\1\GINC-AC16\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\18-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,1,B5,5,A4,4,D3,0\H,1,B6,5,A5,4,D4,0\H,5,B7,4,A6,3,D5,0\H,5,B8,4,A7,3,D6,0\N,4,B9,3,A8,2,D7,0\H,3,B10,2,A9,1,D8,0\H,3,B11,2,A10,1,D9,0\H,2,B12,1,A11,5,D10,0\H,2,B13,1,A12,5,D11,0\H,10,B14,4,A13,3,D12,0\C,4,B15,3,A14,2,D13,0\H,16,B16,4,A15,3,D14,0\H,16,B17,4,A16,3,D15,0\H,16,B18,4,A17,3,D16,0\\B1=1.54212725\B2=1.88453444\B3=1.94228202\B4=1.54405242\B5=1.08627681\B6=1.08476118\B7=1.08981133\B8=1.0874798\B9=1.4197799\B10=1.48156368\B11=1.47619219\B12=1.08445706\B13=1.0874178\B14=1.01542671\B15=1.52605915\B16=1.0883414\B17=1.08726675\B18=1.0856723\A1=103.92989485\A2=96.1063101\A3=99.83117493\A4=111.11473575\A5=108.33083359\A6=109.04798775\A7=109.56528608\A8=103.13970076\A9=113.08367227\A10=116.04876558\A11=112.19580918\A12=110.48735427\A13=108.20213453\A14=115.49423151\A15=110.26455979\A16=111.34588841\A17=111.66420623\D1=-6.84427012\D2=-19.29068852\D3=-175.32477075\D4=66.86238437\D5=-78.24834787\D6=164.58019214\D7=92.9993118\D8=-122.08683428\D9=112.22341412\D10=156.23477974\D11=-84.32434306\D12=93.69170114\D13=-140.79124343\D14=177.00311372\D15=-63.39415403\D16=57.09495847\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8540491\S2=0.756876\S2-1=0.\S2A=0.750032\RMSD=0.000e+00\RMSF=2.342e-05\Thermal=0.\Dipole=0.1539168,-0.4735497,0.1954642\PG=C01 [X(C5H12N1Si1)]\\@

6-*endo* transition state

1\1\GINC-AC21\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\29-Jul-2006\1\\# BHandHLYP/6-311G** opt=(ts,noeigentest,Z-matrix,calcFC,MaxCycle=500) freq=noraman scf=verytight\\geom & freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,6,A7,5,D6,0\H,1,B9,6,A8,5,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,3,B12,2,A11,1,D10,0\H,3,B13,2,A12,1,D11,0\C,5,B14,4,A13,3,D12,0\H,15,B15,5,A14,4,D13,0\H,15,B16,5,A15,4,D14,0\H,15,B17,5,A16,4,D15,0\H,4,B18,3,A17,2,D16,0\\B1=1.53224284\B2=1.90202151\B3=2.22825212\B4=1.2717961\B5=1.50264968\B6=1.08667267\B7=1.08890419\B8=1.08801161\B9=1.08911357\B10=1.08693396\B11=1.09132425\B12=1.48132966\B13=1.51278174\B14=1.49633237\B15=1.08840479\B16=1.08406949\B17=1.08688786\B18=1.00954815\A1=114.87140472\A2=86.73405253\A3=128.63633549\A4=119.47547691\A5=108.82560896\A6=109.3487515\A7=106.98473258\A8=108.82579484\A9=108.74181601\A10=106.98368709\A11=112.22713168\A12=104.64053323\A13=123.41960992\A14=109.89810979\A15=111.96289485\A16=110.21909047\A17=112.64188745\D1=-46.14752402\D2=30.27636215\D3=-27.36978019\D4=-167.19356339\D5=-51.50049453\D6=178.13440277\D7=64.1005669\D8=160.20210081\D9=-85.78081228\D10=-133.25169611\D11=114.20878348\D12=152.73291769\D13=-114.66859076\D14=6.33859604\D15=-232.26817333\D16=-176.73287742\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8422241\S2=0.759494\S2-1=0.\S2A=0.750037\RMSD=6.255e-09\RMSF=2.361e-05\Thermal=0.\Dipole=0.1084615,-1.0823781,-1.7334399\PG=C01 [X(C5H12N1Si1)]\\@

6-*endo* product

1\1\GINC-AC42\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\22-Sep-2006\1\\# BHandHLYP/6-311G** opt=(calcfc,maxcycle=500,z-matrix) scf=verytight

freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\
H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,6,A7,5,D6,0\H,1,B9,6,A8,5,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A1
0,4,D9,0\H,3,B12,2,A11,1,D10,0\H,3,B13,2,A12,1,D11,0\C,5,B14,4,A13,3,D12,0\H,15,B15,5,A14,4,D13,0\H,15,B16,
5,A15,4,D14,0\H,15,B17,5,A16,4,D15,0\H,4,B18,3,A17,2,D16,0\\B1=1.53469838\B2=1.86762155\B3=1.73435008\B
4=1.40408431\B5=1.49703004\B6=1.08704817\B7=1.08853427\B8=1.0873104\B9=1.08901746\B10=1.08674793\B1
1=1.09905209\B12=1.47752454\B13=1.48421196\B14=1.4894853\B15=1.08820993\B16=1.09616438\B17=1.085204
35\B18=1.00192846\A1=109.64233733\A2=103.78610888\A3=123.70848353\A4=117.13866239\A5=110.68763984\
A6=109.63354576\A7=108.93379109\A8=108.93115384\A9=108.25128099\A10=109.55503971\A11=114.35561258\
A12=109.66871652\A13=115.68166608\A14=111.40928689\A15=111.90817182\A16=111.0729309\A17=119.325518
82\D1=-39.17440394\D2=29.78420274\D3=-34.92188759\D4=179.94419402\D5=-
62.40241362\D6=174.92007124\D7=59.16686293\D8=170.86060497\D9=-73.9949137\D10=-
157.66192648\D11=81.90631944\D12=178.24938725\D13=-48.05423864\D14=71.90098836\D15=-
168.05198014\D16=-172.58419182\\Version=IA64L-G03RevD.01\State=2-A\HF=-541.8950537\S2=0.755446\S2-
1=0.\S2A=0.750022\RMSD=7.019e-09\RMSF=2.934e-05\Thermal=0.\Dipole=0.021542,-0.1232908,-
0.0614638\PG=C01 [X(C5H12N1Si1)]\\@

Cyclization of *E*-5b:

***E*-5b**

1\1\GINC-AC27\FOpt\UBHandHLYP\6-311G(d,p)\C7H16N1Si1(2)\UXW563\28-Jul-2006\0\\# BHandHLYP/6-
311G** opt=(Z-matrix,calcFC,MaxCycle=500) freq=noraman scf=verytight\\geom &
freq\\0,2\Si,2.4118295506,0.2248671798,-0.4279276775\C,0.9780584468,-0.8917447206,0.0946442783\C,-
0.4152731005,-0.2880770344,-0.0733941807\C,-1.5217027284,-1.2383288985,0.3548250976\C,-2.9085943451,-
0.6907072975,0.2300862837\H,-3.7140217307,-1.3720697819,0.5227768375\H,-1.4710776875,-2.1617306099,-
0.2243734875\H,-1.3750683103,-1.5462504986,1.3915820449\H,-0.5037068101,0.6301021539,0.5001121998\H,-
0.5801192495,-0.0010041431,-1.1082877199\H,1.0525584191,-1.8226277976,-0.4668636717\H,1.1418552978,-
1.1618348417,1.1413655204\N,-3.1539014278,0.466955968,-0.1778266571\C,-4.5287914817,0.890210289,-
0.2559842491\H,-4.7573747127,1.1779088361,-1.2780546393\H,-5.2387573111,0.1231394638,0.0621700808\H,-
4.6670988051,1.7738137499,0.3603085801\C,2.375120192,1.8534873036,0.5172685466\H,3.2056221213,2.4911179
167,0.2288867306\H,1.456623631,2.4019970979,0.3339042185\H,2.4494106943,1.6752124782,1.5898964048\C,4.04
86709599,-0.6595846116,-0.133321625\H,4.0958497865,-1.5987346578,-0.67655766\H,4.8891993953,-
0.0496540693,-0.4508062975\H,4.1798012057,-0.8801754744,0.9256970417\\Version=IA64L-G03RevD.01\State=2-
A\HF=-620.4550124\S2=0.751505\S2-1=0.\S2A=0.750001\RMSD=9.444e-09\RMSF=6.949e-06\Thermal=0.\Dipole=-
0.3049064,-0.4673403,0.3698125\PG=C01 [X(C7H16N1Si1)]\\@

5-*exo* transition state

1\1\GINC-AC42\FTS\UBHandHLYP\6-311G(d,p)\C7H16N1Si1(2)\UXW563\24-Jul-2006\1\\# BHandHLYP/6-
311G** opt=(TS,NoEigentest,Z-matrix,calcFC,MaxCycle=500) freq=noraman scf=verytight\\geom &
freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\H,1,B5,5,A4,4,D3,0\H,1,B6,5,A5,4,D4,0\H,5
,B7,4,A6,1,D5,0\H,5,B8,4,A7,1,D6,0\N,4,B9,1,A8,5,D7,0\H,4,B10,1,A9,5,D8,0\H,2,B11,1,A10,5,D9,0\H,2,B12,1,A11
,5,D10,0\C,10,B13,4,A12,1,D11,0\H,14,B14,10,A13,4,D12,0\H,14,B15,10,A14,4,D13,0\H,14,B16,10,A15,4,D14,0\C,3
,B17,2,A16,1,D15,0\H,18,B18,3,A17,2,D16,0\H,18,B19,3,A18,2,D17,0\H,18,B20,3,A19,2,D18,0\C,3,B21,2,A20,1,D1
9,0\H,22,B22,3,A21,2,D20,0\H,22,B23,3,A22,2,D21,0\H,22,B24,3,A23,2,D22,0\\B1=1.53133574\B2=1.88788016\B3=
2.53212654\B4=1.51210657\B5=1.08725173\B6=1.08576968\B7=1.08826629\B8=1.08827663\B9=1.28719933\B10=
1.08937578\B11=1.08898126\B12=1.08947855\B13=1.43714192\B14=1.08674216\B15=1.08839835\B16=1.0926358
2\B17=1.87688839\B18=1.08878753\B19=1.08622747\B20=1.08510693\B21=1.88459987\B22=1.08604361\B23=1.0
8966663\B24=1.08588562\A1=111.24598679\A2=95.05067573\A3=33.69489621\A4=109.88237243\A5=108.270963
71\A6=109.15269318\A7=107.56533252\A8=98.87168797\A9=139.89438071\A10=110.89559425\A11=109.5142144
5\A12=117.26672528\A13=109.26012342\A14=109.81822775\A15=113.6626697\A16=112.34341763\A17=110.4940
1453\A18=111.65842051\A19=110.4439341\A20=111.56747146\A21=111.35093573\A22=110.5009578\A23=111.50
242449\D1=16.34623686\D2=120.28409932\D3=170.95597194\D4=54.34058512\D5=-
122.50324934\D6=121.77484869\D7=131.60876326\D8=-59.25959316\D9=170.35645281\D10=-
72.35305698\D11=160.83659729\D12=128.27801795\D13=-
115.00082379\D14=6.68542304\D15=87.56269596\D16=62.5253604\D17=-177.68985597\D18=-57.19688697\D19=-
147.7240803\D20=177.9354527\D21=-62.48040078\D22=57.29938997\\Version=IA64L-G03RevD.01\State=2-
A\HF=-620.4440747\S2=0.79608\S2-1=0.\S2A=0.750229\RMSD=2.738e-09\RMSF=4.273e-
05\Thermal=0.\Dipole=0.0452474,-0.3550997,0.3917843\PG=C01 [X(C7H16N1Si1)]\\@

5-*exo* product

1\1\GINC-AC47\FOpt\UBHandHLYP\6-311G(d,p)\C7H16N1Si1(2)\UXW563\20-Sep-2006\1\\# BHandHLYP/6-
311G** opt=(calcfc,maxcycle=500,z-matrix) scf=(qc,direct)
freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,1,B4,2,A3,3,D2,0\H,1,B5,5,A4,4,D3,0\
H,1,B6,5,A5,4,D4,0\H,5,B7,1,A6,2,D5,0\H,5,B8,1,A7,2,D6,0\N,4,B9,3,A8,2,D7,0\H,4,B10,3,A9,2,D8,0\H,2,B11,1,A1

0,5,D9,0\H,2,B12,1,A11,5,D10,0\C,10,B13,4,A12,3,D11,0\H,14,B14,10,A13,4,D12,0\H,14,B15,10,A14,4,D13,0\H,14,B16,10,A15,4,D14,0\C,3,B17,2,A16,1,D15,0\H,18,B18,3,A17,2,D16,0\H,18,B19,3,A18,2,D17,0\H,18,B20,3,A19,2,D18,0\C,3,B21,2,A20,1,D19,0\H,22,B22,3,A21,2,D20,0\H,22,B23,3,A22,2,D21,0\H,22,B24,3,A23,2,D22,0\\B1=1.53936314\B2=1.89076444\B3=1.93897936\B4=1.52854487\B5=1.08670768\B6=1.08593957\B7=1.09004017\B8=1.08646826\B9=1.41923112\B10=1.09388563\B11=1.08575412\B12=1.08869473\B13=1.43266446\B14=1.09342534\B15=1.08422456\B16=1.09283827\B17=1.87250375\B18=1.08740192\B19=1.08679345\B20=1.08546453\B21=1.87692914\B22=1.0868975\B23=1.08764537\B24=1.08671449\A1=104.50832549\A2=95.07163028\A3=108.45164165\A4=111.19550987\A5=108.2846179\A6=109.60499653\A7=111.7051224\A8=108.72613917\A9=111.3970213\A10=112.04562009\A11=110.18523591\A12=113.54283627\A13=109.91557157\A14=110.54850037\A15=112.54660131\A16=114.14608558\A17=110.3601836\A18=111.82640374\A19=110.93324768\A20=112.5572951\A21=111.43842912\A22=110.7427858\A23=111.39637855\D1=-8.46112595\D2=33.97328682\D3=-175.53677422\D4=66.91956546\D5=67.00381219\D6=-174.30676861\D7=98.33383448\D8=-136.45781587\D9=157.64522426\D10=-83.54068319\D11=99.40540982\D12=69.91696511\D13=-170.69205485\D14=-48.80327084\D15=110.22117347\D16=65.22528924\D17=-175.20183658\D18=-54.59230647\D19=-123.5504798\D20=175.23605099\D21=-65.0253519\D22=54.70135123\\Version=IA64L-G03RevD.01\State=2-A\HF=-620.4763687\S2=0.756732\S2-1=0.\S2A=0.750034\RMSD=0.000e+00\RMSF=2.608e-05\Thermal=0.\Dipole=0.2916122,-0.3488659,0.4274993\PG=C01 [X(C7H16N1Si1)]\\@

6-*endo* transition state

1\1\GINC-AC31\FTS\UBHandHLYP\6-311G(d,p)\C7H16N1Si1(2)\UXW563\25-Jul-2006\1\\# BHandHLYP/6-311G** opt=(TS,NoEigentest,z-matrix,calcFC,maxcycle=500) freq=noraman scf=(qc,direct)\\geom & freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,6,A7,5,D6,0\H,1,B9,6,A8,5,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11,3,D10,0\C,4,B13,3,A12,2,D11,0\H,14,B14,4,A13,3,D12,0\H,14,B15,4,A14,3,D13,0\H,14,B16,4,A15,3,D14,0\C,3,B17,2,A16,1,D15,0\H,18,B18,3,A17,2,D16,0\H,18,B19,3,A18,2,D17,0\H,18,B20,3,A19,2,D18,0\C,3,B21,2,A20,1,D19,0\H,22,B22,3,A21,2,D20,0\H,22,B23,3,A22,2,D21,0\H,22,B24,3,A23,2,D22,0\\B1=1.5310137\B2=1.89940878\B3=2.26808935\B4=1.27409287\B5=1.49672609\B6=1.08854805\B7=1.08965876\B8=1.08809594\B9=1.08922574\B10=1.08649119\B11=1.09155047\B12=1.08795052\B13=1.45176966\B14=1.08642004\B15=1.0882035\B16=1.08263498\B17=1.88669858\B18=1.08692851\B19=1.08891669\B20=1.08540723\B21=1.91178452\B22=1.09156102\B23=1.08657138\B24=1.08702348\A1=114.46413493\A2=87.78868727\A3=122.03347543\A4=122.9448043\A5=109.19280783\A6=109.20032964\A7=107.25765936\A8=109.09158463\A9=108.37832724\A10=107.94086238\A11=119.67956147\A12=114.61240357\A13=108.93359932\A14=112.32599864\A15=109.75589146\A16=110.27718735\A17=111.86783759\A18=109.9478091\A19=111.69229809\A20=105.75417741\A21=110.93180117\A22=111.36260594\A23=111.29259068\D1=-49.37102883\D2=34.6302015\D3=-33.68306167\D4=-166.37068091\D5=-50.64423363\D6=178.4562363\D7=64.09066866\D8=-194.89397523\D9=-80.33492145\D10=145.59084448\D11=186.7020935\D12=107.08125487\D13=-132.38562848\D14=-11.19194734\D15=-142.61502869\D16=185.32009124\D17=-55.82704514\D18=63.80065964\D19=103.16628893\D20=59.49949152\D21=-180.37934161\D22=-60.40226072\\Version=IA64L-G03RevD.01\State=2-A\HF=-620.4431183\S2=0.770219\S2-1=0.\S2A=0.750079\RMSD=0.000e+00\RMSF=2.410e-05\Thermal=0.\Dipole=0.1143944,-0.6808792,-0.8000353\PG=C01 [X(C7H16N1Si1)]\\@

6-*endo* product

1\1\GINC-AC49\FOpt\UBHandHLYP\6-311G(d,p)\C7H16N1Si1(2)\UXW563\24-Jul-2006\1\\# BhandHLYP/6-311G** opt=(Z-matrix,readFC,MaxCycle=500) geom=checkpoint guess=check freq=noraman scf=(qc,direct)\\geom & freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,6,A7,5,D6,0\H,1,B9,6,A8,5,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11,3,D10,0\C,4,B13,3,A12,2,D11,0\H,14,B14,4,A13,3,D12,0\H,14,B15,4,A14,3,D13,0\H,14,B16,4,A15,3,D14,0\C,3,B17,2,A16,1,D15,0\H,18,B18,3,A17,2,D16,0\H,18,B19,3,A18,2,D17,0\H,18,B20,3,A19,2,D18,0\C,3,B21,2,A20,1,D19,0\H,22,B22,3,A21,2,D20,0\H,22,B23,3,A22,2,D21,0\H,22,B24,3,A23,2,D22,0\\B1=1.53189945\B2=1.87363173\B3=1.75233754\B4=1.39313397\B5=1.49265376\B6=1.08841124\B7=1.08962859\B8=1.08772266\B9=1.08879073\B10=1.08677448\B11=1.09787802\B12=1.07886892\B13=1.44917108\B14=1.08793681\B15=1.09048403\B16=1.08476384\B17=1.87208369\B18=1.08663409\B19=1.08783215\B20=1.08611222\B21=1.87655897\B22=1.08775862\B23=1.08735672\B24=1.08667797\A1=111.77570309\A2=104.25044154\A3=121.53115655\A4=120.69592149\A5=110.70486221\A6=109.18498624\A7=109.36180996\A8=108.95665411\A9=108.09355022\A10=110.51367601\A11=114.77778777\A12=120.22746308\A13=110.45322825\A14=112.05761172\A15=110.57931386\A16=111.86379954\A17=112.49084697\A18=110.06643826\A19=111.11614261\A20=111.01588531\A21=111.05915154\A22=111.56031633\A23=111.09524314\D1=-35.93989093\D2=24.20075463\D3=-32.44407547\D4=179.16529505\D5=-64.11127106\D6=175.16317792\D7=59.0358648\D8=172.32587048\D9=-72.02559897\D10=176.8600586\D11=-177.63239276\D12=143.31447919\D13=-96.18565659\D14=24.45233077\D15=-154.72637403\D16=-180.21431399\D17=-60.8618995\D18=58.58882215\D19=83.48386856\D20=64.80921232\D21=184.63118647\D22=-55.32342741\\Version=IA64L-G03RevD.01\State=2-A\HF=-620.505086\S2=0.755635\S2-

1=0.\S2A=0.750023\RMSD=0.000e+00\RMSF=3.041e-
05\Thermal=0.\Dipole=0.0893222,0.0123884,0.2684438\PG=C01[X(C7H16N1Si1)]\\@

Cyclization of *E*-6b:

***E*-6b**

1\1\GINC-AC20\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1O1Si1(2)\UXW563\19-Jul-2006\1\\# BHandHLYP/6-311G** opt=(Z-matrix,readFC,MaxCycle=500) geom=checkpoint guess=check freq=noraman scf=(qc,direct)\\geom & freq\\0,2\Si\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,5,B5,4,A4,3,D3,0\H,4,B6,3,A5,2,D4,0\H,4,B7,3,A6,2,D5,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\H,2,B10,1,A9,3,D8,0\H,2,B11,1,A10,3,D9,0\H,1,B12,2,A11,3,D10,0\H,1,B13,2,A12,3,D11,0\N,5,B14,4,A13,3,D12,0\O,15,B15,5,A14,4,D13,0\C,16,B16,15,A15,5,D14,0\H,17,B17,16,A16,15,D15,0\H,17,B18,16,A17,15,D16,0\H,17,B19,16,A18,15,D17,0\\B1=1.88628352\B2=1.52778779\B3=1.52162341\B4=1.49252344\B5=1.08439196\B6=1.09057201\B7=1.09060426\B8=1.08647689\B9=1.08629663\B10=1.08878851\B11=1.09120355\B12=1.48153781\B13=1.48108765\B14=1.25683586\B15=1.37515538\B16=1.40574695\B17=1.08636492\B18=1.0824781\B19=1.08635537\A1=114.5346407\A2=112.25923569\A3=115.22706998\A4=118.81686793\A5=109.92012578\A6=109.95690661\A7=110.31836994\A8=110.28470266\A9=108.19521352\A10=107.27072457\A11=111.52697063\A12=111.25117355\A13=121.46375192\A14=111.82269636\A15=109.76857378\A16=111.02151312\A17=105.87347311\A18=111.02086766\D1=-178.81554905\D2=-179.88654412\D3=-179.98569933\D4=-57.59784383\D5=57.81942311\D6=-57.05048438\D7=59.4088193\D8=123.46952573\D9=-122.50049149\D10=57.25754229\D11=-180.01385044\D12=0.001579\D13=-179.98995353\D14=-180.02902861\D15=60.98188271\D16=180.03069204\D17=-60.91902354\\Version=IA64L-G03RevD.01\State=2-A\HF=-616.9897315\S2=0.751605\S2-1=0.\S2A=0.750001\RMSD=0.000e+00\RMSF=9.307e-06\Thermal=0.\Dipole=-0.1448159,0.0514556,0.3475204\PG=C01 [X(C5H12N1O1Si1)]\\@

5-*exo* transition state

1\1\GINC-AC33\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1O1Si1(2)\UXW563\25-Jul-2006\1\\# BHandHLYP/6-311G** opt=(TS,NoEigentest,calcFC,z-matrix,MaxCycle=100) freq=noraman scf=verytight\\geom & freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\H,1,B5,5,A4,4,D3,0\H,1,B6,5,A5,4,D4,0\H,5,B7,4,A6,1,D5,0\H,5,B8,4,A7,1,D6,0\N,4,B9,1,A8,5,D7,0\H,4,B10,1,A9,5,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\H,2,B13,1,A12,5,D11,0\H,2,B14,1,A13,5,D12,0\O,10,B15,4,A14,1,D13,0\C,16,B16,10,A15,4,D14,0\H,17,B17,16,A16,10,D15,0\H,17,B18,16,A17,10,D16,0\H,17,B19,16,A18,10,D17,0\\B1=1.52992553\B2=1.8883124\B3=2.52878439\B4=1.506577\B5=1.08711537\B6=1.0857336\B7=1.08716978\B8=1.08754443\B9=1.28749522\B10=1.08091076\B11=1.48437909\B12=1.47759478\B13=1.08769598\B14=1.08886671\B15=1.36508928\B16=1.4078855\B17=1.0821615\B18=1.08592217\B19=1.08568859\A1=112.17780044\A2=95.04894444\A3=33.82938425\A4=109.47247333\A5=108.54313584\A6=108.58617516\A7=108.51641414\A8=97.31744445\A9=142.00030827\A10=110.88964069\A11=113.26948237\A12=110.75876245\A13=109.70058922\A14=111.08711773\A15=110.11151299\A16=105.879602 46\A17=110.78327599\A18=110.88219011\D1=17.18702301\D2=121.75913109\D3=172.50666212\D4=56.08961996\D5=-121.92777832\D6=122.27570168\D7=131.55493807\D8=-64.43147733\D9=-154.24895763\D10=82.3929901\D11=170.86720263\D12=-71.79595575\D13=158.7450213\D14=-177.89183757\D15=-179.60464056\D16=-60.53818016\D17=61.29276496\\Version=IA64L-G03RevD.01\State=2-A\HF=-616.9814141\S2=0.806544\S2-1=0.\S2A=0.75032\RMSD=5.756e-09\RMSF=3.629e-05\Thermal=0.\Dipole=-0.2245876,-0.0997608,-0.2886583\PG=C01 [X(C5H12N1O1Si1)]\\@

5-*exo* product

1\1\GINC-AC34\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1O1Si1(2)\UXW563\18-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(readfc,maxcycle=500,z-matrix) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\H,1,B5,5,A4,4,D3,0\H,1,B6,5,A5,4,D4,0\H,5,B7,4,A6,1,D5,0\H,5,B8,4,A7,1,D6,0\N,4,B9,1,A8,5,D7,0\H,4,B10,1,A9,5,D8,0\H,3,B11,2,A10,1,D9,0\H,3,B12,2,A11,1,D10,0\H,2,B13,1,A12,5,D11,0\H,2,B14,1,A13,5,D12,0\O,10,B15,4,A14,1,D13,0\C,16,B16,10,A15,4,D14,0\H,17,B17,16,A16,10,D15,0\H,17,B18,16,A17,10,D16,0\H,17,B19,16,A18,10,D17,0\\B1=1.53958211\B2=1.88899396\B3=2.50118851\B4=1.53525227\B5=1.08647754\B6=1.08731727\B7=1.08869494\B8=1.08607631\B9=1.43500403\B10=1.08840422\B11=1.47912694\B12=1.47539443\B13=1.08474347\B14=1.0878666\B15=1.34844665\B16=1.41162768\B17=1.08188597\B18=1.08491331\B19=1.08500973\A1=103.62806936\A2=84.9672285\A3=35.27290498\A4=111.15473599\A5=108.66666287\A6=108.59287243\A7=110.44535545\A8=100.42902698\A9=143.45203454\A10=113.41211438\A11=114.17790302\A12=112.27358372\A13=110.1804558\A14=107.01993606\A15=110.70690703\A16=106.13830637\A17=110.35002257\A18=110.47201884\D1=10.51618681\D2=132.5288804\D3=-174.09127133\D4=68.41289276\D5=-119.21400718\D6=123.34384714\D7=108.46323033\D8=-36.83104195\D9=-131.21664498\D10=103.47711339\D11=160.8813872\D12=-79.83492523\D13=157.27445294\D14=-178.05472385\D15=-178.61071967\D16=-59.32579427\D17=62.08206507\\Version=IA64L-G03RevD.01\State=2-A\HF=-617.0214363\S2=0.756578\S2-1=0.\S2A=0.750033\RMSD=0.000e+00\RMSF=1.656e-05\Thermal=0.\Dipole=-0.0086825,0.0493722,-0.0621126\PG=C01 [X(C5H12N1O1Si1)]\\@

6-*endo* transition state

1\1\GINC-AC36\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1O1Si1(2)\UXW563\24-Jul-2006\1\\# BHandHLYP/6-311G** opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman scf=(qc,direct)\\geom & freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11,3,D10,0\H,3,B13,2,A12,1,D11,0\H,3,B14,2,A13,1,D12,0\C,4,B15,3,A14,2,D13,0\H,16,B16,4,A15,3,D14,0\H,16,B17,4,A16,3,D15,0\H,16,B18,4,A17,3,D16,0\O,4,B19,3,A18,2,D17,0\\B1=1.52998763\B2=1.89571616\B3=2.24546016\B4=1.28802021\B5=1.49394176\B6=1.08697468\B7=1.08822747\B8=1.08752953\B9=1.08903947\B10=1.08531792\B11=1.09028793\B12=1.07999272\B13=1.47900406\B14=1.50089909\B15=2.29569249\B16=1.08198428\B17=1.08527759\B18=1.08629019\B19=1.38272648\A1=114.51364437\A2=89.22938429\A3=119.17972436\A4=121.12986677\A5=109.61031041\A6=109.35121829\A7=109.97702739\A8=110.33803026\A9=108.08521719\A10=108.80991015\A11=117.97480658\A12=110.39128557\A13=106.67296474\A14=100.70948942\A15=139.72989026\A16=93.04884281\A17=92.04236284\A18=114.63162585\D1=-48.57019675\D2=38.85308196\D3=-43.32639836\D4=-169.38765519\D5=-53.19254237\D6=-169.91131852\D7=-53.08100299\D8=-185.571457\D9=-70.23117933\D10=133.84279699\D11=-145.93886073\D12=98.32235031\D13=-152.85750205\D14=-119.22816364\D15=6.43630632\D16=116.27015404\D17=173.24039662\\Version=IA64L-G03RevD.01\State=2-A\HF=-616.9745465\S2=0.78828\S2-1=0.\S2A=0.750195\RMSD=0.000e+00\RMSF=2.406e-05\Thermal=0.\Dipole=-0.226768,-0.6231055,-0.589724\PG=C01 [X(C5H12N1O1Si1)]\\@

6-*endo* product

1\1\GINC-AC48\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1O1Si1(2)\UXW563\24-Jul-2006\1\\# BHandHLYP/6-311G** opt=(Z-matrix,readFC,MaxCycle=500) geom=checkpoint guess=check freq=noraman scf=(qc,direct)\\geom & freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,6,A7,5,D6,0\H,1,B9,6,A8,5,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11,3,D10,0\H,3,B13,2,A12,1,D11,0\H,3,B14,2,A13,1,D12,0\C,4,B15,3,A14,2,D13,0\H,16,B16,4,A15,3,D14,0\H,16,B17,4,A16,3,D15,0\H,16,B18,4,A17,3,D16,0\O,4,B19,3,A18,2,D17,0\\B1=1.53520999\B2=1.87207071\B3=1.75318959\B4=1.39319202\B5=1.49308057\B6=1.08735325\B7=1.08864144\B8=1.08734332\B9=1.08834014\B10=1.08589911\B11=1.09653413\B12=1.07604341\B13=1.47437697\B14=1.47887081\B15=2.30524207\B16=1.08338499\B17=1.08695888\B18=1.08701718\B19=1.40137229\A1=110.75373678\A2=102.16543485\A3=121.34338616\A4=117.21807483\A5=110.63186051\A6=109.65144236\A7=109.10682431\A8=108.77144992\A9=108.2322945\A10=110.58896185\A11=114.86196905\A12=114.2178935\A13=111.53705182\A14=122.79082015\A15=140.71801479\A16=92.4658776\A17=91.8611518\A18=113.16154206\D1=-40.836083\D2=36.3853932\D3=-44.82695053\D4=179.03205669\D5=-63.59624119\D6=175.77289178\D7=59.750235\D8=176.10127333\D9=-67.76394201\D10=164.19786736\D11=-157.84282476\D12=78.652957\D13=-145.54309317\D14=-84.94540687\D15=40.91811282\D16=150.36164191\D17=-183.89161341\\Version=IA64L-G03RevD.01\State=2-A\HF=-617.0210153\S2=0.755705\S2-1=0.\S2A=0.750023\RMSD=0.000e+00\RMSF=1.692e-05\Thermal=0.\Dipole=-0.4135695,-0.4389356,0.0984252\PG=C01 [X(C5H12N1O1Si1)]\\@

Cyclization of *E*-7b:

***E*-7b**

1\1\GINC-AC6\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1O1Si1(2)\UXW563\20-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\Si,-2.7443170709,-0.359475091,0.1067224446\C,-1.1923287692,0.7081652681,0.0176263952\C,0.1117741778,-0.0791317999,-0.1024149765\C,1.3292837603,0.8291104346,-0.1205427718\C,2.6372678947,0.1068942503,-0.2289489805\H,1.2737376178,1.5322930829,-0.9497084584\H,1.3673359085,1.4408635769,0.7789855056\H,0.2078798565,-0.7813051036,0.7205185375\H,0.1075311174,-0.6839735643,-1.0041091381\H,-1.2987164976,1.3956872143,-0.8199478804\H,-1.1749190453,1.3279105225,0.9157660963\H,-2.6861431728,-1.3101985429,1.2415165727\H,-3.9642163338,0.4735766476,0.2207745468\N,2.7181559732,-1.1424738772,-0.3086580653\H,3.6648701627,-1.4810491341,-0.3752785578\O,3.6505260508,0.9985414013,-0.2246296987\C,4.9697038108,0.5150188966,-0.3199260893\H,5.6105573226,1.3846982609,-0.3004557798\H,5.2153482743,-0.1303850897,0.520352985\H,5.1254883123,-0.0249185632,-1.2502078358\\Version=IA64L-G03RevD.01\HF=-617.0503434\S2=0.751606\S2-1=0.\S2A=0.750001\RMSD=4.961e-09\RMSF=9.437e-05\Thermal=0.\Dipole=1.1160499,0.5085968,-0.0931934\PG=C01 [X(C5H12N1O1Si1)]\\@

5-*exo* transition state

1\1\GINC-AC44\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1O1Si1(2)\UXW563\20-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,0.0985724844,1.6108086828,-0.4558026538\C,1.3262535007,0.7074573057,-0.2769542448\Si,0.7566592861,-1.0190081708,0.2229306962\C,-1.44215076,-0.1110119357,0.5326555251\C,-0.9333651056,1.3141537894,0.6218490171\H,0.3817184921,2.6591119565,-0.4178725242\H,-0.3547954193,1.4317229182,-1.4243235687\H,-0.5210561884,1.4715114352,1.614188228\H,-1.7988642601,1.965823799,0.5241724507\N,-1.8426021236,-0.5445657887,-0.6323869639\H,1.5581003967,-

1.5545449514,1.3534539203\H,0.7488126871,-2.0144560732,-0.8661984554\H,1.9406059702,0.6911213899,-1.1721761381\H,1.9510819911,1.0870430168,0.5288408936\H,-2.3474191489,-1.4157859862,-0.5682583635\O,-1.941337833,-0.5035755923,1.7408885362\C,-2.5374744017,-1.7699585494,1.8245043226\H,-1.8494167219,-2.5470031475,1.4928854401\H,-2.7753632186,-1.927596605,2.8670447552\H,-3.4538006471,-1.8257323444,1.2412944974\\Version=IA64L-G03RevD.01\HF=-617.0281504\S2=0.783542\S2-1=0.\S2A=0.750167\RMSD=5.854e-09\RMSF=4.721e-05\Thermal=0.\Dipole=-0.2197349,-0.247259,0.4275132\PG=C01 [X(C5H12N1O1Si1)]\\@

5-*exo* product
1\1\GINC-AC57\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1O1Si1(2)\UXW563\20-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,0.8610399819,1.2622801503,-0.411553302\C,1.630983381,-0.0571687336,-0.2076004668\Si,0.2862207397,-1.3254233543,0.1578130523\C,-1.1549088961,-0.0186582595,0.31248315\C,-0.3521292619,1.2836534574,0.5160817894\H,1.4955928608,2.1260545151,-0.2353173479\H,0.5103002074,1.3227583909,-1.4366528465\H,-0.0302261982,1.3213879805,1.5553071049\H,-0.9742174408,2.1535818183,0.3266000343\N,-1.7661882522,-0.0266138655,-0.949124525\H,0.4767603075,-2.0380597085,1.4366390076\H,0.0382303977,-2.3112029328,-0.9103695136\H,2.2500496803,-0.3041609596,-1.0630773138\H,2.2903329248,0.0195061582,0.6537180759\H,-2.5897501306,-0.6177555204,-0.8931475114\O,-1.9821204832,-0.3634517688,1.4007301535\C,-2.984495921,0.5698686268,1.7222463764\H,-3.6000677546,0.8143325482,0.8575065775\H,-3.6095583174,0.1122156972,2.4780685003\H,-2.5659767732,1.4900995617,2.1246964367\\Version=IA64L-G03RevD.01\HF=-617.0432669\S2=0.757225\S2-1=0.\S2A=0.750035\RMSD=5.405e-09\RMSF=2.758e-05\Thermal=0.\Dipole=-0.0147354,0.3203014,0.3037277\PG=C01 [X(C5H12N1O1Si1)]\\@

6-*endo* transition state
1\1\GINC-AC57\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1O1Si1(2)\UXW563\24-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,0.2343301825,0.1028294082,-0.041761083\C,0.1400142002,0.0976051653,1.4863345153\Si,1.827706631,0.2030401848,2.3592800059\N,2.5405036895,-1.2820481196,1.0751440188\C,2.2314064937,-1.4586221751,-0.156235071\C,0.8462862028,-1.1657404935,-0.6448591061\H,-0.4639759507,0.9420163869,1.8052789229\H,-0.3862811191,-0.7981993879,1.8118191698\H,-0.755223358,0.2113398975,-0.4799290689\H,0.8088273253,0.9649155967,-0.3774029568\H,0.8385363042,-1.0828635599,-1.7243687117\H,0.2177611389,-2.019843979,-0.3932605905\H,1.8954730091,-0.6875077114,3.5397862175\H,1.8455168514,1.6042858261,2.9388400259\H,3.5032942669,-1.5203867039,1.2600353482\O,3.2091128468,-1.8463498378,-0.9902332885\C,2.9390331686,-2.2115547381,-2.328219354\H,3.8633794151,-2.6224107334,-2.708367399\H,2.1627872104,-2.9677606656,-2.3869093204\H,2.6621034921,-1.3507763584,-2.928530839\\Version=IA64L-G03RevD.01\HF=-617.0376604\S2=0.767183\S2-1=0.\S2A=0.750079\RMSD=8.553e-09\RMSF=8.131e-06\Thermal=0.\Dipole=-0.0790805,-1.0661257,-2.1713934\PG=C01 [X(C5H12N1O1Si1)]\\@

6-*endo* product
1\1\GINC-AC59\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1O1Si1(2)\UXW563\20-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.0598862769,-1.1622288881,0.3993821497\C,0.2144252254,-1.4599990962,-0.4027283118\Si,1.5115901138,-0.162305732,-0.0443439755\N,0.5939987857,1.302487028,0.0650261551\C,-0.7267473022,1.3544583125,0.516488573\C,-1.632571907,0.2258006086,0.1140528837\H,0.5891667247,-2.4528907799,-0.167420397\H,-0.0141459485,-1.4522842709,-1.4668447429\H,-1.8182607051,-1.9075685196,0.1744439376\H,-0.8531639429,-1.2459568103,1.4652085622\H,-2.5804078391,0.3307524048,0.6326950408\H,-1.85045277,0.3157000153,-0.9564154486\H,2.531672462,-0.0118253903,-1.1012649891\H,2.2247154613,-0.4991743417,1.2121424047\H,1.0411971387,2.1975529209,0.127865674\O,-1.2149825344,2.628832952,0.3708932374\C,-2.2687766781,2.9914397982,1.2265007935\H,-2.4174981849,4.0565449587,1.103110783\H,-3.1948440325,2.4811128815,0.9715972512\H,-2.0212005297,2.7782922682,2.2639360294\\Version=IA64L-G03RevD.01\HF=-617.0852281\S2=0.754525\S2-1=0.\S2A=0.750014\RMSD=6.845e-09\RMSF=5.217e-05\Thermal=0.\Dipole=-0.3397514,-0.1373088,0.2118134\PG=C01 [X(C5H12N1O1Si1)]\\@

Cyclization of *E*-8b:

***E*-8b**
1\1\GINC-AC28\FOpt\UBHandHLYP\6-311G(d,p)\C5H16N1Si3(2)\UXW563\13-Apr-2007\0\\# BHandHLYP/6-311G** opt=(grad,maxcycle=500,readfc) geom=checkpoint guess=check scf=direct freq=noraman\\freq&geom\\0,2\C,0.8491285314,-1.2316802032,-0.1927730408\C,-0.0023921944,-0.1784087755,0.5168449074\Si,-1.7945327941,-0.0590338201,-0.0897599231\N,2.7788886273,0.7914286197,-

0.8096160709\C,3.1571268056,-0.1426416368,-0.0674110523\C,2.2836687183,-1.2976702967,0.3156931448\H,-0.0256855085,-0.3807180837,1.5889186902\H,0.4559657674,0.7973424815,0.3902074561\H,0.3996766234,-2.2144025758,-0.0680880111\H,0.8673824651,-1.0264017697,-1.2588038019\H,2.7683053973,-2.2015771315,-0.0558963211\H,2.2992429258,-1.3917237964,1.4023168677\H,4.174587633,-0.1709086639,0.3349354349\C,3.7163717036,1.8368517767,-1.1330046822\H,3.3131792147,2.7928106026,-0.8118925309\H,4.6983091557,1.6957867328,-0.6760483369\H,3.8348164375,1.8891528362,-2.2112830722\H,-2.2479892623,3.0221862781,0.4716909639\H,-4.3130520946,1.8133321421,0.2649980624\H,-3.0455032249,1.6964829184,2.2932317995\H,-3.0202561625,-2.6640858607,1.3401661752\H,-4.3642360362,-1.8468301181,-0.4674986375\H,-2.355528783,-3.0781503577,-0.9155354716\Si,-2.9748059418,-2.0776018809,-0.0203666346\Si,-2.9429951633,1.7634655434,0.8163802445\\Version=IA64L-G03RevD.01\State=2-A\HF=-1123.2429116\S2=0.753821\S2-1=0.\S2A=0.750007\RMSD=5.283e-09\RMSF=1.160e-06\Thermal=0.\Dipole=1.0642458,-0.1348312,0.2614561\PG=C01 [X(C5H16N1Si3)]\\@

5-*exo* transition state

1\1\GINC-AC45\FTS\UBHandHLYP\6-311G(d,p)\C5H16N1Si3(2)\UXW563\17-Apr-2007\0\\# BHandHLYP/6-311G** opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,-1.3050987177,-1.6749487609,1.3257418891\C,0.2081617,-1.4423126258,1.3821668805\Si,0.7069257061,-0.0992306238,0.13223297\C,-1.6174945745,-0.4250000509,-0.8446465207\C,-1.7737570021,-1.7458359763,-0.1227051573\H,-1.5693231383,-2.589314526,1.8511362737\H,-1.830307601,-0.8598546811,1.8137709105\H,-1.2193071192,-2.5148072793,-0.6566885093\H,-2.8250532094,-2.0217926743,-0.1665113789\N,-2.2449833266,0.6128250698,-0.3939781438\H,-1.3020498885,-0.4639944053,-1.8870785814\H,0.5274834497,-1.1780320531,2.3865492483\H,0.7276730423,-2.3621380223,1.121160315\C,-2.2440736484,1.791848557,-1.2135906051\H,-1.6785852988,2.5806831836,-0.7199935623\H,-1.8256421505,1.635367627,-2.2100893503\H,-3.2621421634,2.1577452336,-1.3126584539\Si,2.5164858196,-0.7160942687,-1.2188443296\H,2.7733208786,0.3314749344,-2.229655951\H,3.766098944,-0.9308506738,-0.4526199045\H,2.2013677484,-1.9782895549,-1.924485974\Si,0.9342360527,2.0304699906,1.0731627471\H,2.0231412763,2.0615420042,2.076312079\H,1.2557252599,3.0190903379,0.0215027505\H,-0.317297039,2.4418612387,1.7411723586\\Version=IA64L-G03RevD.01\State=2-A\HF=-1123.229665\S2=0.803882\S2-1=0.\S2A=0.750473\RMSD=7.208e-09\RMSF=1.848e-06\Thermal=0.\Dipole=-0.1122822,-0.3545238,-0.2312168\PG=C01 [X(C5H16N1Si3)]\\@

5-*exo* product

1\1\GINC-AC57\FOpt\UBHandHLYP\6-311G(d,p)\C5H16N1Si3(2)\UXW563\17-Apr-2007\0\\# BHandHLYP/6-311G** opt=(grad,maxcycle=500,calcfc) scf=direct freq=noraman\\freq&geom\\0,2\C,-1.2832624202,-1.8576951651,1.1767027035\C,0.2031210813,-1.5400173521,1.4082649564\Si,0.552006581,-0.1255593314,0.1841264209\C,-1.1106439593,-0.3411123808,-0.8105928433\C,-1.5786038984,-1.7216641838,-0.3143972666\H,-1.5405679418,-2.8494899806,1.538649092\H,-1.8991444013,-1.1457533943,1.7182848255\H,-1.0380420906,-2.4907395179,-0.8649145508\H,-2.6357193951,-1.8531427154,-0.5273919676\N,-2.0042355435,0.6788654535,-0.3907375446\H,-0.9419033375,-0.3475075177,-1.8898947312\H,0.4122511572,-1.2831382239,2.4413173578\H,0.8158734705,-2.4048214816,1.1642931742\C,-2.1277215074,1.754856581,-1.329970604\H,-2.7118665652,2.5632096405,-0.9058216637\H,-1.1579983465,2.1479553879,-1.6442798768\H,-2.6321643391,1.4025314748,-2.2335291811\Si,2.4132629501,-0.5282916801,-1.193723268\H,2.5770535968,0.5551669074,-2.1874599701\H,3.6542247086,-0.6128666391,-0.3932616715\H,2.247014178,-1.8044010873,-1.9250656353\Si,0.7400481563,1.9632006673,1.2430924367\H,2.0867538036,2.0816142448,1.8460396313\H,0.578590986,3.0720770089,0.2783812539\H,-0.2621509235,2.1150762848,2.3169889224\\Version=IA64L-G03RevD.01\State=2-A\HF=-1123.25195\S2=0.757117\S2-1=0.\S2A=0.750038\RMSD=3.994e-09\RMSF=1.652e-05\Thermal=0.\Dipole=0.005879,-0.2510256,-0.3353348\PG=C01 [X(C5H16N1Si3)]\\@

6-*endo* transition state

1\1\GINC-AC59\FTS\UBHandHLYP\6-311G(d,p)\C5H16N1Si3(2)\UXW563\11-Apr-2007\1\\# BHandHLYP/6-311G** opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman scf=direct\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2,B7,1,A6,6,D5,0\H,1,B8,6,A7,5,D6,0\H,1,B9,6,A8,5,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,5,B12,4,A11,3,D10,0\C,4,B13,3,A12,2,D11,0\H,14,B14,4,A13,3,D12,0\H,14,B15,4,A14,3,D13,0\H,14,B16,4,A15,3,D14,0\H,3,B17,2,A16,1,D15,0\H,3,B18,2,A17,1,D16,0\H,3,B19,2,A18,1,D17,0\H,3,B20,2,A19,1,D18,0\H,3,B21,2,A20,1,D19,0\H,3,B22,2,A21,1,D20,0\Si,3,B23,2,A22,1,D21,0\Si,3,B24,2,A23,1,D22,0\\B1=1.53034499\B2=1.90299695\B3=2.1814721\B4=1.27571821\B5=1.49480781\B6=1.0865311\B7=1.08885294\B8=1.08754996\B9=1.08878237\B10=1.08621265\B11=1.09218194\B12=1.0867224\B13=1.45466308\B14=1.08242724\B15=1.08539125\B16=1.0868333\B17=3.18715715\B18=3.21882223\B19=3.17974237\B20=3.33801953\B21=3.17892903\B22=3.18027705\B23=2.36885673\B24=2.33892303\A1=112.55054609\A2=88.85847899\A3=122.18738067\A4=123.9381695\A5=109.79488325\A6=109.44905759\A7=107.40220933\A8=109.27952293\A9=108.22440252\A10=107.1868135\A11=119.05841589\A12=115.34693216\A13=109.78141792\A14=108.81879945\A15=111.91371298\A16=133.48429198\A17=89.

63793343\A18=106.28576299\A19=92.82684628\A20=133.15034871\A21=95.55072788\A22=107.09281004\A23=11
0.69704836\D1=-52.10014121\D2=36.28479401\D3=-31.54162634\D4=-166.6372608\D5=-
50.39063967\D6=182.00134686\D7=67.34325246\D8=160.63795156\D9=-85.48420125\D10=148.91210862\D11=-
169.28033524\D12=-16.84999307\D13=-258.49481369\D14=-137.88644956\D15=-166.81033768\D16=-
166.65156059\D17=-
125.70598641\D18=106.92352957\D19=90.35626874\D20=64.27660741\D21=88.28319996\D22=-
152.65507948\\Version=IA64L-G03RevD.01\State=2-A\HF=-1123.2344511\S2=0.76682\S2-
1=0.\S2A=0.750127\RMSD=7.002e-09\RMSF=3.511e-05\Thermal=0.\Dipole=-0.1283078,-1.3144263,-
1.4639485\PG=C01 [X(C5H16N1Si3)]\\@

6-*endo* product
1\1\GINC-AC43\FOpt\UBHandHLYP\6-311G(d,p)\C5H16N1Si3(2)\UXW563\04-Apr-2007\0\\# BHandHLYP/6-
311G** geom=checkpoint guess=check opt=(grad,maxcycle=500,readfc) scf=direct freq=noraman\\freq&geom\\0,2\C,-
2.1025101161,-1.0691010397,0.2200714627\C,-0.8078669852,-1.588798743,-0.4131086436\Si,0.6287114611,-
0.4244961003,-0.0548714065\N,-0.0760855642,1.1791368103,-0.1333098725\C,-
1.4317266137,1.3783227661,0.1175691271\C,-2.4388592943,0.3431194651,-0.2572247299\H,-0.5768902711,-
2.5910991053,-0.0605423561\H,-0.9411866244,-1.6620411035,-1.4913677416\H,-2.924595037,-1.7370254115,-
0.0263827365\H,-2.0152584875,-1.0676162954,1.3049128283\H,-3.3996713269,0.6451800955,0.149940591\H,-
2.5668860807,0.3105831338,-1.3466807525\H,-
1.7419490897,2.4109053047,0.1261915754\C,0.7580275443,2.3537810816,0.0372359986\H,0.4017508806,3.163114
8043,-0.5953910666\H,0.7624539139,2.7051777956,1.069047007\H,1.7820403898,2.1382045682,-
0.248637209\H,3.4032375506,0.3439723291,-1.4920828462\H,2.9083419273,-1.9928970873,-
1.6036075959\H,1.7555403406,-0.4554363351,-3.0399756092\H,2.185558211,-
2.2014512664,2.0921342426\H,2.5447859898,0.134912632,2.4556447738\H,0.4812414996,-
0.8736627741,3.1299214732\Si,1.5280935551,-0.8746055361,2.084322922\Si,2.3150372271,-0.6397149883,-
1.6832004358\\Version=IA64L-G03RevD.01\State=2-A\HF=-1123.2752109\S2=0.75576\S2-
1=0.\S2A=0.750024\RMSD=9.980e-09\RMSF=6.595e-06\Thermal=0.\Dipole=-0.2567459,0.1472185,-
0.1772228\PG=C01 [X(C5H16N1Si3)]\\@

Cyclization of *E*-9b:
***E*-1b**
1\1\GINC-AC14\FOpt\UBHandHLYP\6-311G(d,p)\C8H16N1Si1(2)\UXW563\13-Aug-2006\1\\# BHandHLYP/6-
311G** geom=checkpoint guess=check scf=(qc,direct) opt=(z-matrix,readfc,maxcycle=500) freq=noraman\\geom &
freq\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,1,B4,4,A3,3,D2,0\H,2,B5,1,A4,5,D3,0\H,3,B6,2,A5,1,D4,0\H,3,
B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\H,5,B10,1,A9,4,D8,0\H,5,B11,1,A10,4,D9,0\H,2,B12,1,A11,
5,D10,0\C,1,B13,5,A12,4,D11,0\H,14,B14,1,A13,5,D12,0\H,14,B15,1,A14,5,D13,0\C,14,B16,1,A15,5,D14,0\H,17,B1
7,14,A16,1,D15,0\H,17,B18,14,A17,1,D16,0\C,17,B19,14,A18,1,D17,0\H,20,B20,17,A19,14,D18,0\H,20,B21,17,A20,
14,D19,0\Si,20,B22,17,A21,14,D20,0\H,23,B23,20,A22,17,D21,0\H,23,B24,20,A23,17,D22,0\N,1,B25,5,A24,4,D23,0\
\B1=2.36221128\B2=1.52103574\B3=1.51902264\B4=1.51425512\B5=1.08641212\B6=1.08874574\B7=1.08662549\
B8=1.08585704\B9=1.08880257\B10=1.0897098\B11=1.08754591\B12=1.08996461\B13=1.506096\B14=1.089689\B
15=1.08459818\B16=1.53220083\B17=1.08741965\B18=1.08865407\B19=1.53263685\B20=1.08794626\B21=1.0908
0633\B22=1.88777075\B23=1.48526531\B24=1.48211863\B25=1.26055708\A1=89.54326094\A2=109.66276432\A3
=33.91469288\A4=125.94047601\A5=109.59499663\A6=109.81005463\A7=111.4772678\A8=109.42320243\A9=108
.52122323\A10=108.68984251\A11=113.41281733\A12=116.54056448\A13=108.18142525\A14=107.35280742\A15
=15.73621973\A16=107.07808449\A17=110.32894922\A18=114.58489347\A19=109.77870614\A20=108.98744043\
A21=117.99966259\A22=110.35349553\A23=110.11100221\A24=125.45484038\D1=-
38.06252019\D2=138.66756767\D3=129.1758171\D4=81.92071699\D5=-160.77298412\D6=180.50214696\D7=-
61.43841177\D8=-121.83046105\D9=123.58292177\D10=-
98.07671076\D11=196.22104282\D12=54.7411365\D13=170.62497514\D14=-
66.68897535\D15=170.89933611\D16=56.47241687\D17=-68.86980951\D18=-44.30087098\D19=-
159.94112929\D20=80.68441824\D21=56.84544248\D22=177.25068233\D23=14.81907758\\Version=IA64L-
G03RevD.01\State=2-A\HF=-658.527493\S2=0.751757\S2-1=0.\S2A=0.750001\RMSD=0.000e+00\RMSF=1.885e-
05\Thermal=0.\Dipole=0.4598735,-0.4101336,-0.2974544\PG=C01 [X(C8H16N1Si1)]\\@

5-*exo* transition state
1\1\GINC-AC42\FTS\UBHandHLYP\6-311G(d,p)\C8H16N1Si1(2)\UXW563\16-Aug-2006\1\\# BHandHLYP/6-
311G** scf=verytight opt=(ts,noeigentest,z-matrix,calcfc,maxcycle=500) freq=noraman\\geom &
freq\\0,2\C\C,1,B1\C,1,B2,2,A1\C,1,B3,3,A2,2,D1,0\C,4,B4,1,A3,3,D2,0\C,4,B5,1,A4,3,D3,0\C,5,B6,4,A5,1,D4,0\C,7,
B7,5,A6,4,D5,0\N,4,B8,1,A7,3,D6,0\H,1,B9,3,A8,2,D7,0\H,1,B10,3,A9,2,D8,0\H,2,B11,1,A10,3,D9,0\H,2,B12,1,A11,
3,D10,0\H,3,B13,1,A12,4,D11,0\H,3,B14,1,A13,4,D12,0\H,5,B15,4,A14,1,D13,0\H,5,B16,4,A15,1,D14,0\H,6,B17,4,A
16,1,D15,0\H,6,B18,4,A17,1,D16,0\H,7,B19,5,A18,4,D17,0\H,7,B20,5,A19,4,D18,0\H,8,B21,7,A20,5,D19,0\H,8,B22,
7,A21,5,D20,0\Si,2,B23,1,A22,3,D21,0\H,24,B24,2,A23,1,D22,0\H,24,B25,2,A24,1,D23,0\\B1=2.50625709\B2=1.521

10751\B3=1.52282317\B4=1.52721137\B5=2.38346701\B6=1.52424467\B7=1.51874097\B8=1.30471385\B9=1.0892
1186\B10=1.08980065\B11=1.08850577\B12=1.08640817\B13=1.08699579\B14=1.08396097\B15=1.08887272\B16=
1.08517813\B17=1.09096153\B18=1.08853586\B19=1.08569078\B20=1.08879178\B21=1.08862637\B22=1.0864641
4\B23=1.88468125\B24=1.48777162\B25=1.47737963\A1=35.04449828\A2=113.03334964\A3=114.79209079\A4=1
46.74409026\A5=112.64188957\A6=109.63247319\A7=115.52844213\A8=110.26816119\A9=110.56188055\A10=99.
45955835\A11=144.12244498\A12=110.07203875\A13=108.29216007\A14=107.17533366\A15=110.01614585\A16=
117.94667427\A17=123.09470427\A18=110.31567041\A19=109.6514022\A20=109.62264451\A21=111.35976032\A
22=82.31033565\A23=111.41877297\A24=114.89786622\D1=-64.38148732\D2=159.31783996\D3=-
54.44493474\D4=154.01888889\D5=38.01958482\D6=-
46.75062753\D7=58.19070055\D8=175.79659347\D9=111.37604925\D10=-
25.41481606\D11=173.24587333\D12=55.96829282\D13=32.78662801\D14=-82.00912281\D15=-
59.07736631\D16=75.89693813\D17=161.23387022\D18=-
81.45826736\D19=60.58957235\D20=178.68243889\D21=-142.4518599\D22=-
119.39431147\D23=116.9143835\\Version=IA64L-G03RevD.01\State=2-A\HF=-658.5139966\S2=0.799287\S2-
1=0.\S2A=0.750301\RMSD=9.911e-09\RMSF=4.007e-05\Thermal=0.\Dipole=-0.3212963,0.1718892,-
0.5245255\PG=C01 [X(C8H16N1Si1)]\\@

5-*exo* product

1\1\GINC-AC3\FOpt\UBHandHLYP\6-311G(d,p)\C8H16N1Si1(2)\UXW563\16-Aug-2006\1\\# BHandHLYP/6-
311G** geom=checkpoint guess=check scf=(qc,direct) opt=(z-matrix,readfc,maxcycle=500) freq=noraman\\geom &
freq\\0,2\C\C,1,B1\C,2,B2,1,A1\C,1,B3,3,A2,2,D1,0\C,4,B4,1,A3,3,D2,0\C,4,B5,1,A4,3,D3,0\C,5,B6,4,A5,1,D4,0\C,6,
B7,4,A6,1,D5,0\N,6,B8,4,A7,1,D6,0\H,1,B9,4,A8,9,D7,0\H,1,B10,4,A9,9,D8,0\H,2,B11,1,A10,4,D9,0\H,2,B12,1,A11,
4,D10,0\H,3,B13,2,A12,1,D11,0\H,3,B14,2,A13,1,D12,0\H,5,B15,4,A14,1,D13,0\H,5,B16,4,A15,1,D14,0\H,6,B17,4,A
16,1,D15,0\H,6,B18,4,A17,1,D16,0\H,7,B19,5,A18,4,D17,0\H,7,B20,5,A19,4,D18,0\H,8,B21,6,A20,4,D19,0\H,8,B22,
6,A21,4,D20,0\Si,4,B23,1,A22,3,D21,0\H,24,B24,4,A23,1,D22,0\H,24,B25,4,A24,1,D23,0\\B1=2.50456101\B2=1.541
89962\B3=1.55883721\B4=1.53551691\B5=2.47075745\B6=1.52196392\B7=1.5238265\B8=1.44074234\B9=1.08968
75\B10=1.08748054\B11=1.08731208\B12=1.08435021\B13=1.08673596\B14=1.08424223\B15=1.08695751\B16=1.
08970687\B17=1.09676194\B18=1.08628705\B19=1.0867875\B20=1.08920745\B21=1.08897014\B22=1.08692757\B
23=1.91611628\B24=1.48350316\B25=1.47519057\A1=35.22494328\A2=109.86177253\A3=112.90863432\A4=106.1
9123463\A5=112.95011704\A6=90.93420625\A7=31.28742326\A8=
107.77142518\A9=111.19107276\A10=105.16784193\A11=141.59648377\A12=111.49951558\A13=109.382487\A14
=109.14533722\A15=109.29187182\A16=100.96608635\A17=137.02263969\A18=110.22485863\A19=110.50144276
\A20=109.51022108\A21=109.19633704\A22=100.01535886\A23=111.08989504\A24=112.99952612\D1=-
49.49414903\D2=164.78300827\D3=-99.23504156\D4=80.59876524\D5=-
116.7760678\D6=95.11858749\D7=173.77510658\D8=56.89757763\D9=-
121.63592261\D10=92.37030601\D11=122.43938435\D12=-119.01050131\D13=-43.67635336\D14=-
159.37468171\D15=-7.6038437\D16=120.04140544\D17=176.80193298\D18=-65.45133753\D19=-
88.94289311\D20=154.35561838\D21=41.34332872\D22=96.09386024\D23=-142.30062024\\Version=IA64L-
G03RevD.01\State=2-A\HF=-658.5360798\S2=0.756478\S2-1=0.\S2A=0.750033\RMSD=6.536e-09\RMSF=4.753e-
05\Thermal=0.\Dipole=-0.006851,0.2553639,-0.6022473\PG=C01 [X(C8H16N1Si1)]\\@

6-*endo* transition state

1\1\GINC-AC21\FTS\UBHandHLYP\6-311G(d,p)\C8H16N1Si1(2)\UXW563\25-Aug-2006\1\\# BHandHLYP/6-
311G** scf=(qc,direct) opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\geom &
freq\\0,2\C\C,1,B1\Si,2,B2,1,A1\N,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\C,5,B5,4,A4,3,D3,0\H,2,B6,1,A5,6,D4,0\H,2
,B7,1,A6,6,D5,0\H,1,B8,6,A7,5,D6,0\H,1,B9,6,A8,5,D7,0\H,6,B10,5,A9,4,D8,0\H,6,B11,5,A10,4,D9,0\H,3,B12,2,A11
,1,D10,0\H,3,B13,2,A12,1,D11,0\C,5,B14,4,A13,3,D12,0\H,15,B15,5,A14,4,D13,0\H,15,B16,5,A15,4,D14,0\C,15,B17
,5,A16,4,D15,0\H,18,B18,15,A17,5,D16,0\H,18,B19,15,A18,5,D17,0\C,4,B20,3,A19,2,D18,0\H,21,B21,4,A20,3,D19,0
\H,21,B22,4,A21,3,D20,0\C,21,B23,4,A22,3,D21,0\H,24,B24,21,A23,4,D22,0\H,24,B25,21,A24,4,D23,0\\B1=1.52857
517\B2=1.89664477\B3=2.09737928\B4=1.28601557\B5=1.50426865\B6=1.08629859\B7=1.08866571\B8=1.088191
98\B9=1.08932282\B10=1.0866426\B11=1.09187395\B12=1.48274249\B13=1.51811349\B14=1.50463558\B15=1.08
957983\B16=1.09119013\B17=1.52160642\B18=1.08535731\B19=1.08784068\B20=1.46816216\B21=1.08594482\B2
2=1.08532565\B23=1.5141933\B24=1.08601792\B25=1.08877878\A1=113.31907382\A2=92.2372329\A3=126.27763
258\A4=120.03981591\A5=109.57250346\A6=109.26981757\A7=107.47867611\A8=109.20322426\A9=108.3799535
9\A10=107.31212569\A11=112.35054983\A12=103.9451856\A13=124.66297019\A14=108.37778649\A15=106.6620
9373\A16=114.63641758\A17=110.21514986\A18=109.86361897\A19=110.62226222\A20=108.96467823\A21=106.
34981238\A22=113.26116923\A23=109.2476062\A24=110.05478949\D1=-43.3367119\D2=28.13332117\D3=-
28.11228223\D4=-172.05639427\D5=-55.83080554\D6=176.38603414\D7=61.80106921\D8=164.29371568\D9=-
81.61994594\D10=-135.19054342\D11=113.41165895\D12=153.90194127\D13=-
125.84071285\D14=121.3899977\D15=-1.15217941\D16=156.64766459\D17=-85.87063821\D18=-
171.57643666\D19=-62.61422534\D20=52.11782446\D21=175.15674173\D22=176.98399847\D23=-
65.54905588\\Version=IA64L-G03RevD.01\State=2-A\HF=-658.5257388\S2=0.768253\S2-

1=0.\S2A=0.750093\RMSD=0.000e+00\RMSF=4.182e-05\Thermal=0.\Dipole=0.4236662,-1.0866711,-1.5128128\PG=C01 [X(C8H16N1Si1)]\\@

6-*endo* product
1\1\GINC-AC56\FOpt\UBHandHLYP\6-311G(d,p)\C8H16N1Si1(2)\UXW563\16-Aug-2006\1\\# BHandHLYP/6-311G** scf=(qc,direct) geom=checkpoint guess=check opt=(z-matrix,readfc,maxcycle=500) freq=noraman\\geom & freq\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,3,B5,2,A4,1,D3,0\H,2,B6,1,A5,5,D4,0\H,2,B7,1,A6,5,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\H,5,B10,4,A9,3,D8,0\H,5,B11,4,A10,3,D9,0\H,3,B12,2,A11,1,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\C,14,B16,1,A15,2,D14,0\H,17,B17,14,A16,1,D15,0\H,17,B18,14,A17,1,D16,0\C,17,B19,14,A18,1,D17,0\H,20,B20,17,A19,14,D18,0\H,20,B21,17,A20,14,D19,0\Si,20,B22,17,A21,14,D20,0\H,23,B23,20,A22,17,D21,0\H,23,B24,20,A23,17,D22,0\N,1,B25,2,A24,3,D23,0\\B1=1.499631\B2=1.52171273\B3=1.51895566\B4=1.51675143\B5=1.0865343\B6=1.0988495\B7=1.08701089\B8=1.08861731\B9=1.08710612\B10=1.08726998\B11=1.09339885\B12=1.08896975\B13=1.49946408\B14=1.08714029\B15=1.09914841\B16=1.5255539\B17=1.08724776\B18=1.08900722\B19=1.53175811\B20=1.08712314\B21=1.08815499\B22=1.86488713\B23=1.48515695\B24=1.47876022\B25=1.40495347\A1=113.81857316\A2=109.56271029\A3=109.59581713\A4=110.27047079\A5=108.85349674\A6=109.04145633\A7=109.9074413\A8=111.21360584\A9=109.94495011\A10=108.82267349\A11=109.63417478\A12=114.77411576\A13=107.47723599\A14=109.53297736\A15=116.43155674\A16=109.09562468\A17=109.27533397\A18=111.66716533\A19=111.23259999\A20=109.69896306\A21=108.74889174\A22=110.10191344\A23=114.07760621\A24=117.03708901\D1=49.55317393\D2=-57.36448963\D3=172.00199188\D4=100.09256131\D5=-144.71820785\D6=62.90048838\D7=-178.20117545\D8=176.74079221\D9=-66.40135361\D10=-70.32764028\D11=-185.62587086\D12=-47.7443055\D13=66.45008887\D14=-170.66887058\D15=172.65029126\D16=56.5591179\D17=-65.45036928\D18=-180.03770467\D19=-62.00569321\D20=58.37446204\D21=84.33840002\D22=204.26633407\D23=-39.99030859\\Version=IA64L-G03RevD.01\State=2-A\HF=-658.5770465\S2=0.755675\S2-1=0.\S2A=0.750023\RMSD=0.000e+00\RMSF=1.317e-05\Thermal=0.\Dipole=-0.0718311,0.0083119,0.0842831\PG=C01 [X(C8H16N1Si1)]\\@

Cyclization of *E*-10a:
***E*-10a**
1\1\GINC-AC7\FOpt\UBHandHLYP\6-311G(d,p)\C3H8Ge1N1(2)\UXW563\14-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\N,3.9782356362,0.2709022647,-0.3260207625\H,4.587108527,0.7145738607,0.3485949316\C,3.022125357,-0.3125892567,0.2420576447\H,2.8951459139,-0.3274028095,1.3264418577\C,1.985082474,-1.0633736677,-0.5342264622\H,2.1874347204,-0.9125945419,-1.5890230137\H,1.0073251434,-0.6357776238,-0.3165456639\C,1.9899923238,-2.5547098179,-0.1757573504\H,1.8046483713,-2.6939321332,0.8859938888\H,2.964268805,-2.9838732424,-0.3886864634\H,0.8921132902,-3.5339745407,-2.6768224839\H,-0.7758448022,-3.06957604,-0.8623794902\Ge,0.6374914899,-3.5965702316,-1.162705383\\Version=IA64L-G03RevD.01\HF=-2250.6909747\S2=0.751594\S2-1=0.\S2A=0.750001\RMSD=4.224e-09\RMSF=7.513e-06\Thermal=0.\Dipole=-0.0981939,-0.0608732,0.8352891\PG=C01 [X(C3H8Ge1N1)]\\@

4-*exo* transition state
1\1\GINC-AC11\FTS\UBHandHLYP\6-311G(d,p)\C3H8Ge1N1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.5255099891,1.1262427923,-0.1835341019\C,-0.0995393685,1.6428160016,0.0513003783\H,-1.7339280869,1.041869563,-1.245230125\H,-2.2970875444,1.7584912217,0.2522239733\H,1.1383415746,-0.6338367259,-1.3726403303\H,1.805638166,-0.4606332554,1.0535489115\H,0.2449242518,2.3655481383,-0.676884266\H,0.019354849,2.0693164054,1.0419892703\N,-2.2061142305,-1.2318263186,-0.273605544\H,-2.2752053517,-2.064173933,0.2987322749\C,-1.5716829767,-0.2830459831,0.3941936512\H,-1.5068089953,-0.3272721694,1.4821316095\Ge,0.7217627016,-0.1441887368,0.0142552977\\Version=IA64L-G03RevD.01\HF=-2250.6638568\S2=0.798605\S2-1=0.\S2A=0.750279\RMSD=5.792e-09\RMSF=6.644e-06\Thermal=0.\Dipole=0.363557,0.3052517,0.6611538\PG=C01 [X(C3H8Ge1N1)]\\@

4-*exo* product
1\1\GINC-AC11\FOpt\UBHandHLYP\6-311G(d,p)\C3H8Ge1N1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.48409307,1.1586043958,-0.1389394695\C,-0.0446794461,1.6980884588,0.0136093148\H,-1.7569388018,1.0969414784,-1.1879712293\H,-2.2424999416,1.7533547106,0.3638843033\H,1.0442630445,-0.7186994729,-1.3371024835\H,1.6037425628,-0.6079487253,1.1071787924\H,0.2839628338,2.3752053696,-0.7630324225\H,0.1229731122,2.1650515604,0.9780112167\N,-2.1114833859,-1.2475650476,-0.2986039919\H,-2.124467852,-2.0976270021,0.2550155572\C,-1.3841471967,-0.286260351,0.3925325379\H,-1.4661295193,-0.3271660613,1.4815176673\Ge,0.6270026599,-0.1541783136,0.018504207\\Version=IA64L-G03RevD.01\HF=-

2250.6682651\S2=0.760059\S2-1=0.\S2A=0.750054\RMSD=4.167e-09\RMSF=1.846e-05\Thermal=0.\Dipole=0.4707277,0.1798521,0.6175493\PG=C01 [X(C3H8Ge1N1)]\\@

5-*endo* transition state
1\1\GINC-AC59\FTS\UBHandHLYP\6-311G(d,p)\C3H8Ge1N1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,2.0230095597,0.7015668041,0.2478989634\C,2.0162882466,-0.7337409733,-0.1735721136\C,0.685018515,1.3507789042,-0.1557290401\H,2.1266751686,0.7417119767,1.3316048922\H,2.8740217045,1.2264634591,-0.1746804724\H,2.8138814983,-1.1424327632,-0.781151215\H,0.9038561148,-2.3292123867,-0.2618588804\H,1.9372730429,0.5447118144,-0.9374658198\H,-1.3176875748,-0.0992808391,1.4087555849\H,0.7227888555,1.6797314182,-1.1911051854\H,0.4827840538,2.2266933016,0.4498639216\N,0.9464523812,-1.3918173783,0.1051139251\Ge,-0.7833524803,0.0272326623,-0.0238095616\\Version=IA64L-G03RevD.01\HF=-2250.6820949\S2=0.776417\S2-1=0.\S2A=0.750136\RMSD=4.788e-09\RMSF=2.459e-05\Thermal=0.\Dipole=1.0351133,-0.2802237,-0.3085712\PG=C01 [X(C3H8Ge1N1)]\\@

5-*endo* product
1\1\GINC-AC57\FOpt\UBHandHLYP\6-311G(d,p)\C3H8Ge1N1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-2.0224328804,-0.6012592484,0.2058541418\C,-1.8787697322,0.8359075943,-0.1912967732\C,-0.7366736047,-1.3674388148,-0.1641028781\H,-2.1779156745,-0.682786693,1.2871273591\H,-2.8939991798,-1.0470726016,-0.2650788132\H,-2.707718419,1.517662985,-0.0880813003\H,-0.4336059618,2.2949461313,-0.1876253888\H,1.6134431587,0.1001409275,-1.1946024001\H,1.4947503507,-0.0278458766,1.2898727838\H,-0.7667503938,-1.6920439682,-1.1992672877\H,-0.5808215757,-2.2397370625,0.4581356294\N,-0.5987569723,1.3382607781,0.0483105793\Ge,0.6655068848,-0.0092321512,0.0047753479\\Version=IA64L-G03RevD.01\HF=-2250.7103453\S2=0.755696\S2-1=0.\S2A=0.750022\RMSD=6.058e-09\RMSF=5.293e-05\Thermal=0.\Dipole=0.138151,-0.0144476,-0.0373591\PG=C01 [X(C3H8Ge1N1)]\\@

Cyclization of *E*-10b:

***E*-10b**
1\1\GINC-AC57\FOpt\UBHandHLYP\6-311G(d,p)\C4H10Ge1N1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\N,4.1283177569,-0.4098341051,-0.5104812297\H,4.8386552504,-1.0423680021,-0.1669524289\C,3.2381751109,-0.217304368,0.3552137555\H,3.2585177021,-0.6918976102,1.3384778547\C,2.0631482148,0.6679921763,0.0934457283\H,2.1982634215,1.1293685871,-0.8793167557\H,2.0445351522,1.4604955607,0.8416931128\C,0.7393422174,-0.0994301768,0.1469342816\H,0.6467172427,-0.592998672,1.11310637\H,0.7632396752,-0.8889263592,-0.6007857918\C,-0.4677015957,0.8070893274,-0.0892474745\H,-0.3875678141,1.2951770024,-1.0564670405\H,-0.5023207259,1.5943150764,0.6591149736\Ge,-2.1916313335,-0.1483843811,-0.0378234994\H,-2.4172996513,-0.8003299766,1.33691951\H,-2.2536036237,-1.2334820788,-1.1252843659\\Version=IA64L-G03RevD.01\HF=-2289.9883159\S2=0.751601\S2-1=0.\S2A=0.750001\RMSD=7.379e-09\RMSF=8.400e-06\Thermal=0.\Dipole=0.0106441,0.0046385,0.683148\PG=C01 [X(C4H10Ge1N1)]\\@

5-*exo* transition state
1\1\GINC-AC1\FTS\UBHandHLYP\6-311G(d,p)\C4H10Ge1N1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.0591353372,1.4853561138,-0.4020595279\C,0.4640439921,1.5089767389,-0.2697062221\,-1.3301748007,-0.8828096249,0.4270325071\C,-1.6824881266,0.5724191579,0.649686009\H,-1.4634192708,2.4902134752,-0.3080043655\H,-1.3430615531,1.1149311529,-1.3815783953\H,-1.368455859,0.8754216252,1.6464717551\H,-2.7675602043,0.6517562069,0.6192837656\N,-1.5816198769,-1.4061532127,-0.7357133713\H,-1.2132103612,-1.4951378026,1.3165877556\H,2.2514624419,-0.3516117588,1.1090273577\H,1.564219307,-1.0652145875,-1.199263396\H,0.9365246633,1.9302686011,-1.1508665957\H,0.7629440107,2.1135092166,0.5822589009\H,-1.4366678964,-2.4063810352,-0.7112626818\Ge,1.1237568711,-0.3164752667,0.0607325045\\Version=IA64L-G03RevD.01\HF=-2289.9754362\S2=0.798497\S2-1=0.\S2A=0.750247\RMSD=9.207e-09\RMSF=1.061e-05\Thermal=0.\Dipole=0.0086916,0.0840493,0.5977983\PG=C01 [X(C4H10Ge1N1)]\\@

5-*exo* product
1\1\GINC-AC3\FOpt\UBHandHLYP\6-311G(d,p)\C4H10Ge1N1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.1888502864,1.4131355246,-0.3543120097\C,0.3337132142,1.6010549097,-0.2917013954\C,-0.8380054422,-0.9455523434,0.4250749788\C,-1.6182457559,0.3536508744,0.6611995801\H,-1.7097483897,2.35049358,-

0.1777133546\H,-1.4729225127,1.0698342108,-1.344824306\H,-1.4179098983,0.7108602358,1.6709733272\H,-2.684822954,0.1573169045,0.5928046731\N,-1.2575171676,-1.596796466,-0.7523540287\H,-0.8106843375,-1.5790481211,1.3110877628\H,1.9253874244,-0.3192776111,1.2740023151\H,1.6807450378,-0.9052708301,-1.1385954361\H,0.7358500266,2.0399226279,-1.196849057\H,0.6135522171,2.2408988847,0.5399453637\H,-0.9393868872,-2.5592292282,-0.7160114458\Ge,1.0125027112,-0.2133801526,0.0476180324\\Version=IA64L-G03RevD.01\HF=-2289.9920981\S2=0.757246\S2-1=0.\S2A=0.750035\RMSD=5.269e-09\RMSF=3.913e-05\Thermal=0.\Dipole=0.2937228,0.0448221,0.4993829\PG=C01 [X(C4H10Ge1N1)]\\@

6-*endo* transition state
1\1\GINC-AC59\FTS\UBHandHLYP\6-311G(d,p)\C4H10Ge1N1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.3016630149,1.331652627,-0.3252017719\C,0.047148487,1.3921136083,0.3935023223\C,-1.7234444418,-1.1590740725,-0.1513031794\C,-2.2273955882,0.2113769446,0.1694938604\H,0.5757597532,2.2932889852,0.0975169219\H,-0.114349214,1.4602563048,1.4661850609\H,-1.8272567201,2.2739381317,-0.1842436375\H,-1.1542352114,1.2282245952,-1.3995973296\H,-3.2142790585,0.3378721636,-0.2648073768\H,-2.3387068583,0.3011600292,1.2493854653\H,-2.3149137991,-1.7803816692,-0.8153912374\H,1.9835252276,-0.5342704086,1.3441151833\H,2.3237152854,0.3309748342,-0.9804526443\N,-0.5804788087,-1.5502521763,0.2820651826\H,-0.3367080208,-2.4756555371,-0.0372680185\Ge,1.2521819826,-0.1427263601,0.0530871984\\Version=IA64L-G03RevD.01\HF=-2289.9792765\S2=0.77719\S2-1=0.\S2A=0.750132\RMSD=8.822e-09\RMSF=1.331e-05\Thermal=0.\Dipole=-1.117077,-0.2583104,-0.2951254\PG=C01 [X(C4H10Ge1N1)]\\@

6-*endo* product
1\1\GINC-AC29\FOpt\UBHandHLYP\6-311G(d,p)\C4H10Ge1N1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.469930001,-1.1880295725,0.3449056445\C,-0.1023018972,-1.5023643394,-0.2686381534\C,-1.3358913552,1.3503900428,0.1415217436\C,-2.0875951545,0.1051330511,-0.1969208839\H,0.314033705,-2.413775426,0.1492005652\H,-0.2002629812,-1.6550141424,-1.3403922354\H,-2.1500583914,-2.014425675,0.1485757776\H,-1.3813159989,-1.109801987,1.4271849645\H,-3.097905103,0.2033063705,0.1900771936\H,-2.1849915318,0.002743556,-1.2853682984\H,-1.8757132727,2.2832820257,0.1514560268\H,2.2638244423,0.0920118795,-0.9897307096\H,1.719541927,-0.0488487098,1.4416757964\N,0.0113267606,1.4434967547,-0.2073622175\H,0.3984613114,2.3574530341,-0.0767565487\Ge,1.1245855406,-0.0140798622,0.0243553351\\Version=IA64L-G03RevD.01\HF=-2290.0123087\S2=0.755673\S2-1=0.\S2A=0.750023\RMSD=3.662e-09\RMSF=1.027e-05\Thermal=0.\Dipole=0.0917991,-0.0559543,-0.0169098\PG=C01 [X(C4H10Ge1N1)]\\@

Cyclization of *E*-10c:
***E*-10c**
1\1\GINC-AC30\FOpt\UBHandHLYP\6-311G(d,p)\C5H12Ge1N1(2)\UXW563\14-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,3.2117031063,-0.648702342,-5.0453971396\C,2.9746251899,-1.3543366898,-3.7150553112\C,3.2683945222,-0.4626990226,-2.5149140881\C,3.031003767,-1.1682872827,-1.1913197465\C,3.30669293,-0.3365448376,0.021594896\H,3.13568039,-0.8420269465,0.9734417916\H,3.6432469567,-2.0692211725,-1.1232090887\H,2.000254861,-1.5209671173,-1.1255553611\H,2.6532529945,0.432263212,-2.5578625241\H,4.2971144546,-0.1144396243,-2.5547117308\H,3.5946477022,-2.2484366266,-3.6605058864\H,1.9424657704,-1.6996507707,-3.6631193131\H,2.5911749831,0.2434924596,-5.1166885795\N,3.7045064558,0.8527573891,-0.0517794665\H,3.8354609219,1.2502122014,0.8680487689\H,1.3623991572,-2.2709550892,-6.5887853008\H,3.0196269558,-0.9491571176,-7.9296662705\H,4.2435197163,-0.317196096,-5.1228099643\Ge,2.8083013346,-1.7461713257,-6.6320791762\\Version=IA64L-G03RevD.01\HF=-2329.2866396\S2=0.75156\S2-1=0.\S2A=0.750001\RMSD=7.464e-09\RMSF=7.334e-06\Thermal=0.\Dipole=-0.074091,-0.357513,0.8165489\PG=C01 [X(C5H12Ge1N1)]\\@

6-*exo* transition state
1\1\GINC-AC29\FTS\UBHandHLYP\6-311G(d,p)\C5H12Ge1N1(2)\UXW563\16-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.4526115018,-0.5420620741,-3.2450723169\C,-1.2358608593,1.3691238701,-0.4423286583\C,-0.5011693156,0.1259450552,0.0024189903\C,-0.7769670806,-1.1702624394,-0.7623565064\C,0.0062216529,-1.3849254889,-2.0578522158\H,1.1378593776,1.8546657848,-2.8257466784\H,-1.0566410859,2.2100284295,-3.9955335507\H,-1.4890488369,-0.7654012443,-3.4857587394\H,0.1347090031,-0.7804256777,-4.1285749602\H,0.5632994461,0.3407720776,0.0406612116\H,-0.807264886,-0.0222697371,1.0380115423\H,-

0.5408844094,-1.9953834368,-0.0957806765\H,-1.8451408572,-1.2532610355,-0.9666014435\H,1.0630444993,-1.2052112076,-1.8641044689\H,-0.0720349362,-2.4360941025,-2.3298299357\H,-2.2314852384,1.2018087496,-0.8522790812\N,-0.8732585477,2.5139569535,0.0290369548\H,-1.5474790278,3.225660555,-0.2189669168\Ge,-0.3222376764,1.3945121206,-2.9189438297\\Version=IA64L-G03RevD.01\HF=-2329.2679661\S2=0.796919\S2-1=0.\S2A=0.750232\RMSD=3.708e-09\RMSF=5.393e-06\Thermal=0.\Dipole=-0.5621987,-0.7376776,-0.3273211\PG=C01 [X(C5H12Ge1N1)]\\@

6-*exo* product
1\1\GINC-AC55\FOpt\UBHandHLYP\6-311G(d,p)\C5H12Ge1N1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-0.5863218002,-1.6719418267,-0.2367574944\C,-0.1435413039,1.3841819011,-0.4058916707\C,-1.5474386131,1.3462963395,0.2070444039\C,-2.3996891191,0.1483956514,-0.2137595171\C,-1.9285031851,-1.2016697049,0.3280355944\H,1.2340416462,-0.2689923097,1.5158530345\H,2.0349651773,-0.5244453911,-0.8416928733\H,-0.6721874853,-1.8434958206,-1.3073206938\H,-0.2873920069,-2.6148495866,0.2108880367\H,-1.4620824728,1.3615327891,1.2947909911\H,-2.0633317981,2.2642933795,-0.0703321779\H,-3.4187049467,0.3193450265,0.1237478473\H,-2.4462960258,0.1043967201,-1.3022016875\H,-1.8674433334,-1.1415869277,1.4144441775\H,-2.6891917726,-1.9490756769,0.1112709578\H,-0.2115689299,1.3584994114,-1.493877747\N,0.6973956764,2.4491505067,-0.0224448421\H,0.469777774,2.6946558486,0.937521162\Ge,0.8085195188,-0.3201093297,0.044545497\\Version=IA64L-G03RevD.01\HF=-2329.2920095\S2=0.756871\S2-1=0.\S2A=0.750032\RMSD=4.192e-09\RMSF=1.616e-05\Thermal=0.\Dipole=-0.8064187,-0.636299,0.2226591\PG=C01 [X(C5H12Ge1N1)]\\@

7-*endo* transition state
1\1\GINC-AC18\FTS\UBHandHLYP\6-311G(d,p)\C5H12Ge1N1(2)\UXW563\17-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,0.9310753392,-3.1309511778,0.1263202741\C,2.4517538419,-2.9581741518,0.1712845306\C,0.130135534,-2.3963936564,1.1987242088\C,0.1295435971,-0.8642097323,1.1012868598\C,1.3758912411,-0.210157447,1.5913314745\H,0.5524607095,-2.8464524266,-0.8545394545\H,2.8058713596,-3.0210091567,1.198921973\H,2.4763473546,-1.0014086991,-1.942198491\H,0.4823877864,-2.6967780681,2.1852925341\H,-0.6997158,-0.4851336211,1.6967759658\H,0.7054203735,-4.1907968109,0.2337650701\H,2.9178902502,-3.7869530009,-0.3560869708\H,4.7010427011,-1.7087264553,-1.066795833\H,-0.9020582814,-2.7323422119,1.1327700616\H,3.0250325136,0.6966140876,1.2549113397\H,-0.0448394517,-0.5565496424,0.0736956849\H,1.5400821248,-0.2080262008,2.6655652765\N,2.2399422122,0.2820132933,0.7756591177\Ge,3.2443415941,-1.3433539219,-0.656286622\\Version=IA64L-G03RevD.01\HF=-2329.2736476\S2=0.777643\S2-1=0.\S2A=0.750132\RMSD=4.362e-09\RMSF=5.378e-06\Thermal=0.\Dipole=-0.4388999,-0.1123392,0.9649507\PG=C01 [X(C5H12Ge1N1)]\\@

7-*endo* product
1\1\GINC-AC29\FOpt\UBHandHLYP\6-311G(d,p)\C5H12Ge1N1(2)\UXW563\16-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.8758281272,-3.2182716403,0.1145043842\C,2.3959688606,-3.0880662385,0.0170243928\C,0.2066405888,-2.4336591969,1.2415292532\C,0.1971288715,-0.8967366969,1.1056240961\C,1.3891332366,-0.1525287455,1.6042820069\H,0.4227841688,-2.9282830251,-0.8335682124\H,2.860592077,-3.363744405,0.9608880853\H,2.4387355973,-0.8682326554,-1.7983165663\H,0.6587418833,-2.7007202459,2.1948526355\H,-0.657121017,-0.527047599,1.6650615214\H,0.6311158319,-4.2704182378,0.2501520017\H,2.7757340354,-3.7770222611,-0.7341404683\H,4.5679663885,-1.2322163364,-0.5453072362\H,-0.8286641432,-2.7650682102,1.2887648944\H,3.2744429748,0.4844947033,1.2337867345\H,-0.0098008273,-0.6455495893,0.0577892704\H,1.240208715,0.6821978524,2.2672534785\N,2.580749737,-0.1499472178,0.8953806927\Ge,3.0424204829,-1.3079694677,-0.4551659717\\Version=IA64L-G03RevD.01\HF=-2329.3065436\S2=0.755648\S2-1=0.\S2A=0.750023\RMSD=8.053e-09\RMSF=9.060e-06\Thermal=0.\Dipole=0.1350515,-0.1097747,0.0082563\PG=C01 [X(C5H12Ge1N1)]\\@

Cyclization of *E*-11a:

***E*-11a**
1\1\GINC-AC28\FOpt\UBHandHLYP\Gen\C3H8N1Sn1(2)\UXW563\14-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\N,3.9934836554,0.3121418779,-0.3202008854\H,4.6131518006,0.7301349586,0.3610428084\C,3.0520453862,-0.3014700295,0.2410227831\H,2.9468550848,-0.3640381017,1.3260828159\C,2.004822243,-1.0280309002,-

0.5449979583\H,2.1876752839,-0.830059779,-1.5958786586\H,1.0298280581,-0.6125191167,-0.2929774577\C,2.0250849743,-2.5317723132,-0.2465188732\H,1.8493173019,-2.7178618286,0.8096002076\H,2.9995201193,-2.9463292045,-0.4857709625\H,0.813413445,-3.4163242939,-3.0448383618\H,-1.0158426888,-3.0098895319,-0.9882698097\Sn,0.5400592655,-3.6395568091,-1.3634541742\\Version=IA64L-G03RevD.01\HF=-177.0873572\S2=0.751668\S2-1=0.\S2A=0.750001\RMSD=3.379e-09\RMSF=1.465e-05\Thermal=0.\Dipole=-0.0849302,-0.3389875,0.8781734\PG=C01 [X(C3H8N1Sn1)]\\@

5-*endo* transition state
1\1\GINC-AC7\FTS\UBHandHLYP\Gen\C3H8N1Sn1(2)\UXW563\16-Nov-2007\0\\# BHandHLYP/gen scf=direct freq=noraman nosymm pseudo=read opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,2.070463,0.708332,0.232541\C,2.036414,-0.726527,-0.187583\C,0.748647,1.416244,-0.137942\H,2.191902,0.745958,1.315505\H,2.93173,1.209297,-0.199324\H,2.799272,-1.138208,-0.833345\H,0.925931,-2.338534,-0.227454\H,-2.086614,0.440472,-1.126656\H,-1.53315,-0.140894,1.559778\H,0.779497,1.769556,-1.165371\H,0.584044,2.281505,0.492879\Sn,-0.848466,-0.028927,-0.002418\N,0.956793,-1.395868,0.123255\\Version=IA64L-G03RevD.01\HF=-177.0802672\S2=0.779882\S2-1=0.\S2A=0.750171\RMSD=6.250e-09\RMSF=3.823e-05\Thermal=0.\Dipole=0.806626,-0.339561,-0.341199\Polar=161.7347714,-6.6796751,69.2609462,7.4319441,-2.767892,63.58874\PG=C01 [X(C3H8N1Sn1)]\\@

5-*endo* product
1\1\GINC-AC7\FOpt\UBHandHLYP\Gen\C3H8N1Sn1(2)\UXW563\16-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-2.0428620257,-0.5989340978,0.2092073544\C,-1.9010377381,0.8342226901,-0.2082685106\C,-0.8006864778,-1.4287040221,-0.1770668645\H,-2.170309757,-0.6617900879,1.2965404562\H,-2.9412149028,-1.0269417999,-0.2280487719\H,-2.7576904425,1.4873313422,-0.154877748\H,-0.5613676465,2.3709727642,-0.1355378128\H,1.8438365668,0.1233617601,-1.3224502444\H,1.7146497283,-0.0027800808,1.4431919887\H,-0.8500438369,-1.7371166758,-1.2166906365\H,-0.6954911054,-2.316801444,0.4329622234\Sn,0.7885798037,-0.0172689534,0.0122063879\N,-0.6501061662,1.3939506052,0.0528531781\\Version=IA64L-G03RevD.01\HF=-177.0942294\S2=0.755753\S2-1=0.\S2A=0.750023\RMSD=4.791e-09\RMSF=7.725e-07\Thermal=0.\Dipole=0.2516136,-0.0548979,-0.0122065\PG=C01 [X(C3H8N1Sn1)]\\@

Cyclization of *E*-11b:
***E*-11b**
1\1\GINC-AC20\FOpt\UBHandHLYP\Gen\C4H10N1Sn1(2)\UXW563\14-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\N,4.6627526405,-0.6433010917,-0.3594423849\H,5.490522791,-0.0684411755,-0.2754839766\C,3.7538831291,-0.2409560511,0.4094246456\H,3.8789669302,0.6182010156,1.0718199512\C, 2.429087518,-0.9272249989,0.4914991783\H,2.4068688558,-1.7106249014,-0.2589570035\H,1.6440094727,-0.2099125169,0.2520105669\C,2.163849448,-1.5079724481,1.884020847\H,2.2422398509,-0.712577359,2.6240137662\H,2.9517943389,-2.2209809216,2.1171488754\C,0.7973275423,-2.1819902462,1.9856483149\H,0.7157169787,-2.9845516071,1.2581720765\H,0.0047722718,-1.4728029178,1.7628002118\H,0.4699537466,-1.7659580262,5.1135650209\H,1.6162854362,-4.1709107484,4.3236650216\Sn,0.3976996785,-3.0206729354,3.9387991401\\Version=IA64L-G03RevD.01\HF=-216.3845543\S2=0.751672\S2-1=0.\S2A=0.750001\RMSD=6.780e-09\RMSF=5.525e-06\Thermal=0.\Dipole=-0.3819148,0.5087223,0.2481998\PG=C01 [X(C4H10N1Sn1)]\\@

5-*exo* transition state
1\1\GINC-AC18\FTS\UBHandHLYP\Gen\C4H10N1Sn1(2)\UXW563\17-Nov-2007\0\\# BHandHLYP/gen scf=direct freq=noraman nosymm pseudo=read opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.634011,1.315786,-0.35774\C,-0.150218,1.68789,-0.304618\C,-1.375365,-1.08699,0.422956\C,-1.996887,0.270558,0.695278\H,-2.252561,2.199302,-0.217157\H,-1.879644,0.906971,-1.332193\H,-1.705381,0.613688,1.686353\H,-3.076267,0.126614,0.716694\N,-1.539103,-1.600628,-0.774529\H,-1.223396,-1.719949,1.292542\H,2.237065,0.136212,1.194418\H,1.64614,-0.81872,-1.358608\H,0.170602,2.188863,-1.211055\H,0.04946,2.358671,0.526537\Sn,0.980019,-0.106795,0.043414\H,-1.254371,-2.570969,-0.781786\\Version=IA64L-G03RevD.01\HF=-216.3685137\S2=0.796489\S2-1=0.\S2A=0.750244\RMSD=4.952e-09\RMSF=9.751e-06\Thermal=0.\Dipole=-0.0611177,-0.040474,0.6217321\Polar=116.0754481,2.0194449,86.8366802,3.8822339,5.7396564,76.5927362\PG=C01 [X(C4H10N1Sn1)]\\@

5-*exo* product

1\1\GINC-AC28\FOpt\UBHandHLYP\Gen\C4H10N1Sn1(2)\UXW563\17-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.6788239785,1.2339438684,-0.3393417204\C,-0.227814122,1.7351819403,-0.2931312776\C,-1.0188732636,-1.0957216744,0.4279534203\C,-1.9213374318,0.1184269062,0.680241278\H,-2.3746670042,2.0511777412,-0.1644409454\H,-1.8964215365,0.8380832161,-1.3268641198\H,-1.7388322438,0.4953354257,1.6866636669\H,-2.9604410348,-0.2010362758,0.6437227332\N,-1.3017988907,-1.7296933655,-0.7826170851\H,-0.936246339,-1.7403116142,1.3018131022\H,1.9421454068,0.0017632626,1.395452139\H,1.7628762024,-0.6912184383,-1.290140094\H,0.052257355,2.2644096588,-1.1957677046\H,-0.0723529522,2.4067213949,0.5461118676\Sn,0.9066953016,-0.0520656827,0.035142671\H,-0.9194844687,-2.6679453631,-0.7555129315\\Version=IA64L-G03RevD.01\HF=-216.3753039\S2=0.759219\S2-1=0.\S2A=0.750047\RMSD=5.177e-09\RMSF=3.912e-06\Thermal=0.\Dipole=0.3142271,0.0829993,0.5120835\PG=C01 [X(C4H10N1Sn1)]\\@

6-*endo* transition state
1\1\GINC-AC24\FTS\UBHandHLYP\Gen\C4H10N1Sn1(2)\UXW563\17-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.7702315348,1.2634053554,-0.3412543703\C,-0.3936619601,1.539939394,0.2644061515\C,-1.8707307976,-1.2694429024,-0.1609414731\C,-2.4770973834,0.0315590321,0.2479763605\H,0.0176527748,2.4520664269,-0.1572252161\H,-0.4927216089,1.7081960579,1.3338841121\H,-2.419454529,2.1218847795,-0.1773797256\H,-1.6948629635,1.1487758609,-1.4220960436\H,-3.5204134602,0.0379488539,-0.0521530687\H,-2.4559929458,0.1085388323,1.3349523658\H,-2.4332445761,-1.9136515549,-0.8250607104\H,1.9126292842,-0.3390838556,1.4217225566\H,2.1998878341,0.5619610094,-1.2060178737\N,-0.6538812101,-1.5795701973,0.1846875298\H,-0.3711091909,-2.4795785761,-0.169854994\Sn,1.0579222674,-0.0342145154,-0.0292856018\\Version=IA64L-G03RevD.01\HF=-216.3778119\S2=0.782094\S2-1=0.\S2A=0.750186\RMSD=7.495e-09\RMSF=3.640e-06\Thermal=0.\Dipole=-1.0083489,-0.4220015,-0.3132943\PG=C01 [X(C4H10N1Sn1)]\\@

6-*endo* product
1\1\GINC-AC22\FOpt\UBHandHLYP\Gen\C4H10N1Sn1(2)\UXW563\16-Nov-2007\0\\# BHandHLYP/gen scf=direct freq=noraman nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.800279,-1.184835,0.341424\C,-0.437045,-1.596824,-0.226511\C,-1.6557,1.373313,0.173773\C,-2.353976,0.120725,-0.246722\H,-0.074544,-2.5022,0.24962\H,-0.524706,-1.808992,-1.288761\H,-2.51653,-1.982407,0.150666\H,-1.738241,-1.080641,1.423308\H,-3.396957,0.212067,0.043061\H,-2.349697,0.026059,-1.340733\H,-2.238431,2.278912,0.225255\H,2.14052,0.13838,-1.215499\H,1.768181,-0.052399,1.527682\N,-0.30231,1.542282,-0.112825\H,0.021619,2.475178,0.049967\Sn,0.970139,-0.015484,0.014269\\Version=IA64L-G03RevD.01\HF=-216.3956065\S2=0.75575\S2-1=0.\S2A=0.750024\RMSD=5.792e-09\RMSF=8.191e-06\Thermal=0.\Dipole=0.1761037,-0.123255,-0.0170419\Polar=96.5223865,2.0293464,77.8791371,-0.4785998,0.5339732,69.05406\PG=C01 [X(C4H10N1Sn1)]\\@

Cyclization of *E*-11c:

***E*-11c**
1\1\GINC-AC30\FOpt\UBHandHLYP\Gen\C5H12N1Sn1(2)\UXW563\16-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.5547559053,-0.3529571472,3.9995580998\H,-0.7169423483,0.4752830878,3.3150086544\H,-1.4190870622,-1.0058218811,3.9147985263\C,0.7231676142,-1.1070544651,3.6366778371\H,0.8806707019,-1.9288542517,4.3332669697\H,1.5861848386,-0.4510277992,3.7430220998\C,0.7000513498,-1.664835812,2.2166522797\H,-0.157717372,-2.3249266634,2.1018050388\H,0.5560437127,-0.8452482917,1.5130771322\C,1.9730224621,-2.4319151219,1.8623477883\H,2.1074785851,-3.2815063987,2.5240653947\H,2.8330941199,-1.7729299958,1.985861023\C,1.9558459175,-2.9388092427,0.4571067464\H,1.8849051161,-2.171441437,-0.3167458338\N,2.0041499628,-4.1663772052,0.1930462955\H,1.9728772186,-4.3245312095,-0.8052816844\Sn,-0.5329855631,0.4530257307,6.006128222\H,0.7844233322,1.5489859581,6.1589545577\H,-0.2840167901,-0.8255113016,7.1292479865\\Version=IA64L-G03RevD.01\HF=-255.6819473\S2=0.751672\S2-1=0.\S2A=0.750001\RMSD=5.783e-09\RMSF=1.067e-05\Thermal=0.\Dipole=-0.3083802,0.7129379,-0.5428323\PG=C01 [X(C5H12N1Sn1)]\\@

6-*exo* transition state
1\1\GINC-AC28\FTS\UBHandHLYP\Gen\C5H12N1Sn1(2)\UXW563\14-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.701564991,-0.4814856033,-3.4538418714\C,-1.2602980423,1.4177408295,-0.4553350282\C,-0.3310013674,0.2474098457,-0.2070434063\C,-0.6215249171,-1.0685177376,-0.9362911342\C,-0.0044945424,-1.239301639,-2.3262033554\H,0.6806244815,2.3963977576,-3.3142971477\H,-1.9685023851,2.3625116584,-

4.1829935423\H,-1.7166540916,-0.849897642,-3.580286553\H,-0.187950439,-0.6446912421,-4.3973798998\H,0.6949834808,0.5673320015,-0.3699387764\H,-0.4084107536,0.062726482,0.8642822154\H,-0.2425471073,-1.871851195,-0.3105017553\H,-1.6992183859,-1.2262737103,-0.9942539772\H,1.0452620348,-0.9521550714,-2.2789106885\H,-0.0090464253,-2.3016856529,-2.5662451155\H,-2.3024277228,1.1486996032,-0.6246776439\N,-0.9250038747,2.5810032259,0.0216997866\H,-1.7077031646,3.2195770935,-0.0326923648\Sn,-0.8406630025,1.6391594149,-3.1062364025\\Version=IA64L-G03RevD.01\HF=-255.6596981\S2=0.800536\S2-1=0.\S2A=0.750261\RMSD=3.687e-09\RMSF=1.644e-05\Thermal=0.\Dipole=-0.5657984,-0.7348481,-0.1351437\PG=C01 [X(C5H12N1Sn1)]\\@

6-*exo* product
1\1\GINC-AC29\FOpt\UBHandHLYP\Gen\C5H12N1Sn1(2)\UXW563\16-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.742881145,-1.7356014911,-0.4100918335\C,-0.3534990032,1.5332994546,-0.672454766\C,-1.7185123602,1.3730772145,-0.0005917155\C,-2.525677541,0.138156019,-0.4100460808\C,-2.0570355807,-1.2006055091,0.1670027133\H,1.4363168959,-0.2032402271,1.3646651939\H,2.0918713674,-0.4809738147,-1.332748435\H,-0.8618744254,-1.9552280208,-1.4683271009\H,-0.4585164456,-2.6638862427,0.075266306\H,-1.5828365483,1.3879055659,1.0798018425\H,-2.3010364357,2.2625698185,-0.2354984925\H,-3.5529884315,0.2959962854,-0.0920086814\H,-2.5597198475,0.0692225566,-1.4983232294\H,-1.971727888,-1.1023036093,1.2490420779\H,-2.8413671589,-1.9368790612,-0.0019186947\H,-0.4637860214,1.5102392037,-1.7609412023\N,0.3686298718,2.62682594,-0.1768111484\Sn,0.8131100068,-0.2771340571,-0.218208602\H,1.0563224314,2.8971159646,-0.8718513549\\Version=IA64L-G03RevD.01\HF=-255.672773\S2=0.757815\S2-1=0.\S2A=0.750038\RMSD=3.131e-09\RMSF=2.888e-05\Thermal=0.\Dipole=-0.224816,-0.6842811,-0.5875859\PG=C01 [X(C5H12N1Sn1)]\\@

7-*endo* transition state
1\1\GINC-AC30\FTS\UBHandHLYP\Gen\C5H12N1Sn1(2)\UXW563\17-Nov-2007\0\\# BHandHLYP/gen scf=direct nosymm pseudo=read opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.2139574377,-1.6552680795,-0.6920005595\C,-1.4127843273,-1.3140105179,0.1956322712\C,-1.1514433601,1.8086884308,-0.1589230574\C,-2.4569392397,-0.3941416263,-0.4367930967\C,-1.9622704872,0.9289419661,-1.0404214437\H,-0.5339374811,-1.8789592736,-1.7071497379\H,2.3549626328,-0.3207898398,0.6141438936\H,-1.07159836,-0.8799359294,1.1311573115\H,-3.2166223227,-0.171396204,0.3092268041\H,0.2664409822,-2.5569524193,-0.3215835327\H,2.322824356,-0.5081697557,-2.1583330593\H,-1.9332625462,-2.2318030595,0.4672030533\H,-2.9633269187,-0.9345574715,-1.2351314261\H,-2.8197232456,1.4817625151,-1.4110369472\H,-1.3392985436,0.7076650423,-1.9165589099\N,-0.0128300161,1.3913457685,0.2979267833\Sn,1.3368556096,-0.1526989984,-0.7569761044\H,0.5011202255,2.1000885057,0.7988477998\H,-1.4551855204,2.8380259461,-0.0211260412\\Version=IA64L-G03RevD.01\HF=-255.6745195\S2=0.777176\S2-1=0.\S2A=0.75016\RMSD=9.581e-09\RMSF=2.625e-05\Thermal=0.\Dipole=-0.9527955,0.8350441,0.1940148\PG=C01 [X(C5H12N1Sn1)]\\@

7-*endo* product
1\1\GINC-AC3\FOpt\UBHandHLYP\Gen\C5H12N1Sn1(2)\UXW563\16-Nov-2007\0\\# BHandHLYP/gen scf=direct freq=noraman nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.2406129321,-1.7381918325,-0.5515831002\C,-1.5022467701,-1.336477986,0.2213727566\C,-1.1028411756,1.7356128274,-0.1084772966\C,-2.4564744822,-0.4109857576,-0.5311227582\C,-1.8565000205,0.8958162842,-1.079959108\H,-0.4868012215,-2.0479978174,-1.5637487685\H,2.5387984391,-0.3910521463,0.4210590325\H,-1.2257028548,-0.866412212,1.1619724578\H,-3.2752039148,-0.1575336432,0.1381393479\H,0.2339144512,-2.5892124083,-0.071791321\H,1.7741280346,0.159499625,-2.1944091692\H,-2.0561391337,-2.2358320036,0.486015542\H,-2.8958316871,-0.9566137577,-1.3665492208\H,-2.6719664055,1.4818614797,-1.4947997402\H,-1.2185856763,0.6545288575,-1.9403058289\N,0.2099388753,1.4040873788,0.1870048647\Sn,1.2012287314,-0.1571701236,-0.6123775365\H,0.6884791522,2.0703929626,0.7589813322\H,-1.418557409,2.7435172734,0.0986825132\\Version=IA64L-G03RevD.01\HF=-255.6913862\S2=0.755867\S2-1=0.\S2A=0.750025\RMSD=8.229e-09\RMSF=8.508e-06\Thermal=0.\Dipole=0.1159686,,-0.1305775,0.0116288\PG=C01 [X(C5H12N1Sn1)]\\@

Gaussian archive entries for Table 2

Cyclization of 12a:

12a

1\1\GINC-AC58\FOpt\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,1.6500397951,0.2234640488,0.4617484778\H,1.6316867641,1.2705957309,0.1474792102\H,1.4472775257,0.1959477256,1.5294238261\C,0.5790467191,-0.5765071042,-0.2807423117\H,0.6417700063,-1.6163656131,0.0291895826\H,0.7941148328,-0.5609413055,-1.3468953239\H,-1.3758384981,1.4066244364,-0.5507099558\H,-1.5603704686,0.0137280035,1.4172469196\N,2.9513251614,-0.3758517504,0.2564111746\C,3.8475870969,0.3255090632,-0.2630862706\H,3.7003507406,1.364580531,-0.5608279931\H,4.8270303247,-0.1014626797,-0.4330657306\Si,-1.1825080001,0.0393519135,-0.0146176052\\Version=IA64L-G03RevD.01\HF=-463.2319749\S2=0.751683\S2-1=0.\S2A=0.750001\RMSD=3.780e-09\RMSF=2.068e-05\Thermal=0.\Dipole=0.2263876,0.3959816,-0.2618259\PG=C01 [X(C3H8N1Si1)]\\@

4-*exo* transition state

1\1\GINC-AC33\FTS\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,-1.5346037358,1.079138878,0.002331738\C,-0.0841392474,1.5705415897,-0.0250167455\H,-2.081165566,1.323948641,-0.9061168518\H,-2.1019849242,1.4553990652,0.8485888569\H,1.9528163456,-0.135600738,-0.8848362602\H,1.1048322896,-0.6896299358,1.274579874\H,0.1499784594,2.1404081469,-0.9170955606\H,0.1686187743,2.1822115558,0.8341343374\C,-2.3320533633,-1.1801998411,-0.1041198485\H,-2.189020476,-2.2359560601,0.0619749267\H,-3.2659643807,-0.8452326164,-0.5374717891\N,-1.3803784282,-0.3712162601,0.1666820999\Si,0.7115952528,-0.1525164243,-0.0430267765\\Version=IA64L-G03RevD.01\HF=-463.217142\S2=0.780158\S2-1=0.\S2A=0.75015\RMSD=9.904e-09\RMSF=1.275e-05\Thermal=0.\Dipole=-1.0937135,0.1275868,-0.1477717\PG=C01 [X(C3H8N1Si1)]\\@

4-*exo* product

1\1\GINC-AC58\FOpt\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,1.4639153409,1.1416926475,0.0199696273\C,0.0014986031,1.6625469774,-0.0126054249\H,1.9934153621,1.4283560007,0.9269503954\H,2.0538261155,1.4666121924,-0.8355104938\H,-1.2293269206,-0.6569963533,1.1890824264\H,-1.2405637692,-0.6792666676,-1.1884837677\H,-0.268155532,2.2510691907,0.8552168681\H,-0.2339245003,2.2293311107,-0.9047212676\C,2.1775977396,-1.2550214086,0.0447389556\H,1.8922784291,-2.2840000014,-0.0681814271\H,3.1944263991,-0.9581262711,-0.1384853813\N,1.1983488564,-0.2998576903,-0.0198775335\Si,-0.5262091236,-0.1438307274,-0.0082369763\\Version=IA64L-G03RevD.01\HF=-463.2534542\S2=0.755356\S2-1=0.\S2A=0.750019\RMSD=8.260e-09\RMSF=5.822e-06\Thermal=0.\Dipole=-0.1696001,0.3897955,-0.0932184\PG=C01 [X(C3H8N1Si1)]\\@

5-*endo* transition state

1\1\GINC-AC58\FTS\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,1.9542239905,0.7181753317,0.2481616225\C,0.605293543,1.3652869136,-0.1257038716\H,2.0125014145,0.5931574777,1.3328524555\H,2.782719499,1.3428296612,-0.0650051057\H,-1.6389886057,0.0333608536,-1.1994298467\H,-1.5653656353,0.1509454826,1.2207824415\H,0.6500879301,1.7176441003,-1.1523678\H,0.397766352,2.224859621,0.5046571724\C,1.3485444912,-1.4861597486,0.1390223571\H,1.2183921344,-2.4326690351,-0.3641178607\H,1.1223361673,-1.4733259399,1.2052201246\N,2.0118455752,-0.5503988737,-0.4411409641\Si,-0.7560008563,0.0553821552,-0.0157217243\\Version=IA64L-G03RevD.01\HF=-463.2173232\S2=0.801257\S2-1=0.\S2A=0.750289\RMSD=7.807e-09\RMSF=5.969e-05\Thermal=0.\Dipole=-0.1715122,0.1408669,0.5106899\PG=C01 [X(C3H8N1Si1)]\\@

5-*endo* product

1\1\GINC-AC56\FOpt\UBHandHLYP\6-311G(d,p)\C3H8N1Si1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,-2.0233055856,-0.5361053541,0.1954481849\C,-0.729291105,-1.3463413953,-0.0494336204\H,-2.2007474791,-0.4530457224,1.2725199728\H,-2.8927919576,-1.0152377458,-0.2396425508\H,1.4347389776,0.047979369,-1.212757051\H,1.5079086519,-0.088929328,1.1784221721\H,-0.7596446295,-1.8065724222,-1.0322676912\H,-

0.6077728153,-2.140953876,0.6780898682\C,-0.6735379798,1.3910911876,0.1406158937\H,-0.4574407177,2.3162638696,-0.3788764802\H,-0.7854946321,1.6264297093,1.2053294907\N,-1.8872511595,0.796238419,-0.3542504826\Si,0.6081274322,-0.0134937101,0.0086872971\\Version=IA64L-G03RevD.01\HF=-463.2548307\S2=0.756161\S2-1=0.\S2A=0.750029\RMSD=9.778e-09\RMSF=4.462e-06\Thermal=0.\Dipole=0.3419484,-0.3698317,0.4449723\PG=C01 [X(C3H8N1Si1)]\\@

Cyclization of 12b:

12b

1\1\GINC-AC50\FOpt\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,2.5691180209,0.6056010411,0.0910318596\H,2.7034931249,1.003857654,-0.9194642538\H,2.5635507051,1.4475812249,0.7803757882\C,1.234095637,-0.1225891449,0.1924149609\H,1.1461896146,-0.535843892,1.1933152531\H,1.2463551767,-0.9687393421,-0.4911845708\C,0.0459404381,0.7914692156,-0.1190613309\H,0.1494527793,1.2128789179,-1.1175849759\H,0.0381788938,1.6361012427,0.567824464\H,-1.8864936222,-0.5957704611,1.3442369856\H,-1.7342507493,-1.1696477907,-0.9998166667\C,4.5676107074,-0.4801766641,-0.3449136998\H,4.5964375278,-0.0314783996,-1.3389332509\H,5.3841395754,-1.1377145877,-0.0774744305\N,3.651027713,-0.2683937,0.4793761683\Si,-1.6290055426,-0.0678073127,-0.0153423019\\Version=IA64L-G03RevD.01\HF=-502.5292586\S2=0.751657\S2-1=0.\S2A=0.750001\RMSD=4.720e-09\RMSF=7.428e-06\Thermal=0.\Dipole=0.3087401,0.3839014,-0.5539685\PG=C01 [X(C4H10N1Si1)]\\@

5-*exo* transition state

1\1\GINC-AC29\FTS\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** freq=noraman opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) scf=direct\\freq&geom\\0,2\C,1.2892703683,1.6808246458,0.2899914984\C,-0.2014958791,1.6199234997,-0.0444296093\C,1.990875928,0.5047081181,-0.368455565\H,1.74471792,2.61507832,-0.0286408079\H,1.4323600003,1.6043822869,1.3652566522\H,1.9504396441,0.5981097822,-1.4515299451\H,3.0332932718,0.4167707443,-0.0764977064\H,-2.1936868005,-0.0638754053,-0.7479410651\H,-1.0912322998,-0.7671013355,1.2307572639\H,-0.7830839325,2.2111463725,0.6575578011\H,-0.3828219471,2.0531342467,-1.0273131332\C,1.8233049587,-1.8154097756,0.1000889246\H,1.2524000495,-2.6765360088,0.4115337479\H,2.8635149216,-1.9541495927,-0.1660457381\N,1.2490165212,-0.6871784684,0.032079676\Si,-0.833418725,-0.1745634302,-0.1024089417\\Version=IA64L-G03RevD.01\State=2-A\HF=-502.5243551\S2=0.76955\S2-1=0.\S2A=0.750094\RMSD=2.530e-09\RMSF=2.373e-05\Thermal=0.\Dipole=1.5319011,-0.1619281,-0.0759274\PG=C01 [X(C4H10N1Si1)]\\@

5-*exo* product

1\1\GINC-AC1\FOpt\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,-1.2656478494,1.7006285155,-0.2825371566\C,0.2052658182,1.6646492712,0.1698852545\C,-1.9533455832,0.4217543161,0.1892448183\H,-1.7862755069,2.5775197659,0.091109816\H,-1.306246594,1.739610579,-1.3682786212\H,-2.2319423609,0.501624848,1.2421736162\H,-2.8653544041,0.236088518,-0.3736720878\H,1.4385215153,-0.7085921154,1.0943842595\H,1.3373954576,-0.5055414697,-1.2753494678\H,0.8241314986,2.3480387675,-0.4006577411\H,0.2894419602,1.9481231594,1.2168207453\C,-1.4892870489,-1.9720461452,0.0652217658\H,-0.7978575181,-2.773125221,-0.1215981396\H,-2.5406168965,-2.14069488,-0.0867508424\N,-1.0187286781,-0.6799880515,-0.0102156358\Si,0.6395611902,-0.1520108582,-0.0196085817\\Version=IA64L-G03RevD.01\HF=-502.5757111\S2=0.755312\S2-1=0.\S2A=0.750019\RMSD=5.376e-09\RMSF=2.131e-05\Thermal=0.\Dipole=-0.0803851,0.5418792,-0.0584512\PG=C01 [X(C4H10N1Si1)]\\@

6-*endo* transition state

1\1\GINC-AC57\FTS\UBHandHLYP\6-311G(d,p)\C4H10N1Si1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,1.6717551678,1.163580144,0.4560799852\C,0.3024301371,1.4627637673,-0.1638459543\C,2.4382258811,0.0589036599,-0.2725643419\H,-0.1199766765,2.3454733102,0.3097068804\H,0.4201019287,1.7030308879,-1.21837035\H,2.2898251746,2.0583146182,0.4420490817\H,1.5466148916,0.9032804409,1.5047677243\H,3.3247949282,-0.2114824604,0.3023173107\H,2.7873452266,0.4362193371,-1.228341125\H,-1.4327919695,-0.4550179236,-1.2939080467\H,-2.1517218817,0.5191903576,0.7913169878\N,1.6529377467,-1.1340658537,-0.5461699167\C,1.026897936,-1.6643538626,0.4310009648\H,1.1649172183,-1.3784476658,1.4716122538\H,0.4608803153,-2.5675414491,0.2554595223\Si,-0.9723720244,0.0681866922,0.0072860246\\Version=IA64L-G03RevD.01\HF=-502.5152373\S2=0.791216\S2-

1=0.\S2A=0.750201\RMSD=4.502e-09\RMSF=1.141e-
05\Thermal=0.\Dipole=0.3024956,0.3239936,0.6277942\PG=C01 [X(C4H10N1Si1)]\\@

6-*endo* product
1\1\GINC-AC58\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\13-Jul-
2007\0\\# BHandHLYP/6-311G** nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman
scf=direct\\freq&geom\\0,2\C,-0.4979038604,-1.6040897674,-0.2944806931\C,-
1.5509259384,1.2986582429,0.272166943\C,-2.368175956,0.1195493556,-0.237361209\C,-1.8826136671,-
1.2403454343,0.2575619224\H,1.2413805995,-0.4204913283,1.481037629\H,1.8999706472,-0.2268206799,-
0.8120932506\H,-0.5583573371,-1.7262222138,-1.3743623116\H,-0.161026793,-2.5554074837,0.1099582431\H,-
1.6524805076,1.3703759883,1.3585009867\H,-1.9629955067,2.216423262,-0.1392669094\H,-
3.3984559616,0.2716875876,0.0757628706\H,-2.3632317178,0.1299799226,-1.3260180556\H,-1.8567271618,-
1.2347511435,1.347364243\H,-2.6035446109,-2.0037653011,-0.0244439213\N,-0.1436702523,1.2361541849,-
0.1076530228\C,0.5333667204,2.4422799431,-0.1564330822\H,1.555171335,2.4256529386,-0.4912930346\H,-
0.0464611827,3.3369184239,-0.3014180547\Si,0.7365981513,-0.2545944974,0.095379707\\Version=IA64L-
G03RevD.01\HF=-541.8765479\S2=0.755565\S2-1=0.\S2A=0.75002\RMSD=6.239e-09\RMSF=1.898e-
05\Thermal=0.\Dipole=-0.5185724,-0.3396541,-0.093378\PG=C01 [X(C5H12N1Si1)]\\@

Cyclization of 12c:
12c
1\1\GINC-AC26\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\05-Mar-2008\0\\# BHandHLYP/6-
311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,0.2939038223,-
0.9405410873,1.8181912947\C,0.4927338963,0.505793977,1.3519631413\C,1.6811590401,0.6625344017,0.41142379
06\C,1.8801652915,2.0981097759,-
0.051885333\H,2.0158100567,2.7356034027,0.8198015364\H,0.9915637922,2.4508565831,-
0.5846420998\H,1.5457969006,0.0247713611,-
0.4603229018\H,2.5920502337,0.3285908056,0.9020263696\H,0.6337621963,1.152060561,2.2169133306\H,-
0.4106537907,0.8562730474,0.8550621155\H,0.1575282475,-1.5903250872,0.9555657201\H,1.1928949476,-
1.2915415383,2.3214992082\H,-2.4494848267,-0.8202426452,2.3267920957\H,-1.016324811,-
0.3979440626,4.2253975725\N,3.0736019257,2.2093253158,-0.8585484861\C,2.9643474084,2.658846139,-
2.0205093822\H,3.8444062461,2.7454485626,-2.6439476478\H,2.0153865649,2.9778404985,-2.4540915183\Si,-
1.1704491455,-1.1852350068,2.9797921954\\Version=IA64L-G03RevD.01\HF=-541.8264156\S2=0.751663\S2-
1=0.\S2A=0.750001\RMSD=4.953e-09\RMSF=1.067e-05\Thermal=0.\Dipole=-0.198482,0.1568563,-
0.4655811\PG=C01 [X(C5H12N1Si1)]\\@

6-*exo* transition state
1\1\GINC-AC3\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G**
nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,-
0.0475921268,-1.5265072195,0.5189835327\C,1.9790002442,0.6239976198,-0.5391518945\C,2.352382395,-
0.7073343379,0.0944313924\C,1.3193712096,-1.8114384482,-0.1142392452\H,-2.1521649044,-0.6403701837,-
0.9870327118\H,-1.6651621275,0.7508612924,0.8481139367\H,0.0834232932,-1.3644393263,1.5878969212\H,-
0.6768209546,-2.4075323141,0.4192529587\H,1.7746571027,0.48270925,-
1.596674133\H,2.7950821916,1.338090697,-0.4507544281\H,3.3060912075,-1.0191882385,-
0.3261972353\H,2.5153205436,-0.5537846726,1.160041716\H,1.202711115,-1.9883123333,-
1.1833203979\H,1.7256386972,-
2.7329830333,0.2989838005\N,0.7754878512,1.1678995305,0.082934091\C,0.7570773574,2.3834173644,0.4358312
004\H,-0.1312553362,2.7792730429,0.9035085709\H,1.5924421768,3.0505908191,0.2597391575\Si,-0.9970869355,-
0.0502065086,-0.2083782324\\Version=IA64L-G03RevD.01\HF=-541.8214562\S2=0.765842\S2-
1=0.\S2A=0.750074\RMSD=6.880e-09\RMSF=6.355e-
05\Thermal=0.\Dipole=1.3896169,0.7428756,0.1269047\PG=C01 [X(C5H12N1Si1)]\\@

6-*exo* product
1\1\GINC-AC58\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-
311G** nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,-0.4979038604,-
1.6040897674,-0.2944806931\C,-1.5509259384,1.2986582429,0.272166943\C,-2.368175956,0.1195493556,-
0.237361209\C,-1.8826136671,-1.2403454343,0.2575619224\H,1.2413805995,-
0.4204913283,1.481037629\H,1.8999706472,-0.2268206799,-0.8120932506\H,-0.5583573371,-1.7262222138,-
1.3743623116\H,-0.161026793,-2.5554074837,0.1099582431\H,-1.6524805076,1.3703759883,1.3585009867\H,-
1.9629955067,2.216423262,-0.1392669094\H,-3.3984559616,0.2716875876,0.0757628706\H,-
2.3632317178,0.1299799226,-1.3260180556\H,-1.8567271618,-1.2347511435,1.347364243\H,-2.6035446109,-
2.0037653011,-0.0244439213\N,-0.1436702523,1.2361541849,-0.1076530228\C,0.5333667204,2.4422799431,-
0.1564330822\H,1.555171335,2.4256529386,-0.4912930346\H,-0.0464611827,3.3369184239,-

0.3014180547\Si,0.7365981513,-0.2545944974,0.095379707\\Version=IA64L-G03RevD.01\HF=-541.8765479\S2=0.755565\S2-1=0.\S2A=0.75002\RMSD=6.239e-09\RMSF=1.898e-05\Thermal=0.\Dipole=-0.5185724,-0.3396541,-0.093378\PG=C01 [X(C5H12N1Si1)]\\@

7-*endo* transition state
1\1\GINC-AC29\FTS\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\12-Jul-2007\0\\# BHandHLYP/6-311G** nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,-0.1118486177,-1.4875203998,-0.3347143693\C,-1.372492339,-1.4630591473,0.5466007107\C,-2.5707072442,-0.7170661554,-0.0389235255\C,-2.2866632766,0.7062030808,-0.5135679942\H,-0.3747782158,-1.483809949,-1.3905672964\H,1.6164213488,-0.2207739863,1.4214381052\H,-1.1390497818,-1.0324241898,1.5167288309\H,-3.3485099566,-0.6841660696,0.7194647456\H,0.4250086563,-2.4217525298,-0.1717318515\H,2.323314034,-0.2531316235,-0.8913498495\H,-1.6884536657,-2.4845740976,0.7426769912\H,-2.9761792159,-1.2758052095,-0.8810062191\H,-3.2363819683,1.2131209309,-0.6724904669\H,-1.7675007411,0.692074188,-1.4764727524\C,-0.4863459463,2.0362626691,0.0727482634\H,0.0958005457,2.6151856123,0.7749527829\N,-1.5397653701,1.4410411223,0.4785458322\H,-0.2517058142,2.168256116,-0.9818333024\Si,1.1551215685,-0.1320423617,0.0173413643\\Version=IA64L-G03RevD.01\HF=-541.8145442\S2=0.792394\S2-1=0.\S2A=0.750208\RMSD=5.832e-09\RMSF=1.018e-05\Thermal=0.\Dipole=-0.0686907,-0.1160918,-0.5647434\PG=C01 [X(C5H12N1Si1)]\\@

7-*endo* product
1\1\GINC-AC59\FOpt\UBHandHLYP\6-311G(d,p)\C5H12N1Si1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman scf=direct\\freq&geom\\0,2\C,0.26847869,-1.431433323,0.373275031\C,1.5478548083,-1.3748856152,-0.4791461789\C,2.6077908241,-0.3799450734,0.0012092103\C,2.0656863056,0.9765952501,0.4659402674\H,0.5082262603,-1.3952846488,1.4344602999\H,-1.4434122013,-0.3334054855,-1.4603035536\H,1.2845166639,-1.1367887302,-1.5070515863\H,3.319717581,-0.220988068,-0.803427403\H,-0.2292265156,-2.3866203068,0.2153935415\H,-2.1600132397,-0.1376860221,0.8232922826\H,2.0054746329,-2.3604152292,-0.5119577215\H,3.1630110974,-0.8082419129,0.8337662474\H,2.9054301402,1.6640132943,0.5581607515\H,1.6272750354,0.8741546651,1.462204254\C,-0.1828097745,1.6335367736,0.02373771\H,-0.7743170155,2.3210368785,-0.5748620969\N,1.1400471756,1.5325659056,-0.4853083612\H,-0.2181238536,1.9571356129,1.0687422481\Si,-0.9840036148,-0.1004849651,-0.0752269428\\Version=IA64L-G03RevD.01\HF=-541.8544461\S2=0.756583\S2-1=0.\S2A=0.750033\RMSD=2.513e-09\RMSF=1.779e-05\Thermal=0.\Dipole=0.0542328,-0.3351607,0.5804418\PG=C01 [X(C5H12N1Si1)]\\@

Cyclization of 13b:
13b
1\1\GINC-AC2\FOpt\UBHandHLYP\6-311G(d,p)\C6H14N1Si1(2)\UXW563\14-Jun-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\Si,-3.8938444154,-0.273641909,-0.03971133\C,-2.2216963485,0.5967848472,-0.0383684307\C,-1.0171355292,-0.3413847392,-0.0525960577\C,0.3089867747,0.3990344493,-0.0141287927\H,0.3672182552,1.0796461524,-0.8665722516\H,0.3484053785,1.0240217267,0.8808905096\H,-1.0529131467,-1.0204247156,0.7960938807\H,-1.0325880745,-0.9674089032,-0.9413954173\H,-2.1875005287,1.2690002007,-0.89442515\H,-2.1898747461,1.234172819,0.8470870177\H,-4.0278907979,-1.1973374416,1.1110093319\H,-5.0100209672,0.7004907998,-0.0251982996\C,3.7122651864,-1.1207736077,-0.0183653339\H,4.3587592066,-0.9499239666,-0.8769022796\H,4.3321942487,-1.0189444309,0.8702072492\H,3.309872884,-2.1235609091,-0.0641317784\C,2.5943728218,-0.1223070986,0.0037331182\C,2.9893064477,1.3323296717,0.0704760058\H,4.0655963892,1.4535008254,0.0843145581\H,2.5950285386,1.8779143482,-0.7830065355\H,2.5819700083,1.800544435,0.9630390205\N,1.4080644146,-0.542052554,-0.0338220347\\Version=IA64L-G03RevD.01\HF=-581.1361761\S2=0.751605\S2-1=0.\S2A=0.750001\RMSD=5.038e-09\RMSF=1.552e-06\Thermal=0.\Dipole=0.7836478,0.7549596,-0.0210404\PG=C01 [X(C6H14N1Si1)]\\@

5-*exo* transition state
1\1\GINC-AC50\FTS\UBHandHLYP\6-311G(d,p)\C6H14N1Si1(2)\UXW563\23-Aug-2006\1\\# Bhandhlyp/6-311G** scf=verytight opt=(ts,noeigentest,z-matrix,calcfc,maxcycle=500) freq=noraman\\geom &
freq\\0,2\C\C,1,B1\C,2,B2,1,A1\H,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,2,B5,1,A4,3,D3,0\H,2,B6,1,A5,3,D4,0\H,3,B7,2,A6,1,D5,0\H,3,B8,2,A7,1,D6,0\H,1,B9,2,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\C,3,B11,2,A10,1,D9,0\C,12,B12,3,A11,2,D10,0\H,13,B13,12,A12,3,D11,0\H,13,B14,12,A13,3,D12,0\H,13,B15,12,A14,3,D13,0\C,12,B16,3,A15,2,D14,0\H,17,B17,12,A16,3,D15,0\H,17,B18,12,A17,3,D16,0\H,17,B19,12,A18,3,D17,0\N,12,B20,3,A19,2,D18,0\Si,1,B21,2,A20,3,D19,0\\B1=1.52472606\B2=1.51966413\B3=1.08956603\B4=1.08655634\B5=1.08762236\B6=1.08768361\B7=1.08490433\B8=1.0894108\B9=2.82603357\B10=2.69288594\B11=2.40624859\B12=1.49345543\B13=1.08354599\B14=1.09219855\B15=1.08505144\B16=1.49698737\B17=1.0871595\B18=1.08055065\B19=1.08975078\B20=1.28161031\

B21=1.89845218\A1=109.35553948\A2=110.25434085\A3=111.27909111\A4=112.38613442\A5=109.80602753\A6=110.89479697\A7=110.43048058\A8=102.48254213\A9=142.79578969\A10=132.11143791\A11=148.35532559\A12=111.97828234\A13=108.81807031\A14=111.21669525\A15=94.61910909\A16=110.17593052\A17=113.64832196\A18=109.17444493\A19=30.81858475\A20=110.64343189\D1=79.29687052\D2=-163.05629873\D3=-122.33811504\D4=118.53455068\D5=171.73386401\D6=-68.84809687\D7=-68.35449698\D8=-29.41072603\D9=61.44462967\D10=-18.7095672\D11=181.22228124\D12=-58.15697322\D13=59.01651785\D14=163.73088872\D15=-123.11354788\D16=-0.79696221\D17=120.13220693\D18=-21.98761094\D19=-39.38626399\\Version=IA64L-G03RevD.01\State=2-A\HF=-581.1337336\S2=0.768149\S2-1=0.\S2A=0.750088\RMSD=7.328e-09\RMSF=7.247e-06\Thermal=0.\Dipole=0.7722195,-0.1666341,1.51346\PG=C01 [X(C6H14N1Si1)]\\@

5-*exo* product

1\1\GINC-AC28\FOpt\UBHandHLYP\6-311G(d,p)\C6H14N1Si1(2)\UXW563\09-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(Z-matrix,readfc,maxcycle=500) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\C,2,B2,1,A1\H,1,B3,3,A2,2,D1,0\H,1,B4,3,A3,2,D2,0\H,2,B5,1,A4,3,D3,0\H,2,B6,1,A5,3,D4,0\H,3,B7,2,A6,1,D5,0\H,3,B8,2,A7,1,D6,0\N,2,B9,1,A8,3,D7,0\Si,1,B10,3,A9,2,D8,0\H,11,B11,1,A10,3,D9,0\H,11,B12,1,A11,3,D10,0\C,10,B13,2,A12,1,D11,0\C,14,B14,10,A13,2,D12,0\H,15,B15,14,A14,10,D13,0\H,15,B16,14,A15,10,D14,0\H,15,B17,14,A16,10,D15,0\C,14,B18,10,A17,2,D16,0\H,19,B19,14,A18,10,D17,0\H,19,B20,14,A19,10,D18,0\H,19,B21,14,A20,10,D19,0\\B1=2.48840447\B2=1.52606842\B3=1.08792323\B4=1.08425841\B5=1.08481844\B6=1.09332092\B7=1.08728034\B8=1.08636464\B9=1.46271631\B10=1.87619856\B11=1.4785729\B12=1.48062775\B13=1.39888201\B14=1.49288723\B15=1.08800533\B16=1.08514447\B17=1.0958955\B18=1.49267321\B19=1.08487807\B20=1.08574895\B21=1.09686134\A1=35.77952722\A2=110.54783028\A3=112.2892383\A4=143.47758432\A5=100.28263106\A6=108.65103302\A7=110.52275424\A8=80.32755606\A9=102.19702175\A10=114.83354036\A11=113.30663759\A12=120.1681747\A13=116.01961737\A14=112.41483341\A15=110.63585942\A16=112.12660473\A17=118.86472928\A18=109.80794717\A19=112.8146816\A20=112.29942482\D1=-79.90430132\D2=160.20885896\D3=28.29234339\D4=-110.42165944\D5=118.91639768\D6=-123.65650189\D7=139.96396369\D8=36.29359425\D9=99.54536711\D10=-137.1555139\D11=166.51333862\D12=172.25395309\D13=47.04269354\D14=-193.3730525\D15=-73.60436368\D16=23.82681383\D17=186.02896126\D18=-54.17689488\D19=67.01038148\\Version=IA64L-G03RevD.01\State=2-A\HF=-581.1759572\S2=0.755507\S2-1=0.\S2A=0.750023\RMSD=0.000e+00\RMSF=1.508e-05\Thermal=0.\Dipole=0.3652093,-0.1991047,-0.018724\PG=C01 [X(C6H14N1Si1)]\\@

6-*endo* transition state

1\1\GINC-AC9\FTS\UBHandHLYP\6-311G(d,p)\C6H14N1Si1(2)\UXW563\22-Aug-2006\1\\# BHandHLYP/6-311G** scf=(qc,direct) opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\geom & freq\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,3,B4,2,A3,1,D2,0\H,2,B5,1,A4,3,D3,0\H,2,B6,1,A5,3,D4,0\H,1,B7,2,A6,3,D5,0\H,1,B8,2,A7,3,D6,0\H,1,B9,2,A8,3,D7,0\H,1,B10,2,A9,3,D8,0\H,3,B11,2,A10,1,D9,0\C,4,B12,3,A11,2,D10,0\H,13,B13,4,A12,3,D11,0\H,13,B14,4,A13,3,D12,0\H,13,B15,4,A14,3,D13,0\C,4,B16,3,A15,2,D14,0\H,17,B17,4,A16,3,D15,0\H,17,B18,4,A17,3,D16,0\H,17,B19,4,A18,3,D17,0\Si,1,B20,2,A19,3,D18,0\N,4,B21,3,A20,2,D19,0\\B1=1.52884727\B2=1.52962904\B3=2.38739009\B4=1.08655316\B5=1.08683716\B6=1.08818194\B7=1.08973886\B8=1.08906816\B9=2.80222068\B10=2.75978075\B11=1.09022159\B12=1.50918091\B13=1.08989211\B14=1.08447316\B15=1.08175078\B16=1.51714624\B17=1.08331639\B18=1.08993707\B19=1.08118594\B20=1.89030197\B21=1.29684152\A1=112.91823978\A2=111.99784918\A3=108.7703037\A4=109.79539999\A5=110.09154442\A6=110.03999085\A7=109.76821476\A8=99.38043648\A9=145.90852539\A10=109.69315068\A11=146.73354316\A12=108.56454342\A13=112.23245193\A14=110.20500488\A15=96.04956907\A16=110.33369924\A17=108.56878133\A18=113.92033177\A19=115.23959223\A20=31.01288325\D1=33.83540721\D2=-179.73740266\D3=120.75255417\D4=-121.62239007\D5=66.87846966\D6=-177.14526554\D7=-81.44012722\D8=-53.43645739\D9=-62.70437803\D10=98.2976839\D11=87.27085119\D12=-153.93177629\D13=-31.1345314\D14=-106.33203444\D15=154.95315983\D16=-87.3173972\D17=32.85800901\D18=-55.54053737\D19=89.588955\\Version=IA64L-G03RevD.01\State=2-A\HF=-581.1219411\S2=0.792485\S2-1=0.\S2A=0.750222\RMSD=0.000e+00\RMSF=1.146e-05\Thermal=0.\Dipole=0.3666812,-0.6422905,-0.0691869\PG=C01 [X(C6H14N1Si1)]\\@

6-*endo* product

1\1\GINC-AC35\FOpt\UBHandHLYP\6-311G(d,p)\C6H14N1Si1(2)\UXW563\09-Sep-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check opt=(Z-matrix,readfc,maxcycle=500) scf=(qc,direct) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\H,2,B4,1,A3,4,D2,0\H,2,B5,1,A4,4,D3,0\H,1,B6,4,A5,2,D4,0\H,1,B7,4,A6,2,D5,0\H,4,B8,1,A7,2,D6,0\H,4,B9,1,A8,2,D7,0\H,3,B10,2,A9,1,D8,0\H,3,B11,2,A10,1,D9,0\C,3,B12,2,A11,1,D10,0\H,13,B13,3,A12,2,D11,0\H,13,B14,3,A13,2,D12,0\H,13,B15,3,A14,2,D13,0\C,13,B16,3,A15,2,D14,0\C,17,B17,13,A16,3,D15,0\H,18,B18,17,A17,13,D16,0\H,18,B19,17,A18,13,D17,0\H,18,B20,17,A19,13,D18,0\N,17,B21,13,A20,3,D19,0\\B1=1.53256414\B2=1.88037137\B3=1.53763988\B4=1.08703966\B5=1.08895912\B6=1.08751354\B7=1.08719781\B8=1.0855074\B9=1.0908826\B10=1.48086451\B11=1.47723379\B12=2.85685667\B13=1.08791885\B14=1.08395093\B15=1.08723455\B16=1.52798913\B17=1.53837995\B18=1.08825226\B19=1.

08510682\B20=1.08441829\B21=1.4341165\A1=110.62972832\A2=112.73883049\A3=110.47694455\A4=109.86734762\A5=108.4067245\A6=108.12473973\A7=108.63416927\A8=109.05461035\A9=112.2299212\A10=111.38252728\A11=132.36801851\A12=148.88362348\A13=89.71103897\A14=89.48747252\A15=38.92343245\A16=109.5737837\A17=109.78098404\A18=109.84586183\A19=113.89034171\A20=108.29437599\D1=50.67788475\D2=173.68763875\D3=-69.3454865\D4=-122.73643196\D5=121.760381\D6=178.39604132\D7=61.41122158\D8=-162.21691763\D9=75.67862429\D10=-31.07491238\D11=-24.17317009\D12=101.47267411\D13=-149.76189109\D14=-22.97140642\D15=-121.64648625\D16=-67.750625\D17=50.62465329\D18=171.18768889\D19=111.73240143\\Version=IA64L-G03RevD.01\State=2-A\HF=-581.1524125\S2=0.75724\S2-1=0.\S2A=0.750038\RMSD=0.000e+00\RMSF=1.623e-05\Thermal=0.\Dipole=-0.5719929,-0.289102,0.2924615\PG=C01 [X(C6H14N1Si1)]\\@

Cyclization of 13c:

13c

1\1\GINC-AC24\FOpt\UBHandHLYP\6-311G(d,p)\C7H16N1Si1(2)\UXW563\08-Mar-2008\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,0.4638889262,-0.8474876204,2.2424915419\C,0.4019629304,0.3544292716,1.2931069079\C,1.6470070791,0.4885418781,0.4264483442\C,1.5909618226,1.6766952191,-0.5167148375\H,1.4566943379,2.5936158533,0.061607002\H,0.7127951358,1.5893307576,-1.1604236539\H,1.7891625356,-0.4153627016,-0.1621597914\H,2.5295417276,0.58600817,1.0549502528\H,0.2648614784,1.2675396624,1.8712025605\H,-0.475393594,0.2675676657,0.653189633\H,0.6004039352,-1.7625980631,1.6690634497\H,1.3369639088,-0.7626278504,2.8870112416\H,-2.2830763337,-1.2737162158,2.5234906998\H,-1.2657683765,0.1225173522,4.2111704182\N,2.8040356714,1.7504708026,-1.3039083714\C,2.9225348531,2.6368790488,-2.1900723336\Si,-1.0603432795,-1.0522026144,3.3311620106\C,4.1889651077,2.6892141582,-2.990509026\H,4.6795807999,3.6525174953,-2.8655665204\H,4.8577753328,1.9005721773,-2.6736904641\H,3.9743928235,2.5783834661,-4.0516337918\C,1.8723406978,3.66886738,-2.5198479923\H,0.963506135,3.1896853123,-2.87558125\H,1.6042601771,4.2436180506,-1.6374570753\H,2.2139511629,4.3559423509,-3.2843859504\\Version=IA64L-G03RevD.01\HF=-620.4332385\S2=0.751667\S2-1=0.\S2A=0.750001\RMSD=6.245e-09\RMSF=1.484e-05\Thermal=0.\Dipole=-0.0332737,0.6252085,-0.5563341\PG=C01 [X(C7H16N1Si1)]\\@

6-*exo* transition state

1\1\GINC-AC31\FTS\UBHandHLYP\6-311G(d,p)\C7H16N1Si1(2)\UXW563\21-Aug-2006\1\\# BHandHLYP/6-311G** scf=(qc,direct) opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\geom & freq\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,1,B6,4,A5,3,D4,0\H,1,B7,4,A6,3,D5,0\H,2,B8,1,A7,4,D6,0\H,2,B9,1,A8,4,D7,0\H,3,B10,2,A9,1,D8,0\H,3,B11,2,A10,1,D9,0\H,4,B12,3,A11,2,D10,0\H,4,B13,3,A12,2,D11,0\C,2,B14,1,A13,4,D12,0\C,15,B15,2,A14,1,D13,0\H,16,B16,15,A15,2,D14,0\H,16,B17,15,A16,2,D15,0\H,16,B18,15,A17,2,D16,0\C,15,B19,2,A18,1,D17,0\H,20,B20,15,A19,2,D18,0\H,20,B21,15,A20,2,D19,0\H,20,B22,15,A21,2,D20,0\N,15,B23,2,A22,1,D21,0\Si,1,B24,4,A23,3,D22,0\\B1=3.14362186\B2=1.52193274\B3=1.52393263\B4=2.73065385\B5=2.77645594\B6=1.08840711\B7=1.08739217\B8=1.08807381\B9=1.08452036\B10=1.08854877\B11=1.0889146\B12=1.0903707\B13=1.08880593\B14=2.37390999\B15=1.49359655\B16=1.09117406\B17=1.08030655\B18=1.08597331\B19=1.50509427\B20=1.08415888\B21=1.08865796\B22=1.08471795\B23=1.28548271\B24=1.89275151\A1=53.60794166\A2=115.31667357\A3=114.31665599\A4=138.62372597\A5=109.19926203\A6=109.74116933\A7=97.38790796\A8=154.13258538\A9=107.4117343\A10=108.37814638\A11=109.04991485\A12=108.24623715\A13=96.1548526\A14=151.83275124\A15=109.93343738\A16=111.70430027\A17=110.37527772\A18=92.0489959\A19=110.10238803\A20=111.51251136\A21=111.8603907\A22=32.7096461\A23=114.32204879\D1=29.67949096\D2=100.1124173\D3=42.43350702\D4=-57.02443122\D5=-173.47521296\D6=76.21594555\D7=-85.04929807\D8=151.66067152\D9=-93.45003653\D10=59.63892662\D11=174.51104697\D12=-173.96942179\D13=4.96306708\D14=-101.3401645\D15=18.61714517\D16=140.62498099\D17=-175.4402789\D18=164.94765889\D19=-76.09907011\D20=44.49771595\D21=-2.8681423\D22=64.79165319\\Version=IA64L-G03RevD.01\State=2-A\HF=-620.425591\S2=0.772121\S2-1=0.\S2A=0.750108\RMSD=0.000e+00\RMSF=3.751e-05\Thermal=0.\Dipole=0.3319022,-0.5035256,1.4391895\PG=C01 [X(C7H16N1Si1)]\\@

6-*exo* product

1\1\GINC-AC29\FOpt\UBHandHLYP\6-311G(d,p)\C7H16N1Si1(2)\UXW563\18-Aug-2006\1\\# BHandHLYP/6-311G** geom=checkpoint guess=check scf=(qc,direct) opt=(readfc,z-matrix,maxcycle=500) freq=noraman\\geom & freq\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\H,1,B4,4,A3,3,D2,0\H,1,B5,4,A4,3,D3,0\H,1,B6,4,A5,3,D4,0\H,1,B7,4,A6,3,D5,0\H,2,B8,1,A7,4,D6,0\H,2,B9,1,A8,4,D7,0\H,3,B10,2,A9,1,D8,0\H,3,B11,2,A10,1,D9,0\H,4,B12,3,A11,2,D10,0\H,4,B13,3,A12,2,D11,0\C,2,B14,1,A13,4,D12,0\C,15,B15,2,A14,1,D13,0\H,16,B16,15,A15,2,D14,0\H,16,B17,15,A16,2,D15,0\H,16,B18,15,A17,2,D16,0\C,15,B19,2,A18,1,D17,0\H,20,B20,15,A19,2,D18,0\H,20,B21,15,A20,2,

D19,0\H,20,B22,15,A21,2,D20,0\N,15,B23,2,A22,1,D21,0\Si,24,B24,15,A23,2,D22,0\\B1=3.10789748\B2=1.5229107
8\B3=1.52549321\B4=2.74580155\B5=2.78409492\B6=1.08881545\B7=1.08769395\B8=1.09390467\B9=1.08257765\
B10=1.08792377\B11=1.08886424\B12=1.09005487\B13=1.08744221\B14=2.44540906\B15=1.49236858\B16=1.086
47666\B17=1.0868054\B18=1.09480376\B19=1.49640349\B20=1.08635741\B21=1.09566913\B22=1.08397311\B23=
1.40685487\B24=1.74141202\A1=54.2270044\A2=113.80714237\A3=104.43372571\A4=138.06408097\A5=109.4529
7076\A6=110.74435454\A7=101.90008148\A8=151.27824706\A9=107.82317208\A10=108.95870011\A11=108.8557
6733\A12=109.58302052\A13=98.07199311\A14=144.02787919\A15=109.99142164\A16=112.09228797\A17=112.8
7044907\A18=99.82277873\A19=110.88565132\A20=110.72734689\A21=113.30921135\A22=32.4684047\A23=123.
88462368\D1=30.5370772\D2=84.25256008\D3=37.12090977\D4=-
66.97333209\D5=175.71926367\D6=70.59226781\D7=-95.35801362\D8=152.05096756\D9=-
92.12008743\D10=57.06803858\D11=-187.17408961\D12=179.6447387\D13=-53.00075783\D14=-
134.46219483\D15=-
14.89841066\D16=106.64398241\D17=125.04729945\D18=131.19224309\D19=249.9854758\D20=9.94705943\D21=
-3.91877535\D22=-159.43704484\\Version=IA64L-G03RevD.01\State=2-A\HF=-620.4726959\S2=0.755593\S2-
1=0.\S2A=0.750023\RMSD=0.000e+00\RMSF=2.017e-
05\Thermal=0.\Dipole=0.2467034,0.2495138,0.0600702\PG=C01 [X(C7H16N1Si1)]\\@

7-*endo* transition state
1\1\GINC-AC7\FTS\UBHandHLYP\6-311G(d,p)\C7H16N1Si1(2)\UXW563\21-Aug-2006\1\\# BHandHLYP/6-
311G** scf=(qc,direct) opt=(ts,noeigentest,z-matrix,calcfc,maxcycle=500) freq=noraman\\geom &
freq\\0,2\C\C,1,B1\C,1,B2,2,A1\C,2,B3,1,A2,3,D1,0\C,4,B4,2,A3,1,D2,0\H,1,B5,2,A4,4,D3,0\H,1,B6,2,A5,4,D4,0\H,2,
B7,1,A6,4,D5,0\H,4,B8,2,A7,1,D6,0\H,1,B9,2,A8,4,D7,0\H,1,B10,2,A9,4,D8,0\H,2,B11,1,A10,4,D9,0\H,4,B12,2,A11,
1,D10,0\H,5,B13,4,A12,2,D11,0\H,5,B14,4,A13,2,D12,0\Si,1,B15,2,A14,4,D13,0\C,3,B16,1,A15,2,D14,0\H,17,B17,3,
A16,1,D15,0\H,17,B18,3,A17,1,D16,0\H,17,B19,3,A18,1,D17,0\C,3,B20,1,A19,2,D18,0\H,21,B21,3,A20,1,D19,0\H,2
1,B22,3,A21,1,D20,0\H,21,B23,3,A22,1,D21,0\N,3,B24,1,A23,2,D22,0\\B1=1.53662452\B2=3.5323113\B3=1.527491
18\B4=1.52476119\B5=2.77426495\B6=1.08735448\B7=1.09048428\B8=1.08760022\B9=2.77081357\B10=1.090048
36\B11=1.08791148\B12=1.08855536\B13=1.08971022\B14=1.09085713\B15=1.88186156\B16=1.5166515\B17=1.0
8364679\B18=1.09013245\B19=1.08107592\B20=1.51047285\B21=1.0898961\B22=1.08446795\B23=1.08211641\B2
4=1.2951158\A1=90.98398151\A2=115.8625381\A3=115.73571809\A4=100.18320218\A5=109.92382336\A6=110.1
1943502\A7=109.55924244\A8=147.33609564\A9=108.98614272\A10=108.25524913\A11=108.09143314\A12=108.
18831219\A13=109.31387074\A14=117.1907753\A15=117.93191052\A16=110.55982239\A17=108.44169889\A18=1
14.02042855\A19=111.63603465\A20=108.60830736\A21=112.4331397\A22=110.26114825\A23=59.88578874\D1=
43.02630694\D2=-66.58548157\D3=109.14707121\D4=-41.4501632\D5=-
124.5413879\D6=56.06989654\D7=81.70335186\D8=-157.47153435\D9=120.57152859\D10=172.2746047\D11=-
169.98565341\D12=-54.25067809\D13=82.6614357\D14=65.99161845\D15=93.16237768\D16=-
149.11737564\D17=-28.9866167\D18=-159.32715329\D19=157.30235705\D20=-
83.80128222\D21=39.00865943\D22=-51.17629467\\Version=IA64L-G03RevD.01\State=2-A\HF=-
620.4150557\S2=0.796898\S2-1=0.\S2A=0.750252\RMSD=0.000e+00\RMSF=2.446e-
05\Thermal=0.\Dipole=0.2639285,-0.2645626,0.3143695\PG=C01 [X(C7H16N1Si1)]\\@

7-*endo* product
1\1\GINC-AC58\FOpt\UBHandHLYP\6-311G(d,p)\C7H16N1Si1(2)\UXW563\18-Aug-2006\1\\# BHandHLYP/6-
311G** geom=checkpoint guess=check scf=(qc,direct) opt=(readfc,z-matrix,maxcycle=500) freq=noraman\\geom &
freq\\0,2\C\C,1,B1\C,1,B2,2,A1\C,2,B3,1,A2,3,D1,0\C,4,B4,2,A3,1,D2,0\H,1,B5,2,A4,4,D3,0\H,1,B6,2,A5,4,D4,0\H,2,
B7,1,A6,3,D5,0\H,4,B8,2,A7,1,D6,0\H,1,B9,2,A8,4,D7,0\H,1,B10,2,A9,4,D8,0\H,2,B11,1,A10,3,D9,0\H,4,B12,2,A11,
1,D10,0\H,5,B13,4,A12,2,D11,0\H,5,B14,4,A13,2,D12,0\Si,3,B15,1,A14,2,D13,0\C,3,B16,1,A15,2,D14,0\H,17,B17,3,
A16,1,D15,0\H,17,B18,3,A17,1,D16,0\H,17,B19,3,A18,1,D17,0\C,3,B20,1,A19,2,D18,0\H,21,B21,3,A20,1,D19,0\H,2
1,B22,3,A21,1,D20,0\H,21,B23,3,A22,1,D21,0\N,5,B24,4,A23,2,D22,0\\B1=1.53489904\B2=3.14624981\B3=1.52647
497\B4=1.53256041\B5=2.749125\B6=1.08875857\B7=1.08979273\B8=1.08705356\B9=2.76780162\B10=1.0891607
6\B11=1.08799535\B12=1.08776784\B13=1.08900841\B14=1.09233923\B15=1.93285151\B16=1.53711971\B17=1.0
8618471\B18=1.08804261\B19=1.08366642\B20=1.53049532\B21=1.08733092\B22=1.0860982\B23=1.085447\B24=
1.43990516\A1=99.98688508\A2=115.57596325\A3=114.66660438\A4=95.00328456\A5=110.09215119\A6=109.236
11201\A7=110.13249362\A8=145.08220536\A9=108.93328806\A10=108.89665268\A11=108.40896205\A12=108.20
206462\A13=109.41822642\A14=33.90195614\A15=133.74961872\A16=110.32918323\A17=109.69367834\A18=113
.1133703\A19=111.86912747\A20=109.56362717\A21=111.74785351\A22=111.04088689\A23=110.32548092\D1=3
7.04443992\D2=-58.26778171\D3=93.68796618\D4=-53.98028123\D5=-
86.09334583\D6=63.64490568\D7=78.75157533\D8=190.09472241\D9=158.71561892\D10=180.5069724\D11=-
164.73367866\D12=-
48.39825974\D13=121.04341074\D14=63.16907401\D15=92.20480362\D16=210.78333525\D17=-
28.24104496\D18=-145.80021984\D19=139.97636094\D20=-
99.77847208\D21=21.39175446\D22=78.58553704\\Version=IA64L-G03RevD.01\State=2-A\HF=-
620.446462\S2=0.756522\S2-1=0.\S2A=0.750033\RMSD=0.000e+00\RMSF=3.673e-05\Thermal=0.\Dipole=-
0.1405289,-0.328378,0.2560813\PG=C01 [X(C7H16N1Si1)]\\@

Cyclization of 14a:

14a

1\1\GINC-AC59\FOpt\UBHandHLYP\6-311G(d,p)\C3H8Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,1.6614107119,0.2124717189,0.4559040546\H,1.636188683,1.2586324472,0.1389673534\H,1.4524772097,0.1853346799,1.5223649907\C,0.6079666014,-0.5992821882,-0.2923264084\H,0.6615841634,-1.6359353167,0.0232455506\H,0.8156724697,-0.5784622849,-1.3578996076\H,-1.4207991734,1.4670235223,-0.566109329\H,-1.6113968208,0.0240099697,1.4743430884\N,2.9696815793,-0.3763229669,0.2597164029\C,3.8613556273,0.3301493661,-0.2609378954\H,3.7057949171,1.3660885952,-0.5652181069\H,4.8452132537,-0.088924765,-0.4250753935\Ge,-1.2336382223,0.0438892208,-0.0154206984\\Version=IA64L-G03RevD.01\HF=-2250.6800909\S2=0.751596\S2-1=0.\S2A=0.750001\RMSD=7.698e-09\RMSF=4.987e-06\Thermal=0.\Dipole=0.2471855,0.4080557,-0.2543205\PG=C01 [X(C3H8Ge1N1)]\\@

4-*exo* transition state

1\1\GINC-AC57\FTS\UBHandHLYP\6-311G(d,p)\C3H8Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.5381154198,1.0789094557,-0.0241854363\C,-0.1086193216,1.6209271772,0.065591453\H,-1.9651821574,1.2431950275,-1.0132103862\H,-2.2166886765,1.5139326862,0.7053077159\H,1.7572535334,-0.316037413,-1.1689374715\H,1.3720640004,-0.6517065941,1.2902139676\H,0.1594433263,2.2723102583,-0.7559551506\H,0.0853936149,2.1409764595,0.9957377598\C,-2.3407767239,-1.173822518,-0.0767648505\H,-2.2578853113,-2.2137502234,0.1913557254\H,-3.1721543486,-0.8611889566,-0.6952979047\N,-1.3950512351,-0.3541511089,0.2675109681\Ge,0.7388497193,-0.1582982503,-0.0107583891\\Version=IA64L-G03RevD.01\HF=-2250.6576181\S2=0.787067\S2-1=0.\S2A=0.750215\RMSD=4.981e-09\RMSF=4.649e-06\Thermal=0.\Dipole=-0.501362,0.2082268,-0.2191722\PG=C01 [
X(C3H8Ge1N1)]\\@

4-*exo* product

1\1\GINC-AC58\FOpt\UBHandHLYP\6-311G(d,p)\C3H8Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,1.4770900653,1.1404072721,0.0203436618\C,0.0313587315,1.6928443672,-0.0227616743\H,1.9864357549,1.4019104302,0.9480427385\H,2.091752292,1.495612595,-0.8065321825\H,-1.2786414292,-0.7027491939,1.2709219734\H,-1.3497862577,-0.7345023043,-1.222377674\H,-0.2374621823,2.2955828709,0.8344022185\H,-0.1991887186,2.2410261848,-0.9269170095\C,2.2018137913,-1.2459855742,0.0562358993\H,1.9256905021,-2.2733704187,-0.0962123898\H,3.2210369027,-0.9465151051,-0.1205077144\N,1.2245199651,-0.2964168669,-0.0709122062\Ge,-0.617492417,-0.1653352571,-0.0038696405\\Version=IA64L-G03RevD.01\HF=-2250.6737795\S2=0.755512\S2-1=0.\S2A=0.75002\RMSD=7.155e-09\RMSF=8.807e-06\Thermal=0.\Dipole=-0.4164049,0.4335253,-0.0859597\PG=C01 [X(C3H8Ge1N1)]\\@

5-*endo* transition state

1\1\GINC-AC58\FTS\UBHandHLYP\6-311G(d,p)\C3H8Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,1.9739702011,0.7208134849,0.227493327\C,0.6331292777,1.4016941098,-0.0992028407\H,2.0647417526,0.5948781288,1.3098287692\H,2.8068401215,1.3262877633,-0.1125146158\H,-1.6095615584,-0.0688432927,-1.2872413629\H,-1.6957946003,0.1660015685,1.2185706289\H,0.650984847,1.7916579948,-1.111172381\H,0.4328316819,2.2265075798,0.5759091536\C,1.3333226891,-1.4789544755,0.1499742758\H,1.1782787084,-2.4257757639,-0.344999974\H,1.1651072095,-1.466386993,1.2266120042\N,1.9874217108,-0.550245342,-0.4606493461\Ge,-0.7779160407,0.0214532371,-0.0053986385\\Version=IA64L-G03RevD.01\HF=-2250.6649293\S2=0.802326\S2-1=0.\S2A=0.750288\RMSD=5.246e-09\RMSF=1.068e-05\Thermal=0.\Dipole=-0.1409755,0.1525854,0.5283137\PG=C01 [X(C3H8Ge1N1)]\\@

5-*endo* product

1\1\GINC-AC47\FOpt\UBHandHLYP\6-311G(d,p)\C3H8Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-2.0262103897,-0.5369510869,0.2016418759\C,-0.7582260819,-1.3744587147,-0.0607448735\H,-2.1789141281,-0.442136075,1.2817329641\H,-2.9109439411,-1.007950494,-0.2118276199\H,1.5180013813,0.0559653764,-1.2535609789\H,1.5759768042,-0.0990298343,1.2366680582\H,-0.7939229081,-1.8201558083,-1.0484515222\H,-0.6413993856,-2.1710372205,0.6637354464\C,-0.7092815286,1.4187980375,0.1409540937\H,-

0.4985123038,2.3397812367,-0.3854666994\H,-0.8225711568,1.6435177048,1.2058252937\N,-1.8857074856,0.7861387931,-0.3699955576\Ge,0.6652081238,-0.0151589148,0.0113745199\\Version=IA64L-G03RevD.01\HF=-2250.6897694\S2=0.756502\S2-1=0.\S2A=0.750032\RMSD=4.221e-09\RMSF=4.670e-05\Thermal=0.\Dipole=0.3430097,-0.3519602,0.4493774\PG=C01 [X(C3H8Ge1N1)]\\@

Cyclization of 14b:

14b

1\1\GINC-AC58\FOpt\UBHandHLYP\6-311G(d,p)\C4H10Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,2.5841431874,0.6135189131,0.0922353592\H,2.7235060763,1.0145715709,-0.9164115913\H,2.5838284916,1.4526339151,0.7849813741\C,1.2424642446,-0.105356359,0.1882524581\H,1.1498438549,-0.5202408772,1.1880572611\H,1.2514255731,-0.9497313944,-0.4975567106\C,0.067084304,0.8185422539,-0.1241696196\H,0.1615305249,1.2341799292,-1.1238688314\H,0.0498508105,1.6576793353,0.5661963953\H,-1.9346739345,-0.6324397461,1.3972166347\H,-1.7719301012,-1.2331843568,-1.0309066419\C,4.5733778055,-0.4882262288,-0.3452734521\H,4.6067233522,-0.0368023417,-1.3378867712\H,5.3840226709,-1.1535671033,-0.0792727678\N,3.6580751831,-0.271016015,0.4790592738\Ge,-1.6834320433,-0.0812334958,-0.0158523715\\Version=IA64L-G03RevD.01\HF=-2289.9773703\S2=0.751586\S2-1=0.\S2A=0.750001\RMSD=9.566e-09\RMSF=6.994e-06\Thermal=0.\Dipole=0.3422154,0.3723183,-0.5480331\PG=C01 [X(C4H10Ge1N1)]\\@

5-*exo* transition state

1\1\GINC-AC57\FTS\UBHandHLYP\6-311G(d,p)\C4H10Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,1.2827449799,1.6955724015,0.3081499995\C,-0.2016942447,1.6880844683,-0.0490439118\C,1.9792917808,0.4864745168,-0.2927727279\H,1.7699960982,2.6067176979,-0.0318128657\H,1.4041092297,1.6527266789,1.3877800479\H,1.9652743821,0.5359375743,-1.3809225996\H,3.0178449068,0.4376026526,0.0208815754\H,-2.125558882,-0.2624655473,-0.9210426001\H,-1.2900851992,-0.6193834852,1.4087786636\H,-0.7714731161,2.3391214727,0.6055660938\H,-0.3502898411,2.0476278222,-1.0643803381\C,1.866130268,-1.8536535372,0.023413125\H,1.3782385178,-2.743909297,0.3855887651\H,2.8048667766,-1.9607356826,-0.5051162543\N,1.2869421528,-0.7160618132,0.1744909969\Ge,-0.8728838095,-0.1683919228,0.0044450304\\Version=IA64L-G03RevD.01\HF=-2289.9654416\S2=0.785203\S2-1=0.\S2A=0.750208\RMSD=4.403e-09\RMSF=1.482e-05\Thermal=0.\Dipole=0.9732473,0.0431014,-0.2209256\PG=C01 [X(C4H10Ge1N1)]\\@

5-*exo* product

1\1\GINC-AC29\FOpt\UBHandHLYP\6-311G(d,p)\C4H10Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.2753097254,1.6974609404,-0.2858790988\C,0.192508771,1.7173915271,0.166338147\C,-1.9462556494,0.4137725344,0.1956716897\H,-1.816176681,2.5667768934,0.0782285501\H,-1.3162686823,1.7238083624,-1.372041644\H,-2.1760826552,0.4848080415,1.2627124484\H,-2.8887932048,0.2557504185,-0.3249087663\H,1.469527576,-0.7428278182,1.192546668\H,1.4515657948,-0.5531927603,-1.2945830687\H,0.793554522,2.4039209947,-0.4170859189\H,0.2753233163,2.0068067608,1.2099473176\C,-1.5220386571,-1.9826770059,0.0536394435\H,-0.8526821806,-2.7880617498,-0.1905584407\H,-2.5811373735,-2.1412480974,-0.0617542415\N,-1.0494062214,-0.6972376655,-0.072650133\Ge,0.7206860505,-0.1592123763,-0.0094509529\\Version=IA64L-G03RevD.01\HF=-2289.9971194\S2=0.755523\S2-1=0.\S2A=0.75002\RMSD=5.883e-09\RMSF=2.201e-05\Thermal=0.\Dipole=0.1263573,0.6382874,-0.0488695\PG=C01 [X(C4H10Ge1N1)]\\@

6-*endo* transition state

1\1\GINC-AC1\FTS\UBHandHLYP\6-311G(d,p)\C4H10Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,1.6764427014,1.1701278028,0.4569957286\C,0.3297252279,1.4845663625,-0.1954648957\C,2.4558450742,0.0614937902,-0.2539050277\H,-0.10033993,2.3739933095,0.2545474963\H,0.4612159037,1.6900429165,-1.2539111803\H,2.304182685,2.0589503909,0.4574708526\H,1.5254727714,0.9132682513,1.5032733848\H,3.3331873778,-0.202266728,0.338503759\H,2.8230234221,0.4387091494,-1.203151094\H,-1.5630265159,-0.4245481531,-1.3497756068\H,-2.1571596645,0.4570967875,0.9246714527\N,1.6904801509,-1.1401957267,-0.5418200939\C,1.0221054067,-1.6603749839,0.4178929153\H,1.1241515831,-1.3656652119,1.4601454021\H,0.4822910946,-2.5774917506,0.2337379567\Ge,-0.9977332883,0.0303277936,-0.0008140503\\Version=IA64L-G03RevD.01\HF=-2289.9628678\S2=0.795187\S2-1=0.\S2A=0.750227\RMSD=9.190e-09\RMSF=8.977e-06\Thermal=0.\Dipole=0.2693195,0.3510322,0.6089497\PG=C01 [X(C4H10Ge1N1)]\\@

6-*endo* product

1\1\GINC-AC34\FOpt\UBHandHLYP\6-311G(d,p)\C4H10Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,1.7468316338,1.052088123,0.4630524695\C,0.4420827305,1.4867393614,-0.2108578871\C,2.3657262861,-0.1933251551,-0.1902453332\H,0.0628799444,2.4015184736,0.2313744311\H,0.6029612021,1.6783766804,-1.2677576123\H,2.4849903656,1.8497514234,0.4216638802\H,1.5643198779,0.8706826194,1.5201923862\H,3.1300069773,-0.6019682776,0.4784595305\H,2.8835224328,0.095797582,-1.1011550732\H,-1.6707456312,-0.2572222391,-1.2599531053\H,-1.7989405533,0.2464416874,1.185791008\N,1.4642014152,-1.2666408102,-0.5387756098\C,0.4112782687,-1.4738294079,0.3846103155\H,0.6979880345,-1.3815264883,1.4350804391\H,-0.0598821932,-2.4356740556,0.2233307344\Ge,-0.853368791,0.0222604831,-0.0005255738\\Version=IA64L-G03RevD.01\HF=-2289.9905702\S2=0.757166\S2-1=0.\S2A=0.750038\RMSD=2.300e-09\RMSF=4.347e-06\Thermal=0.\Dipole=0.0285735,0.5342319,0.5283556\PG=C01 [X(C4H10Ge1N1)]\\@

Cyclization of 14c:

14c

1\1\GINC-AC25\FOpt\UBHandHLYP\6-311G(d,p)\C5H12Ge1N1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.3190453508,-0.9518431274,1.7999908411\C,0.5049425943,0.4947865824,1.3423461185\C,1.6935885714,0.6619158345,0.4023564411\C,1.882452979,2.1000338531,-0.0576120179\H,2.0109456698,2.7368204325,0.8156581712\H,0.9924771174,2.4467637138,-0.5919875363\H,1.5634288457,0.025084855,-0.4708015126\H,2.6063663154,0.3336024137,0.8931383716\H,0.6424637522,1.1394685467,2.2090211019\H,-0.4000535513,0.841403553,0.8457307218\H,0.1707145107,-1.6030584124,0.9428794965\H,1.2113172011,-1.3032113978,2.3108244119\H,-2.5306311108,-0.8070017313,2.3368036625\H,-1.0387761327,-0.3719828451,4.3000958543\N,3.0770858472,2.2217280903,-0.8609089779\C,2.9673268854,2.6714265207,-2.0227759307\H,3.8483628147,2.7656562624,-2.6437108692\H,2.0169892354,2.9831794603,-2.4586455576\Ge,-1.2098498863,-1.2045488326,3.0180813889\\Version=IA64L-G03RevD.01\HF=-2329.2745624\S2=0.75159\S2-1=0.\S2A=0.750001\RMSD=5.430e-09\RMSF=7.281e-06\Thermal=0.\Dipole=-0.1829249,0.1818675,-0.4869439\PG=C01 [X(C5H12Ge1N1)]\\@

6-*exo* transition state

1\1\GINC-AC48\FTS\UBHandHLYP\6-311G(d,p)\C5H12Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-0.0344421314,-1.6198871523,0.5605627391\C,1.9594244752,0.6311476722,-0.4876263346\C,2.3333376613,-0.7191465531,0.1058433459\C,1.3166375346,-1.8356776997,-0.1232060097\H,-2.0473361562,-0.5263739478,-1.1950303559\H,-1.8255798344,0.6264737373,0.9996486178\H,0.1103591521,-1.4892275863,1.6297307057\H,-0.6597564743,-2.4979935603,0.4291422632\H,1.7336141885,0.5220126242,-1.5451807481\H,2.7993241965,1.3171977666,-0.405835027\H,3.2857234298,-1.0160170172,-0.3290754616\H,2.5037369173,-0.5931252476,1.173683357\H,1.172198224,-1.9678647851,-1.1956593913\H,1.7548755787,-2.7660596424,0.2350331551\N,0.8026218568,1.2130846946,0.1982279235\C,0.7926835729,2.4818347477,0.3825955036\H,-0.0403262941,2.9300473022,0.9001814989\H,1.5645925772,3.1309107593,-0.0114164145\Ge,-1.0130854739,-0.0465931121,-0.1176503704\\Version=IA64L-G03RevD.01\HF=-2329.2624757\S2=0.78036\S2-1=0.\S2A=0.750181\RMSD=3.200e-09\RMSF=1.209e-05\Thermal=0.\Dipole=1.0049959,0.4196258,-0.0462998\PG=C01 [X(C5H12Ge1N1)]\\@

6-*exo* product

1\1\GINC-AC47\FOpt\UBHandHLYP\6-311G(d,p)\C5H12Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-0.5337644677,-1.6648953706,-0.2939225752\C,-1.5464818257,1.3042962598,0.2673552623\C,-2.3583110055,0.1228866431,-0.2480087843\C,-1.8976671827,-1.2427496781,0.2585268142\H,1.3199545962,-0.3980355146,1.5270311513\H,1.980744631,-0.2520060292,-0.8816123262\H,-0.5923198607,-1.7934703133,-1.3714588624\H,-0.2205229898,-2.6154114107,0.1267346467\H,-1.626996448,1.3506943437,1.358153784\H,-1.9887021724,2.2226281078,-0.1131472717\H,-3.3920496398,0.2801565538,0.0510767565\H,-2.3400824153,0.1309639063,-1.3366116337\H,-1.8660528209,-1.2254693587,1.3479386261\H,-2.6415349272,-1.9899138289,-0.0096605108\N,-0.1545490905,1.2801674751,-0.1532392168\C,0.5171991249,2.486480638,-0.1378893878\H,1.5315491701,2.492636414,-0.4973545529\H,-0.0696557241,3.3833743251,-0.2461244342\Ge,0.7991600482,-0.2911411626,0.0851215154\\Version=IA64L-G03RevD.01\HF=-2329.2974932\S2=0.75578\S2-1=0.\S2A=0.750021\RMSD=5.918e-09\RMSF=6.394e-06\Thermal=0.\Dipole=-0.4303976,-0.5398058,-0.0642862\PG=C01 [X(C5H12Ge1N1)]\\@

7-*endo* transition state
1\1\GINC-AC23\FTS\UBHandHLYP\6-311G(d,p)\C5H12Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-0.1365049606,-1.5238867138,-0.3307699838\C,-1.3950126556,-1.4814672709,0.5458621253\C,-2.5815041338,-0.7162497805,-0.0395769036\C,-2.2775286799,0.7020440191,-0.5160427442\H,-0.3898748954,-1.5294926023,-1.3873786453\H,1.6848808595,-0.199729661,1.4596080845\H,-1.1572830313,-1.0601317213,1.5189721536\H,-3.3588264118,-0.6707301817,0.7186188738\H,0.412158569,-2.4445727945,-0.1453652883\H,2.3644228931,-0.1815689366,-0.9575983121\H,-1.7272210606,-2.4995663477,0.736340184\H,-2.9955966325,-1.2693304461,-0.8812375808\H,-3.2210120715,1.2168053024,-0.6880181886\H,-1.7486020029,0.6788782366,-1.4733769605\C,-0.4802446531,2.0371025107,0.0771535972\H,0.0914581931,2.6232468031,0.7815996172\N,-1.5360342028,1.4356953748,0.4806636975\H,-0.2544535076,2.1857795216,-0.9770284382\Ge,1.1720623845,-0.0868073116,0.015414712\\Version=IA64L-G03RevD.01\HF=-2329.2620719\S2=0.795122\S2-1=0.\S2A=0.750223\RMSD=7.081e-09\RMSF=1.227e-05\Thermal=0.\Dipole=-0.0929555,-0.1193563,-0.5574915\PG=C01 [X(C5H12Ge1N1)]\\@

7-*endo* product
1\1\GINC-AC57\FOpt\UBHandHLYP\6-311G(d,p)\C5H12Ge1N1(2)\UXW563\13-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,0.2999769794,-1.4896198888,0.3659616164\C,1.5690057188,-1.3805003845,-0.4895654351\C,2.613028785,-0.3813256011,0.0142679726\C,2.0536339974,0.9673879749,0.4768015097\H,0.5384368878,-1.4719236751,1.4264086176\H,-1.583035558,-0.3500315891,-1.4510921864\H,1.2973565077,-1.1198460429,-1.50960298\H,3.3362623754,-0.2116797078,-0.7781619123\H,-0.1899056114,-2.4413873556,0.1793338612\H,-2.1944616303,-0.1150958173,0.9570882218\H,2.0458223942,-2.3562917326,-0.5505222111\H,3.1581232029,-0.8121893442,0.8523798943\H,2.8885338723,1.6553581829,0.6060820758\H,1.582820364,0.8542689233,1.4572719278\C,-0.157057016,1.6985437027,-0.0148461586\H,-0.7313159336,2.3610618698,-0.6533193093\N,1.1603545932,1.5332445026,-0.4990033261\H,-0.203779839,2.0551117913,1.0171964777\Ge,-1.03219709,-0.1022268085,-0.0437806553\\Version=IA64L-G03RevD.01\HF=-2329.2887691\S2=0.757127\S2-1=0.\S2A=0.750037\RMSD=5.047e-09\RMSF=1.037e-05\Thermal=0.\Dipole=0.0356264,-0.3263919,0.5682221\PG=C01 [X(C5H12Ge1N1)]\\@

Cyclization of 15a:

15a
1\1\GINC-AC27\FOpt\UBHandHLYP\Gen\C3H8N1Sn1(2)\UXW563\17-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,1.6923166483,0.1798444482,0.447396211\H,1.653920958,1.227933331,0.1368952348\H,1.4776582991,0.1446641993,1.5126785497\C,0.66083447,-0.64470336,-0.3143579728\H,0.7261593729,-1.6826555942,-0.0054686767\H,0.8752937154,-0.6144906573,-1.3783999675\H,-1.550571417,1.6174037378,-0.6563045151\H,-1.7263368063,0.0794244661,1.653427404\Sn,-1.3733563951,0.0268765492,-0.0280547835\N,3.0148231152,-0.3820776794,0.2613396337\C,3.894301445,0.3411834063,-0.2570183822\H,3.7189075206,1.3728881976,-0.5652041656\H,4.887560074,-0.0576190447,-0.4153745705\\Version=IA64L-G03RevD.01\HF=-177.0764944\S2=0.751605\S2-1=0.\S2A=0.750001\RMSD=3.644e-09\RMSF=1.974e-06\Thermal=0.\Dipole=0.0747155,0.2618827,-0.3586346\PG=C01 [X(C3H8N1Sn1)]\\@

4-*exo* transition state
1\1\GINC-AC25\FTS\UBHandHLYP\Gen\C3H8N1Sn1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/gen scf=direct nosymm pseudo=read opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-1.550534,1.089463,-0.063992\C,-0.154441,1.708138,0.082506\H,-1.948701,1.256686,-1.065118\H,-2.272654,1.489183,0.644582\H,1.937792,-0.397838,-1.312207\H,1.501919,-0.836929,1.406077\H,0.098033,2.398901,-0.711141\H,-0.017411,2.20877,1.03309\Sn,0.807521,-0.208276,-0.018032\C,-2.376868,-1.167446,-0.046741\H,-2.286265,-2.204804,0.224067\H,-3.240223,-0.846794,-0.611496\N,-1.379637,-0.347758,0.209013\\Version=IA64L-G03RevD.01\HF=-177.0536918\S2=0.78079\S2-1=0.\S2A=0.750192\RMSD=9.573e-09\RMSF=4.903e-06\Thermal=0.\Dipole=-0.2534898,0.1531104,-0.2075478\Polar=175.8561219,2.4719253,74.2234172,-11.0660712,-3.1741829,62.0412032\PG=C01 [X(C3H8N1Sn1)]\\@

4-*exo* product
1\1\GINC-AC25\FOpt\UBHandHLYP\Gen\C3H8N1Sn1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/gen scf=direct freq=noraman nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,1.495164,1.125671,0.026581\C,0.083898,1.757286,-0.020285\H,2.018592,1.395661,0.944404\H,2.11458,1.453885,-0.809024\H,-1.530287,-0.811617,1.402791\H,-

1.558949,-0.850662,-1.365234\H,-0.143622,2.380384,0.834504\H,-0.10783,2.32142,-0.923863\Sn,-0.761057,-0.211169,0.001434\C,2.281091,-1.214744,0.049975\H,2.053319,-2.256835,-0.08294\H,3.279906,-0.870718,-0.163239\N,1.252322,-0.316053,-0.035248\\Version=IA64L-G03RevD.01\HF=-177.0603139\S2=0.755473\S2-1=0.\S2A=0.75002\RMSD=5.348e-09\RMSF=8.150e-06\Thermal=0.\Dipole=-0.6571492,0.4012416,-0.1015253\Polar=84.7846512,3.5419603,75.5270637,0.0347087,-0.0477208,59.6897567\PG=C01 [X(C3H8N1Sn1)]\\@

5-*endo* transition state
1\1\GINC-AC25\FTS\UBHandHLYP\Gen\C3H8N1Sn1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/gen scf=direct nosymm pseudo=read opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,2.012121,0.726278,0.198063\C,0.682591,1.46049,-0.05933\H,2.153583,0.598579,1.274884\H,2.851047,1.297292,-0.185007\H,-1.690305,-0.173237,-1.487283\H,-1.990839,0.191209,1.270471\H,0.682055,1.904592,-1.048901\H,0.521397,2.252657,0.663149\Sn,-0.859321,-0.050723,0.000813\C,1.34561,-1.483436,0.177535\H,1.189955,-2.439618,-0.298212\H,1.285169,-1.476609,1.265762\N,1.960293,-0.548386,-0.484735\\Version=IA64L-G03RevD.01\HF=-177.0604441\S2=0.803217\S2-1=0.\S2A=0.750301\RMSD=4.374e-09\RMSF=1.718e-05\Thermal=0.\Dipole=-0.0772488,0.0305875,0.5620168\Polar=103.4422257,0.5297783,71.6332907,-0.5245825,0.1893422,66.4562253\PG=C01 [X(C3H8N1Sn1)]\\@

5-*endo* product
1\1\GINC-AC24\FOpt\UBHandHLYP\Gen\C3H8N1Sn1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-2.0411830031,-0.5284746557,0.197166827\C,-0.8191168304,-1.4386759382,-0.0565678623\H,-2.1691648892,-0.3945671808,1.2762339784\H,-2.9491421627,-0.9777836819,-0.190086522\H,1.7287883523,0.0716178404,-1.4223107484\H,1.8184085617,-0.1018095376,1.3555922103\H,-0.8809977815,-1.8948233942,-1.0381019246\H,-0.7473326459,-2.2295811471,0.6799546802\Sn,0.7921803029,-0.0179046462,-0.0040263252\C,-0.7967518074,1.479566259,0.1572189235\H,-0.6222850908,2.429556275,-0.3276431741\H,-0.934093153,1.6263262349,1.2329115567\N,-1.8458128531,0.7538765724,-0.4484566193\\Version=IA64L-G03RevD.01\HF=-177.0717727\S2=0.758529\S2-1=0.\S2A=0.750049\RMSD=8.875e-09\RMSF=1.618e-06\Thermal=0.\Dipole=0.4173285,-0.3177388,0.4857862\PG=C01 [X(C3H8N1Sn1)]\\@

Cyclization of 15b:
15b
1\1\GINC-AC23\FOpt\UBHandHLYP\Gen\C4H10N1Sn1(2)\UXW563\17-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,2.6184639295,0.630749476,0.0921372064\H,2.7675103624,1.0326056122,-0.9148333155\H,2.6286362104,1.4675378673,0.7875539543\C,1.2636152352,-0.0655146207,0.1805497744\H,1.1643519324,-0.4836307366,1.1787019312\H,1.2652290166,-0.9088070403,-0.5071600252\C,0.1038115136,0.8764681174,-0.1325542078\H,0.2036896743,1.2934870155,-1.1310622033\H,0.0934656417,1.7138892464,0.559887321\H,-2.0459446484,-0.7421045603,1.5543711091\H,-1.8730670208,-1.3898764343,-1.1443430469\Sn,-1.8279216146,-0.0884923081,-0.0207959791\C,4.588808913,-0.5053887581,-0.3437729024\H,4.6309924803,-0.0542696703,-1.3362541797\H,5.3873521646,-1.1851720037,-0.0774750337\N,3.6768462098,-0.2721532027,0.479849597\\Version=IA64L-G03RevD.01\HF=-216.3736194\S2=0.751667\S2-1=0.\S2A=0.750001\RMSD=5.459e-09\RMSF=3.263e-06\Thermal=0.\Dipole=0.1658826,0.5201585,-0.5904201\PG=C01 [X(C4H10N1Sn1)]\\@

5-*exo* transition state
1\1\GINC-AC30\FTS\UBHandHLYP\Gen\C4H10N1Sn1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/gen scf=direct nosymm pseudo=read opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.3173283878,1.7076672894,0.2937831472\C,-0.1767319112,1.7794358734,-0.0246626586\C,1.9685816169,0.4830950028,-0.3329837671\H,1.8394285306,2.6008388522,-0.0443573176\H,1.46113643,1.6462613562,1.3698580312\H,1.9385074657,0.5464461473,-1.420349914\H,3.0123369918,0.4141699383,-0.041108533\H,-2.2983041502,-0.3301811971,-1.0959438609\H,-1.4450671749,-0.8018908809,1.5127883211\H,-0.7001392917,2.4281262965,0.6685381732\H,-0.338791543,2.1811656709,-1.0217917486\Sn,-0.9365986028,-0.2335225328,-0.0158816426\C,1.9121674472,-1.8525500499,0.0664861158\H,1.4414014151,-2.7471945189,0.4371265773\H,2.8752260062,-1.9358813455,-0.4158745112\N,1.2729723827,-0.7207219019,0.1383765878\\Version=IA64L-G03RevD.01\HF=-216.3620769\S2=0.785515\S2-1=0.\S2A=0.75023\RMSD=3.182e-09\RMSF=8.762e-06\Thermal=0.\Dipole=0.8545458,0.0411707,-0.2340029\PG=C01 [X(C4H10N1Sn1)]\\@

5-*exo* product

1\1\GINC-AC24\FOpt\UBHandHLYP\Gen\C4H10N1Sn1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.293519538,1.6910736741,-0.2907102447\C,0.1650658781,1.8143728177,0.1784989034\C,-1.9439461799,0.4019781645,0.2091752137\H,-1.8813678421,2.5451554988,0.0377014982\H,-1.3197099235,1.6868144386,-1.3782002063\H,-2.1482327633,0.4807206717,1.2814912579\H,-2.9039068949,0.259481874,-0.2850753154\H,1.6963347829,-0.8396518622,1.3352554536\H,1.6815075877,-0.6391497808,-1.4345042573\H,0.7167656982,2.5454057973,-0.3991451752\H,0.2168485101,2.1094101815,1.2226143574\Sn,0.8661124906,-0.1917069297,-0.0067621593\C1.6158386124,-1.9939304474,0.0357271353\H,-0.9929968043,-2.829609108,-0.2317131002\H,-2.6834973663,-2.1027421155,-0.0664308619\N,-1.0806040228,-0.7315838747,-0.0777504991\\Version=IA64L-G03RevD.01\HF=-216.3802154\S2=0.755573\S2-1=0.\S2A=0.75002\RMSD=4.122e-09\RMSF=3.126e-06\Thermal=0.\Dipole=0.3202884,0.6649787,-0.0466946\PG=C01 [X(C4H10N1Sn1)]\\@

6-*endo* transition state

1\1\GINC-AC29\FTS\UBHandHLYP\Gen\C4H10N1Sn1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/gen scf=direct nosymm pseudo=read opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.7226416711,1.1884457982,0.4553700051\C,0.3743755834,1.55548382,-0.1646127892\C,2.4521437041,0.0581138933,-0.2758501463\H,-0.0425176545,2.423489811,0.3363194902\H,0.4946257351,1.8161175402,-1.2123415057\H,2.3865683647,2.051360872,0.4511697688\H,1.5879314758,0.926921478,1.503239651\H,3.3421399115,-0.2200294553,0.2911670495\H,2.7959270721,0.4222422561,-1.23872288\H,-1.616689125,-0.5587965697,-1.5444191861\H,-2.4309822613,0.4647508014,0.9195408179\Sn,-1.0671396645,-0.0461415832,-0.0093524643\N,1.6607823209,-1.1332693888,-0.5317833339\C,1.0293280518,-1.6602680259,0.4634891452\H,1.1976077299,-1.3797457171,1.501115839\H,0.523121085,-2.60064153,0.3040675388\\Version=IA64L-G03RevD.01\HF=-216.3584679\S2=0.798935\S2-1=0.\S2A=0.750273\RMSD=6.991e-09\RMSF=8.020e-06\Thermal=0.\Dipole=0.3479588,0.2182872,0.6641881\PG=C01 [X(C4H10N1Sn1)]\\@

6-*endo* product

1\1\GINC-AC26\FOpt\UBHandHLYP\Gen\C4H10N1Sn1(2)\UXW563\22-Nov-2007\0\\# BHandHLYP/gen scf=direct freq=noraman nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,1.7707782312,1.0645753985,0.4598695672\C,0.4951142906,1.5678508564,-0.2249045019\C,2.3672447191,-0.1924001086,-0.1970172584\H,0.1534472668,2.490953687,0.2303542146\H,0.6741358839,1.7693416533,-1.2767154071\H,2.5414194406,1.8328328297,0.4464989189\H,1.5668472364,0.871170608,1.5113583108\H,3.1195074215,-0.611657036,0.4785707632\H,2.890475069,0.0944955766,-1.1048586367\H,-1.8616742392,-0.3371223458,-1.4221758562\H,-2.0490052519,0.2992776526,1.2864782734\Sn,-0.973703419,0.0186141431,-0.014744341\N,1.439492912,-1.2402456879,-0.5547012313\C,0.4858771856,-1.5544846857,0.4267841233\H,0.8007327775,-1.4463348157,1.4668702749\H,0.0531624756,-2.5333977255,0.2626177861\\Version=IA64L-G03RevD.01\HF=-216.3732069\S2=0.758359\S2-1=0.\S2A=0.750047\RMSD=4.406e-09\RMSF=3.649e-06\Thermal=0.\Dipole=-0.0288699,0.4919082,0.5255926\PG=C01 [X(C4H10N1Sn1)]\\@

Cyclization of 15c:

15c

1\1\GINC-AC30\FOpt\UBHandHLYP\Gen\C5H12N1Sn1(2)\UXW563\17-Nov-2007\0\\
BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.9761095509,0.687307411,-0.6840958711\C,-0.6691658171,1.1638369129,-0.0523943331\C,0.468937215,1.287781281,-1.0626611481\C,1.7564053598,1.7600971149,-0.4036435231\H,2.033339842,1.0714604584,0.3930131636\H,1.5848827256,2.7145534746,0.0914304175\H,0.1728036885,1.9824534976,-1.8471288695\H,0.6252525449,0.3225699053,-1.5417853929\H,-0.3680660267,0.4769318704,0.7371507714\H,-0.8207325758,2.1288129254,0.4289909374\H,-2.2931125417,1.3716471307,-1.4663243269\H,-1.8415828562,-0.2844071599,-1.1513079411\H,-3.8711840933,2.0449915157,1.4712217967\H,-3.1565266245,-0.59272206,1.9712573951\Sn,-3.6010325173,0.5149079703,0.7332502851\N,2.9448141806,1.9357148888,-1.2132729887\C,2.9286955777,1.7043814197,-2.4428046093\H,3.8392586405,1.8486682062,-3.0098636313\H,2.0595933715,1.3638877906,-2.9997044747\\Version=IA64L-G03RevD.01\HF=-255.6669197\S2=0.751673\S2-1=0.\S2A=0.750001\RMSD=9.480e-09\RMSF=3.002e-05\Thermal=0.\Dipole=-0.5001473,-0.2547356,-0.6264344\PG=C01 [X(C5H12N1Sn1)]\\@

6-*exo* transition state

1\1\GINC-AC28\FTS\UBHandHLYP\Gen\C5H12N1Sn1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.003667,-1.733695,0.545253\C,1.957675,0.629754,-0.493609\C,2.327968,-0.705246,0.139997\C,1.365915,-1.862761,-0.124096\H,-2.301318,-0.468066,-1.259735\H,-1.947589,0.743682,1.207294\H,0.116768,-1.675924,1.62405\H,-0.601658,-2.616945,0.342137\H,1.768658,0.497346,-1.556145\H,2.797592,1.313867,-0.404369\H,3.309947,-0.978738,-0.241545\H,2.440684,-0.559249,1.21282\H,1.244951,-1.979051,-1.201484\H,1.847387,-2.778064,0.218753\Sn,-1.095604,0.00903,-0.085219\N,0.792215,1.246708,0.155284\C,0.836653,2.532456,0.340463\H,0.018018,3.018127,0.844782\H,1.634008,3.141512,-0.060662\\Version=IA64L-G03RevD.01\HF=-255.6589635\S2=0.783276\S2-1=0.\S2A=0.750221\RMSD=9.115e-09\RMSF=1.258e-05\Thermal=0.\Dipole=0.9518278,0.3186819,-0.1498167\Polar=156.2696505,41.0037269,142.6172789,17.9629137,21.6319755,84.6333892\PG=C01 [X(C5H12N1Sn1)]\\@

6-*exo* product
1\1\GINC-AC29\FOpt\UBHandHLYP\Gen\C5H12N1Sn1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.607933,-1.781306,-0.256068\C,-1.567461,1.327312,0.242939\C,-2.334958,0.125986,-0.297993\C,-1.937854,-1.235722,0.275546\H,1.689015,-0.465776,1.558036\H,2.134717,-0.280674,-1.182674\H,-0.689372,-1.985621,-1.32023\H,-0.352588,-2.718126,0.228575\H,-1.700925,1.376432,1.328545\H,-2.024801,2.229815,-0.160727\H,-3.386391,0.297509,-0.078818\H,-2.243004,0.105372,-1.383158\H,-1.903226,-1.163746,1.362738\H,-2.727451,-1.95039,0.050604\Sn,0.937898,-0.342452,0.027197\N,-0.158323,1.351429,-0.113233\C,0.462808,2.581809,-0.041662\H,1.483161,2.646846,-0.380683\H,-0.153395,3.462495,-0.126025\\Version=IA64L-G03RevD.01\HF=-255.6799755\S2=0.755762\S2-1=0.\S2A=0.750021\RMSD=8.849e-09\RMSF=6.643e-06\Thermal=0.\Dipole=-0.362613,-0.6858143,-0.081435\Polar=102.2027731,4.6543115,99.9286675,-1.4877179,-0.937595,76.9036886\PG=C01 [X(C5H12N1Sn1)]\\@

7-*endo* transition state
1\1\GINC-AC29\FTS\UBHandHLYP\Gen\C5H12N1Sn1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/gen freq=noraman scf=direct nosymm pseudo=read opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.181803,-1.586697,-0.335699\C,-1.441035,-1.52149,0.538139\C,-2.605374,-0.719739,-0.042687\C,-2.264085,0.692579,-0.508324\H,-0.435956,-1.634438,-1.39117\H,1.83644,-0.140893,1.598398\H,-1.200413,-1.119,1.518759\H,-3.383842,-0.659119,0.71343\H,0.371512,-2.49663,-0.116207\H,2.590681,-0.206432,-1.088658\H,-1.80307,-2.532463,0.715994\H,-3.031679,-1.254801,-0.889947\H,-3.193535,1.230353,-0.689507\H,-1.727776,0.662596,-1.461376\Sn,1.257555,-0.009421,-0.011513\C,-0.503705,2.089925,0.078949\H,0.042357,2.695318,0.787379\N,-1.517576,1.41212,0.495734\H,-0.343412,2.31425,-0.973854\\Version=IA64L-G03RevD.01\HF=-255.6570727\S2=0.798513\S2-1=0.\S2A=0.750257\RMSD=8.312e-09\RMSF=5.732e-06\Thermal=0.\Dipole=-0.1902696,0.069457,-0.5807164\Polar=130.3249228,-2.3774176,97.9129471,-1.6766128,0.6959436,85.1383069\PG=C01 [X(C5H12N1Sn1)]\\@

7-*endo* product
1\1\GINC-AC26\FOpt\UBHandHLYP\Gen\C5H12N1Sn1(2)\UXW563\18-Nov-2007\0\\# BHandHLYP/gen scf=direct freq=noraman nosymm pseudo=read opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.3591804608,-1.5963619285,0.3406574677\C,1.6283899059,-1.399967877,-0.5013537515\C,2.6318946453,-0.3848893771,0.0487798798\C,2.0307868609,0.9524354161,0.4829866099\H,0.5971436809,-1.6422010523,1.4003640965\H,-1.9097822418,-0.3777215005,-1.4966822298\H,1.3612671977,-1.1082670025,-1.5140919251\H,3.3843472624,-0.2027972748,-0.7135510611\H,-0.1022638443,-2.5479061307,0.0916687998\H,-2.3329651446,-0.0920918672,1.2411410568\H,2.1446470565,-2.3535053666,-0.595944333\H,3.1489957487,-0.8095647064,0.9078224686\H,2.845417288,1.6551779313,0.6603989129\H,1.5125961133,0.8331167848,1.4395786229\Sn,-1.14817625,-0.1010788177,0.0060229999\C,-0.1054881401,1.8324794835,-0.0729505687\H,-0.6342305058,2.4793459202,-0.7632920946\N,1.178872078,1.5079277511,-0.5353949122\H,-0.1390291718,2.2487286143,0.936737961\\Version=IA64L-G03RevD.01\HF=-255.6723252\S2=0.758206\S2-1=0.\S2A=0.750046\RMSD=6.054e-09\RMSF=9.151e-06\Thermal=0.\Dipole=-0.0123091,-0.2705983,0.5559458\PG=C01 [X(C5H12N1Sn1)]\\@

Gaussian archive entries for Table 3

Addition of $H_3Si•$ to acetonitrile:

Acetonitrile/$H_3Si•$ complex

1\1\GINC-AC28\FOpt\UBHandHLYP\6-311G(d,p)\C2H6N1Si1(2)\UXW563\15-Jan-2008\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(z-matrix,calcfc,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.6726760657,0.197117116,0.0074594378\N,0.5345106222,0.1834295244,-0.0059643535\C,3.1246021853,0.2137378719,0.0248190609\H,3.4945856301,-0.5197542809,0.7315800139\H,3.4802098435,1.1948671059,0.3168524238\H,3.5092684954,-0.0214279888,-0.9606309398\H,-2.3960347633,-0.1284279039,1.2681669789\H,-2.3420883483,-0.7186613721,-1.1006908563\H,-4.2434411634,0.4668123494,-0.1807091118\Si,-2.7766945671,0.2722965777,-0.0988996537\\Version=IA64L-G03RevD.01\HF=-423.9417659\S2=0.751598\S2-1=0.\S2A=0.750001\RMSD=5.538e-09\RMSF=8.266e-06\Thermal=0.\Dipole=1.8963447,0.099757,0.0055626\PG=C01 [X(C2H6N1Si1)]\\@

N-philic transition state

1\1\GINC-NODE051\FTS\UBHandHLYP\6-311G(d,p)\C2H6N1Si1(2)\UWILLE\01-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) OPT=(TS,NOEIGENTEST,CALCFC,Z-MATRIX,MAXCYCLE=500) FREQ=NORAMAN\\geom and freq\\0,2\C,1.2487256462,-0.4343248369,0.17415552\N,0.1243542152,-0.7134958573,0.2132596301\C,2.4842981459,0.3099220761,0.0032473501\H,3.0387194054,0.332483724,0.9341923333\H,2.2579674674,1.3310055058,-0.3033316035\H,3.1019360217,-0.160091226,-0.7531598568\Si,-1.7714590264,0.2497764507,-0.1399552387\H,-2.304299662,-0.0754775933,1.1948564152\H,-2.2173421741,-0.753893124,-1.1224384487\H,-2.3451769478,1.5699899687,-0.5479801294\\Version=AM64L-G03RevC.02\State=2-A\HF=-423.9263854\S2=0.770314\S2-1=0.\S2A=0.750102\RMSD=6.522e-09\RMSF=1.271e-05\Dipole=1.7348571,0.4021445,-0.0521074\PG=C01 [X(C2H6N1Si1)]\\@

N-addition product

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET12\FOpt\UBHandHLYP\6-311G(d,p)\C2H6N1Si1(2)\UWILLE\29-Nov-2006\1\\#BHANDHLYP/6-311G** GEOM=CHECKPOINT GUESS=CHECK SCF=(DIRECT,QC) OPT=(Z-MATRIX,READFC,MAXCYCLE=500) FREQ=NORAMAN\\geometry & frequency\\0,2\C\N,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\H,3,B5,1,A4,2,D3,0\Si,2,B6,1,A5,3,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\\B1=1.22160268\B2=1.48818255\B3=1.08532892\B4=1.08532792\B5=1.08753474\B6=1.73711903\B7=1.47229697\B8=1.47229874\B9=1.47730094\A1=130.48932862\A2=109.39476133\A3=109.39543776\A4=111.18744302\A5=133.46831791\A6=107.79291751\A7=107.79337682\A8=112.93362296\D1=-121.44392546\D2=121.4611435\D3=0.00816227\D4=179.99890896\D5=-121.01430835\D6=120.98752863\D7=-0.01366921\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-423.9649258\S2=0.754995\S2-1=0.\S2A=0.750017\RMSD=0.000e+00\RMSF=1.060e-05\Dipole=0.1335605,0.0000144,-0.3692012\PG=C01 [X(C2H6N1Si1)]\\@

C-philic transition state

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET15\FTS\UBHandHLYP\6-311G(d,p)\C2H6N1Si1(2)\UWILLE\01-Dec-2006\1\\#BHANDHLYP/6-311G** SCF=(DIRECT,QC) OPT=(TS,NOEIGENTEST,CALCFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geometry & frequency\\0,2\C\C,1,B1\H,2,B2,1,A1\H,2,B3,1,A2,3,D1,0\H,2,B4,1,A3,4,D2,0\N,1,B5,2,A4,3,D3,0\Si,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\\B1=1.47256849\B2=1.08301405\B3=1.08301379\B4=1.08487768\B5=1.16100557\B6=2.52851912\B7=1.47216967\B8=1.47216864\B9=1.48339494\A1=110.27850703\A2=110.27886069\A3=108.84734456\A4=154.57664523\A5=98.07003974\A6=100.58126086\A7=100.58011272\A8=123.21011787\D1=-119.86369318\D2=-120.06829755\D3=-120.06564569\D4=180.00030524\D5=57.1580629\D6=-57.14333551\D7=180.00781491\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-423.9255488\S2=0.781\S2-1=0.\S2A=0.750269\RMSD=0.000e+00\RMSF=1.330e-05\Dipole=0.102774,-0.1775416,1.3355918\PG=C01 [X(C2H6N1Si1)]\\@

C-addition product

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET7\FOpt\UBHandHLYP\6-311G(d,p)\C2H6N1Si1(2)\UWILLE\30-Nov-2006\1\\#BHANDHLYP/6-311G** SCF=(DIRECT,QC) GEOM=CHECKPOINT GUESS=CHECK OPT=(Z-MATRIX,READFC,MAXCYCLE=500) FREQ=NORAMAN\\geometry & frequency\\0,2\C\C,1,B1\H,2,B2,1,A1\H,2,B3,1,A2,3,D1,0\H,2,B4,1,A3,4,D2,0\N,1,B5,2,A4,4,D3,0\Si,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\\B1=1.51633128\B2=1.08579879\B3=1.08579863\B4=1.08295127\B5=1.23474743\B6=1.90757962\B7=1.47575569\B8=1.46884277\B9=1.47575563\A1=110.00504371\A2=110.0050441\A3=110.36593514\A4=122.97736397\A5=116.61330953\A6=108.55570464\A7=109.5335727\A8=108.55513336\D1=-118.74432303\D2=-120.62794305\D3=120.62662884\D4=-179.99964245\D5=120.96923415\D6=-0.00558968\D7=-120.98010753\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-423.9585149\S2=0.76746\S2-1=0.\S2A=0.750182\RMSD=0.000e+00\RMSF=4.853e-06\Dipole=0.4018161,-0.6786443,0.6442386\PG=C01 [X(C2H6N1Si1)]\\@

Addition of $H_3Ge^•$ to acetonitrile:

Acetonitrile/$H_3Ge^•$ complex

1\1\GINC-AC6\FOpt\UBHandHLYP\6-311G(d,p)\C2H6Ge1N1(2)\UXW563\15-Jan-2008\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(z-matrix,calcfc,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,1.724232683,0.1448368574,0.0352781242\N,0.5877776492,0.0788619015,0.0502214676\C,3.1738231071,0.22922657,0.0172585953\H,3.5946890154,-0.4853539964,0.7148223494\H,3.4901591279,1.2261092312,0.3008565212\H,3.545008331,0.0114485298,-0.9771164209\H,-2.4855280824,-0.1507498472,1.3190255749\H,-2.4018639224,-0.7587016006,-1.1314191185\H,-4.3402939085,0.555236036,-0.2226760872\Ge,-2.8304100003,0.2890753186,-0.1042690068\\Version=IA64L-G03RevD.01\HF=-2211.3936665\S2=0.751534\S2-1=0.\S2A=0.750001\RMSD=8.301e-09\RMSF=8.540e-05\Thermal=0.\Dipole=1.8678276,0.1221435,-0.0177497\PG=C01 [X(C2H6Ge1N1)]\\@

N-philic transition state

1\1\GINC-AC27\FTS\UBHandHLYP\6-311G(d,p)\C2H6Ge1N1(2)\UXW563\10-Jan-2008\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,1.3229474829,-0.5847579799,0.0020242397\N,0.227790306,-0.9933362922,0.0023749393\C,2.3581842518,0.4416113048,0.0003346891\H,2.985143429,0.3429071332,0.8788369304\H,1.8956532668,1.4298105796,-0.001539684\H,2.9852771747,0.339656385,-0.8776465775\H,-2.3254952023,-0.4625595729,1.250351365\H,-2.3244844215,-0.4676185807,-1.2498826698\H,-1.8984876123,1.6651830582,-0.0039103167\Ge,-1.684614675,0.134438965,-0.0007499147\\Version=IA64L-G03RevD.01\HF=-2211.3733729\S2=0.775517\S2-1=0.\S2A=0.750142\RMSD=7.080e-09\RMSF=8.135e-06\Thermal=0.\Dipole=1.1695089,0.6548391,-0.0009289\PG=C01 [X(C2H6Ge1N1)]\\@

N-addition product

1\1\GINC-AC30\FOpt\UBHandHLYP\6-311G(d,p)\C2H6Ge1N1(2)\UXW563\10-Jan-2008\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.0364368703,0.2867698863,-0.0000380853\N,-0.0731599063,-0.4649713381,0.0003698847\C,-2.4945343185,-0.0202993157,0.0004933274\H,-2.9584108827,0.4246617274,-0.8739323272\H,-2.95840932,0.4270828625,0.8736787477\H,-2.6687223651,-1.0939257239,0.0019592786\H,2.3379408543,-0.5771941984,-1.2505559996\H,2.3381778692,-0.5735965145,1.2511964334\H,1.868938444,1.5547472785,-0.0027104871\Ge,1.7160684954,0.0344013359,-0.0004967726\\Version=IA64L-G03RevD.01\HF=-2211.3920812\S2=0.755157\S2-1=0.\S2A=0.750018\RMSD=5.204e-09\RMSF=1.059e-05\Thermal=0.\Dipole=-0.1514709,0.1809783,-0.0001889\PG=C01 [X(C2H6Ge1N1)]\\@

C-philic transition state

1\1\GINC-AC27\FTS\UBHandHLYP\6-311G(d,p)\C2H6Ge1N1(2)\UXW563\10-Jan-2008\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.9564710723,0.338203965,-0.0026111922\C,-1.6559289034,-0.9604908848,0.0029724827\H,-1.3844320958,-1.5292039635,0.8838254589\H,-1.3855112267,-1.5361674253,-0.8736771849\H,-2.7262502501,-0.7836186298,0.0029241349\N,-0.9418522424,1.5021294168,-0.0073370515\H,2.0060808864,0.5702204738,1.253639737\H,2.0058018933,0.5643115488,-1.2601043922\H,1.9993437289,-1.612201961,0.0019183898\Ge,1.522116282,-0.1495455399,-0.0015263876\\Version=IA64L-G03RevD.01\HF=-2211.3760508\S2=0.783588\S2-1=0.\S2A=0.750317\RMSD=9.746e-09\RMSF=5.524e-06\Thermal=0.\Dipole=-0.3749527,-1.2535523,0.005186\PG=C01 [X(C2H6Ge1N1)]\\@

C-addition product

1\1\GINC-AC29\FOpt\UBHandHLYP\6-311G(d,p)\C2H6Ge1N1(2)\UXW563\10-Jan-2008\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.5793359718,0.2718033613,0.0000340855\C,-1.6020537225,-0.8430847804,0.0000183839\H,-1.4695215521,-1.4682467441,0.8777387634\H,-1.4696431123,-1.4680846533,-0.8778368298\H,-2.6053774797,-0.434923198,0.0001234067\N,-0.8611170707,1.4689756794,0.0000260977\H,1.6606841664,-1.0108785597,1.2444667731\H,2.1714419495,1.109876813,0.0002383775\H,1.6606906385,-1.0104081912,-1.24479938\Ge,1.3623291549,-0.1759517272,-0.0000086775\\Version=IA64L-G03RevD.01\HF=-2211.3973864\S2=0.767532\S2-1=0.\S2A=0.750196\RMSD=7.665e-09\RMSF=3.696e-06\Thermal=0.\Dipole=0.1590932,-1.0353642,-0.0000007\PG=C01 [X(C2H6Ge1N1)]\\@

Addition of $H_3Sn^•$ to acetonitrile:

Acetonitrile/$H_3Sn^•$ complex

1\1\GINC-AC30\FOpt\UBHandHLYP\Gen\C2H6N1Sn1(2)\UXW563\17-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct nosymm opt=(z-matrix,calcfc,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-1.6824920699,-0.0326062807,-0.0447179675\N,-0.5707898177,0.2074892571,-0.0864687394\C,-3.1002191452,-0.3406876387,0.0093754308\H,-3.6708301364,0.4627335527,-0.4414295465\H,-3.41293942,-0.4605829922,1.0399999737\H,-3.2990647826,-1.2600011986,-0.5288573898\H,2.4493392695,-0.7126855282,-1.0912978973\H,2.3333735858,0.326688635,1.5061572463\H,4.3458173684,1.1219950866,-0.2316181027\Sn,2.6792591481,0.6853321069,-0.1311760075\\Version=IA64L-G03RevD.01\HF=-137.7927678\S2=0.75156\S2-1=0.\S2A=0.750001\RMSD=4.680e-09\RMSF=6.958e-06\Thermal=0.\Dipole=-2.1500522,-0.1786674,-0.0309758\PG=C01 [X(C2H6N1Sn1)]\\@

N-philic transition state
1\1\GINC-AC29\FTS\UBHandHLYP\Gen\C2H6N1Sn1(2)\UXW563\15-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-1.2702106752,0.0337307606,0.0013047389\N,-0.2045301447,-0.4670983651,-0.0002878823\C,-2.7287742245,-0.0930943237,0.0053057655\H,-3.1406462744,0.3914920792,-0.873011565\H,-3.1374394594,0.4049336981,0.8775177015\H,-3.0377711962,-1.1375770829,0.0137616659\H,2.4634066227,-0.6013117214,-1.3949002296\H,2.4672388321,-0.5926145623,1.3871236083\H,2.7055828965,1.8112560884,-0.0111470399\Sn,1.954594623,0.2479594302,-0.005701763\\Version=IA64L-G03RevD.01\HF=-137.7612267\S2=0.776918\S2-1=0.\S2A=0.750195\RMSD=8.123e-09\RMSF=2.830e-05\Thermal=0.\Dipole=-1.385174,0.2266604,0.0022393\PG=C01 [X(C2H6N1Sn1)]\\@

N-addition product
1\1\GINC-AC26\FOpt\UBHandHLYP\Gen\C2H6N1Sn1(2)\UXW563\13-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.1141751719,0.275394248,0.0001648812\N,-0.156349647,-0.4827137934,0.0008722816\C,-2.5764179344,-0.0274525831,0.0010082511\H,-3.0379759624,0.4179556951,-0.8744941995\H,-3.0387876106,0.4247284641,0.8725715706\H,-2.7561979621,-1.1003387231,0.0049918909\H,2.4776908727,-0.6439993057,-1.4001729662\H,2.4804086525,-0.6450535434,1.3964148935\H,1.9896648226,1.7355716814,-0.0004497844\Sn,1.8035919406,0.0435838602,-0.000942819\\Version=IA64L-G03RevD.01\HF=-137.7809903\S2=0.755122\S2-1=0.\S2A=0.750017\RMSD=5.379e-09\RMSF=1.024e-05\Thermal=0.\Dipole=-0.0038531,0.177627,-0.0005566\PG=C01 [X(C2H6N1Sn1)]\\@

C-philic transition state
1\1\GINC-AC28\FTS\UBHandHLYP\Gen\C2H6N1Sn1(2)\UXW563\15-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.9567507513,-0.0499692802,0.6199607704\C,-1.7684952827,-0.7816217828,-0.3777954741\H,-1.4668461928,-1.8212150651,-0.4166035403\H,-1.6329117348,-0.3487677354,-1.361427515\H,-2.8143303657,-0.7184824691,-0.0956889126\N,-0.9014372208,0.5854289571,1.5996673741\H,2.0072504139,1.5006955362,-0.067417606\H,2.1682248185,-0.9703506693,-1.3609789659\H,2.263308247,-0.8461713211,1.4282322039\Sn,1.5848860688,-0.1459111702,0.0320766653\\Version=IA64L-G03RevD.01\HF=-137.771743\S2=0.78489\S2-1=0.\S2A=0.750362\RMSD=7.639e-09\RMSF=6.834e-06\Thermal=0.\Dipole=-0.5311091,-0.6867867,-0.9780482\PG=C01 [X(C2H6N1Sn1)]\\@

C-addition product
1\1\GINC-AC29\FOpt\UBHandHLYP\Gen\C2H6N1Sn1(2)\UXW563\15-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.7059427753,0.1471687599,0.2986468674\C,-1.6368909965,-0.9220719139,-0.2313949464\H,-1.4201260734,-1.8733155494,0.2447747304\H,-1.4927304649,-1.0442029472,-1.3004547983\H,-2.6687115402,-0.6528304575,-0.0384437455\N,-1.0501463508,1.1754200758,0.8674057302\H,2.2095638407,1.2990674873,0.7750447102\H,1.8322295096,-0.1795966969,-1.5744041137\H,1.9497664598,-1.4886520258,0.873492971\Sn,1.4658863907,-0.0573507323,0.0853565957\\Version=IA64L-G03RevD.01\HF=-137.7829702\S2=0.768005\S2-1=0.\S2A=0.750223\RMSD=9.009e-09\RMSF=1.211e-06\Thermal=0.\Dipole=0.2553708,-0.8841827,-0.4870157\PG=C01 [X(C2H6N1Sn1)]\\@

Gaussian archive entries for Table 4

Cyclization of 16a:

16a

1\1\GINC-AC15\FOpt\UBHandHLYP\6-311G(d,p)\C4H8N1Si1(2)\UXW563\22-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.7531652831,2.130106365,-0.4567059534\C,-0.2491640698,1.4097675136,0.4399346853\C,0.3959202417,0.2432677197,1.1941963531\C,-0.5479225761,-0.4519288506,2.0593739836\H,0.8092026541,-0.4772850318,0.4938455854\H,-0.6751909936,2.1009355694,1.1617174157\H,-1.0787790821,1.0290837007,-0.1495233631\H,1.579362632,2.5166326392,0.1371999734\H,1.1908849044,1.4274934095,-1.1670899309\H,-1.094281223,3.0971036867,-2.3085180901\H,1.0656490736,4.2021662918,-2.2867969543\H,1.2193930867,0.5993095196,1.8070471337\Si,0.0244133336,3.5589863331,-1.4557898214\N,-1.3004043949,-0.982592946,2.7303459635\\Version=IA64L-G03RevD.01\HF=-501.344935\S2=0.751585\S2-1=0.\S2A=0.750001\RMSD=4.885e-09\RMSF=5.381e-06\Thermal=0.\Dipole=1.0636823,0.6934531,-0.8272605\PG=C01 [X(C4H8N1Si1)]\\@

5-*exo* transition state

1\1\GINC-NODE051\FTS\UBHandHLYP\6-311G(d,p)\C4H8N1Si1(2)\UWILLE\05-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) OPT=(TS,NOEIGENTEST,CALCFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geom and freq\\0,2\C,-0.3145155162,1.5401759806,0.3648534643\C,0.9944497453,1.1407425774,-0.3111103293\C,-1.4798648955,0.6755282954,-0.1228095111\H,-0.2002578843,1.4409013946,1.441518687\H,-0.5008421253,2.5917174397,0.1656159147\H,1.8158778449,1.7696058716,0.0174595247\H,0.90594776831,1.2528320046,-1.3890741456\H,-1.5766555938,-1.9614068736,-1.11504789\H,-1.2617017663,-1.7568409001,1.2807944628\H,-1.7086666185,0.9155857309,-1.1592664642\H,-2.3773730427,0.8782421475,0.4549888508\C,1.390386398,-0.2653850031,-0.0388300625\N,2.1696828211,-1.0930173762,0.2042873221\Si,-0.9876316228,-1.1447061631,-0.0342586831\\Version=AM64L-G03RevC.02\State=2-A\HF=-501.3269447\S2=0.785392\S2-1=0.\S2A=0.75035\RMSD=0.000e+00\RMSF=5.983e-06\Dipole=-0.8912806,1.3078204,-0.2551655\PG=C01 [X(C4H8N1Si1)]\\@

5-*exo* product

1\1\GINC-NODE052\FOpt\UBHandHLYP\6-311G(d,p)\C4H8N1Si1(2)\UWILLE\04-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) OPT=(CALCFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geom and freq\\0,2\C,1.1337415978,1.1779780832,-0.3179803285\C,-0.2663422302,1.4381934233,0.2436475137\C,1.6270073049,-0.2015002613,0.1568517072\H,1.0864365895,1.1909829393,-1.4049276112\H,1.8173506124,1.9690898698,-0.0247299478\H,-0.7527964702,2.2930951795,-0.211199528\H,-0.2081551999,1.6192249665,1.3156475109\H,-0.0941651667,-2.2649128283,1.0916196986\H,0.0342452166,-2.0245206479,-1.3032149122\H,1.9198574525,-0.1531965001,1.2037160617\H,2.4930871532,-0.5370361392,-0.4030482572\C,-1.1026564955,0.1691694529,0.0372998923\N,-2.3202355643,0.1138844857,-0.1119516096\Si,0.1139491215,-1.3137830306,-0.0142224611\\Version=AM64L-G03RevC.02\State=2-A\HF=-501.3560246\S2=0.768802\S2-1=0.\S2A=0.75022\RMSD=0.000e+00\RMSF=3.913e-06\Dipole=1.3681004,0.2003943,0.1528381\PG=C01 [X(C4H8N1Si1)]\\@

6-*endo* transition state

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FTS\UBHandHLYP\6-311G(d,p)\C4H8N1Si1(2)\UWILLE\04-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) OPT=(TS,NOEIGENTEST,CALCFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geometry & frequency\\0,2\C,-0.3608775523,-1.284590708,-0.3525350139\C,0.9862594152,-1.1795303387,0.3707938774\C,1.8322390816,0.0161290658,-0.089430304\C,1.0319144905,1.2454312433,-0.0481121064\H,2.7201994727,0.1285841335,0.5232759876\H,0.8281435755,-1.1043407647,1.4440196215\H,1.5735921526,-2.079567709,0.207063423\H,-0.2002750361,-1.2989550407,-1.429974671\H,-0.8243534078,-2.2374147138,-0.1064461512\H,-2.1035118859,-0.0748867823,1.4361643317\H,-2.7363963422,0.0282155314,-0.8991404569\H,2.1694046705,-0.121692565,-1.1138390463\Si,-1.6025576709,0.0939585634,0.0522222887\N,0.0102559404,1.8085717784,-0.0109333999\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-501.3211826\S2=0.778057\S2-1=0.\S2A=0.750153\RMSD=0.000e+00\RMSF=7.428e-06\Dipole=0.9509052,-1.0947047,-0.1006084\PG=C01 [X(C4H8N1Si1)]\\@

6-*endo* product

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET9\FOpt\UBHandHLYP\6-311G(d,p)\C4H8N1Si1(2)\UWILLE\04-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=VERYTIGHT OPT=(CALCFC,MAXCYCLE=500,Z-MATRIX)

FREQ=NORAMAN\\geometry & frequency\\0,2\C,0.0871349832,1.3977799638,-0.2843270315\C,-1.2350887059,0.9431176456,0.3492160886\C,-1.7079498525,-0.4260150835,-0.1576041757\C,-0.6521139101,-1.4924569363,-0.0417121851\H,-2.5998187501,-0.7457964662,0.3710405015\H,-1.123136942,0.8924714235,1.4306908897\H,-2.0182724792,1.6722575894,0.1572608652\H,-0.0408939632,1.517478039,-1.3591785265\H,0.3755438832,2.3713455429,0.1037569414\H,2.0804826704,0.3132547146,1.3476043095\H,2.452244447,0.0855376118,-1.015518169\H,-1.982144371,-0.3756365375,-1.2108470927\Si,1.4259231833,0.1159653874,0.0405720315\N,0.5630251215,-1.4127115541,0.0591065233\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-501.3617576\S2=0.755956\S2-1=0.\S2A=0.750024\RMSD=6.737e-09\RMSF=4.609e-06\Dipole=-0.5471417,1.068536,-0.1070205\PG=C01 [X(C4H8N1Si1)]\\@

Cyclization of 16b:

16b

1\1\GINC-AC26\FOpt\UBHandHLYP\6-311G(d,p)\C5H10N1Si1(2)\UXW563\22-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.806352569,2.7747403221,2.8248361211\C,-0.7878090774,1.8356832313,2.3748891728\C,-0.9380673847,1.4710353946,0.896612668\C,0.133922559,0.4885164714,0.4420163034\C,-0.0017916734,0.112641043,-1.0365250981\H,0.1865231978,2.2800660931,2.5592860351\H,-0.8866120119,2.3769178771,0.2984074301\H,1.1165438115,0.9218970164,0.6215931206\H,2.6680052075,-0.5421758243,-1.5148467789\H,-0.8523058739,0.9450475189,2.9941044181\H,-1.9239884595,1.0441823034,0.732637335\H,0.0800191894,-0.409550893,1.0553260742\H,1.2264822773,-2.3899835886,-0.9180397912\H,-0.9834755056,-0.3207836233,-1.2183932031\H,0.0523288677,1.0091192799,-1.651379185\Si,1.3041413388,-1.1039764916,-1.6486836275\N,-2.6103645837,3.5093031097,3.1595615456\\Version=IA64L-G03RevD.01\HF=-540.6425989\S2=0.751648\S2-1=0.\S2A=0.750001\RMSD=9.461e-09\RMSF=3.560e-06\Thermal=0.\Dipole=0.8747566,-0.8712587,-0.5865799\PG=C01 [X(C5H10N1Si1)]\\@

6-*exo* transition state

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET18\FTS\UBHandHLYP\6-311G(d,p)\C5H10N1Si1(2)\UWILLE\12-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=VERYTIGHT OPT=(TS,NOEIGENTEST,CALCFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geometry & frequency\\0,2\C,-1.5794201605,-0.0803180939,-0.5629885655\C,1.5301494111,-0.307777121,-0.0434006052\C,1.2292220807,1.0062035328,0.5705535875\C,0.1377692642,1.8015154848,-0.1559442719\C,-1.2936189276,1.3040132282,0.0281770887\H,-1.270405677,-1.6691608072,1.6905658885\H,-0.7008038252,-2.7457312647,-0.4128563044\H,-1.2864269939,-0.1036160899,-1.6109609064\H,-2.6506546998,-0.27288263,-0.5392005437\H,0.9635209781,0.8595357809,1.612670468\H,2.160473021,1.5662124726,0.548045029\H,0.1955809989,2.8218405196,0.2134843046\H,0.3803558422,1.8424947277,-1.2152180625\H,-1.5386805006,1.3096049936,1.0901876143\H,-1.9559719758,2.0327870499,-0.4334840055\N,2.1712070173,-1.0436235078,-0.6714095454\Si,-0.6885747354,-1.4769673131,0.3384464239\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-540.6235135\S2=0.780314\S2-1=0.\S2A=0.750254\RMSD=6.015e-09\RMSF=2.186e-05\Dipole=-0.7746974,1.262536,0.458611\PG=C01 [X(C5H10N1Si1)]\\@

6-*exo* product

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET15\FOpt\UBHandHLYP\6-311G(d,p)\C5H10N1Si1(2)\UWILLE\07-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) GEOM=CHECKPOINT GUESS=CHECK OPT=(READFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geometry & frequency\\0,2\C,-1.3192890888,-1.0454004963,-0.4424160703\C,1.1828107034,0.4964449124,-0.1774592618\C,0.4176311226,1.2908368888,0.8775803754\C,-1.095893977,1.2714309092,0.647883201\C,-1.7339859049,-0.1164846899,0.7085353141\H,1.0021893095,-2.1402152251,0.5950203675\H,1.0433372047,-1.7805411257,-1.7936632181\H,-1.6479194584,-0.6190782805,-1.3890833064\H,-1.815709457,-2.0081914357,-0.3492859021\H,0.6409976645,0.854172997,1.8500919611\H,0.7924051628,2.308765197,0.8830303296\H,-1.5569706376,1.9040519779,1.4018896854\H,-1.3167220894,1.7297528145,-0.314794574\H,-1.4859981353,-0.5803336411,1.6631291862\H,-2.8151733649,-0.0022656252,0.7029009163\N,2.1191543028,0.9582264179,-0.8327861891\Si,0.5441318964,-1.2681905517,-0.5074623909\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-540.6595133\S2=0.767421\S2-1=0.\S2A=0.750186\RMSD=0.000e+00\RMSF=8.709e-06\Dipole=-1.197286,-0.3088217,0.5896444\PG=C01 [X(C5H10N1Si1)]\\@

7-*endo* transition state

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET15\FTS\UBHandHLYP\6-311G(d,p)\C5H10N1Si1(2)\UWILLE\07-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT)

OPT=(TS,NOEIGENTEST,CALCFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geometry &
frequency\\0,2\C,0.9265617068,-1.5060753072,0.0326828958\C,1.9904951285,-
0.5115224538,0.1409991676\C,1.5936889494,0.8872717058,-
0.3553182104\C,0.4378620133,1.5636350302,0.3908344738\C,-0.9581569292,1.3481167898,-
0.2098893318\H,2.2878439739,-0.469136069,1.186066183\H,1.366410469,0.8362572826,-
1.4172933768\H,0.4504289813,1.2611103274,1.4374052331\H,-2.1678951689,-
0.529418687,1.4240037271\H,2.8559291175,-0.8666391837,-0.4105607792\H,2.4853601845,1.5020098078,-
0.263851314\H,0.6347061791,2.6327915678,0.3945663812\H,-3.0453923826,-0.3538649048,-0.8084734659\H,-
1.636943804,2.0794857145,0.2284886225\H,-0.9282124722,1.5792880853,-1.2736240864\Si,-1.8026067051,-
0.3349679636,0.0033423859\N,-0.1440637743,-1.9529838629,-0.0770534997\\Version=x86-Linux-
G03RevB.04\State=2-A\HF=-540.6171736\S2=0.773471\S2-1=0.\S2A=0.750117\RMSD=0.000e+00\RMSF=1.461e-
05\Dipole=1.183157,1.0128892,0.0143082\PG=C01 [X(C5H10N1Si1)]\\@

7-*endo* product
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\FOpt\UBHandHLYP\6-
311G(d,p)\C5H10N1Si1(2)\UWILLE\05-Dec-2006\1\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT)
GEOM=CHECKPOINT GUESS=CHECK OPT=(READFC,MAXCYCLE=500,Z-MATRIX)
FREQ=NORAMAN\\geometry &
frequency\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,4,B4,3,A3,2,D2,0\H,2,B5,1,A4,3,D3,0\H,3,B6,2,A5,1,D4,
0\H,4,B7,3,A6,2,D5,0\H,5,B8,4,A7,3,D6,0\H,2,B9,1,A8,3,D7,0\H,3,B10,2,A9,1,D8,0\H,4,B11,3,A10,2,D9,0\H,5,B12,
4,A11,3,D10,0\H,5,B13,4,A12,3,D11,0\H,5,B14,4,A13,3,D12,0\Si,5,B15,4,A14,3,D13,0\N,16,B16,5,A15,4,D14,0\\B1
=1.49939768\B2=1.53314735\B3=1.53302048\B4=1.53516944\B5=1.09045146\B6=1.088464\B7=1.08980225\B8=2.7
633855\B9=1.08598795\B10=1.08750061\B11=1.08712193\B12=2.76749326\B13=1.08957795\B14=1.08894542\B15
=1.8775196\B16=1.73838691\A1=117.48253732\A2=117.1530178\A3=114.7940267\A4=105.49247347\A5=109.1186
4549\A6=109.59308814\A7=107.88501556\A8=108.10292785\A9=106.24915419\A10=107.823625\A11=141.701099
04\A12=109.63269881\A13=109.03540834\A14=115.30350987\A15=111.25627253\D1=62.69290138\D2=-
88.08559797\D3=123.25827143\D4=-62.11158667\D5=36.82425686\D6=100.71592021\D7=-
124.30533473\D8=184.09518407\D9=151.34827861\D10=51.0075748\D11=-169.00071402\D12=-
53.50420252\D13=69.31335699\D14=-36.1470461\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-
540.658477\S2=0.755806\S2-1=0.\S2A=0.750022\RMSD=0.000e+00\RMSF=4.256e-
05\Dipole=0.4458551,0.127391,1.0793618\PG=C01 [X(C5H10N1Si1)]\\@

Cyclization of 16c:
16c
1\1\GINC-AC27\FOpt\UBHandHLYP\6-311G(d,p)\C6H12N1Si1(2)\UXW563\22-Nov-2007\0\\# BHandHLYP/6-
311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-3.4019440305,-
1.3304570817,2.8735547574\C,-0.8373526219,-0.7565564237,-1.4067847616\C,-2.9825110476,-
1.9455704492,1.621404846\C,-1.6937309667,-1.6696670805,-0.5368470153\C,-2.1233435885,-
1.0124049874,0.7663317603\H,-2.4355922231,-2.8541830124,1.8583539788\H,-1.3932524022,0.1543899281,-
1.6217835259\H,-1.1381204519,-2.5812716359,-0.3187901189\H,0.0419226489,-0.4495088267,-0.8432049368\H,-
3.8740314846,-2.2452347674,1.0771851085\H,-2.5759945832,-1.9752087956,-1.0985470584\H,-2.6844783833,-
0.1051944326,0.5577833544\H,-1.2485946673,-0.7124586067,1.3374958167\H,-0.0735713362,0.9015454393,-
4.2348304206\H,1.9218563872,0.0605126822,-3.1583733823\C,-0.4043723759,-1.4186406556,-2.7188437795\H,-
1.2822159062,-1.7264056832,-3.284335144\H,0.1536839288,-2.328929933,-2.5066834571\N,-3.7212424075,-
0.8347539404,3.8484345191\Si,0.6564319316,-0.3210039975,-3.8270179009\\Version=IA64L-G03RevD.01\HF=-
579.9400058\S2=0.751654\S2-1=0.\S2A=0.750001\RMSD=4.346e-09\RMSF=7.129e-
06\Thermal=0.\Dipole=0.3748516,-0.8018675,-1.3144514\PG=C01 [X(C6H12N1Si1)]\\@

7-*exo* transition state
1\1\GINC-NODE052\FTS\UBHandHLYP\6-311G(d,p)\C6H12N1Si1(2)\UWILLE\09-Dec-2006\0\\#BHANDHLYP/6-
311G** SCF=(QC,DIRECT) OPT=(TS,NOEIGENTEST,CALCFC,MAXCYCLE=500,Z-MATRIX)
FREQ=NORAMAN\\geom and
freq\\0,2\C,1.3080310546,1.4372507341,0.1400336162\C,2.0039532069,0.1148717921,-
0.207726687\C,0.014905677,1.6880565584,-0.6553042391\C,-1.4525315615,-0.9289047616,-0.084549799\C,-
1.2907409447,1.5706501679,0.1272364607\C,-
1.5468489788,0.234007895,0.8292707867\H,1.1055629373,1.4820020349,1.209463749\H,2.2140517424,0.09449962
62,-1.2752704063\H,1.2021288575,-1.7833540358,1.6651291514\H,-0.0221393115,1.0140291111,-1.5085718854\H,-
2.117905758,1.7645907942,-0.5499115167\H,2.0048972791,2.2478194097,-
0.0547580495\H,2.9708377357,0.0648041621,0.2917746594\H,1.4923030892,-2.612484452,-
0.5926302397\H,0.0408044791,2.6895620349,-1.0753941337\H,-1.3265047964,2.3435298138,0.8920754108\H,-
2.5534116548,0.229426169,1.239096518\H,-0.8669010479,0.0962691415,1.6617069535\Si,1.0567516289,-
1.4628698326,0.2238440799\N,-1.8798367254,-1.6923014955,-0.8471840228\\Version=AM64L-

G03RevC.02\State=2-A\HF=-579.9154921\S2=0.781132\S2-1=0.\S2A=0.750272\RMSD=0.000e+00\RMSF=3.275e-06\Dipole=0.4700278,1.3508528,0.6731342\PG=C01 [X(C6H12N1Si1)]\\@

7-*exo* product
1\1\GINC-NODE052\FOpt\UBHandHLYP\6-311G(d,p)\C6H12N1Si1(2)\UWILLE\09-Dec-2006\0\\#BHANDHLYP/6-311G** GEOM=CHECKPOINT GUESS=CHECK SCF=(QC,DIRECT) OPT=(READFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geom and freq\\0,2\C,-1.0224350195,-1.5183687965,-0.6511469906\C,0.4940435058,-1.6338883619,-0.8688643066\C,-1.4049711487,-0.9990229965,0.7438512135\C,0.6515844929,1.1588731408,0.4293285124\C,-1.7750276944,0.4822787628,0.8498143867\C,-0.8204719098,1.4823640025,0.189259408\H,-1.47073075,-0.8939972114,-1.422620078\H,0.9047491165,-2.2982229852,-0.1104994792\H,1.3914346558,0.6544188129,-2.131297267\H,-0.58904426,-1.2107556847,1.4321391026\H,-1.8574569072,0.7305352105,1.9044788081\H,-1.4550409909,-2.5054907021,-0.7887421528\H,0.6969997982,-2.1115367502,-1.8260259696\H,2.8833934035,-0.2534482434,-0.4663831057\H,-2.25375578,-1.5655741155,1.116490348\H,-2.7620288471,0.6384611518,0.4189987922\H,-1.0240859386,2.4799285791,0.5633931395\H,-0.9879213423,1.5052773135,-0.8847255199\Si,1.4722321354,-0.0269486225,-0.8202602784\N,1.3108435127,1.6248958332,1.3607119915\\Version=AM64L-G03RevC.02\State=2-A\HF=-579.9500586\S2=0.76755\S2-1=0.\S2A=0.750189\RMSD=1.840e-09\RMSF=7.464e-05\Dipole=-0.8760797,-0.7150704,-0.6884937\PG=C01 [X(C6H12N1Si1)]\\@

8-*endo* transition state
1\1\GINC-NODE051\FTS\UBHandHLYP\6-311G(d,p)\C6H12N1Si1(2)\UWILLE\09-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) OPT=(TS,NOEIGENTEST,CALCFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geom and freq\\0,2\C,-0.8379684499,-1.6510288261,-0.3675498922\C,0.0701857083,1.4547995176,-0.8458564348\C,-2.0160707564,-0.8851167419,0.0380497499\C,-1.2377405442,1.5785714178,-0.0628967141\C,-1.663274351,0.3984575701,0.8058504415\H,-2.6124801202,-0.6583848337,-0.8415740927\H,-0.0095466924,0.6650084842,-1.5894869124\H,-2.0427100097,1.7966435116,-0.7641390024\H,0.1789967884,2.3751143089,-1.4143548749\H,-2.6212947305,-1.5395247676,0.6589553927\H,-1.159523507,2.4508968216,0.5838451553\H,-2.5494736036,0.6913158038,1.3623474386\H,-0.9016094526,0.1718074043,1.5480207125\H,2.8932280765,-0.9004523592,-0.7365619573\H,2.6349972464,-0.5862249246,1.625283532\C,1.3213765658,1.2585680739,0.0285792781\H,1.1690745179,1.7283642466,0.9987791443\H,2.1576006254,1.7882463797,-0.4241802596\N,0.2851338813,-1.9523866478,-0.4308062178\Si,1.9319824755,-0.5172578292,0.316546477\\Version=AM64L-G03RevC.02\State=2-A\HF=-579.9130254\S2=0.774002\S2-1=0.\S2A=0.750119\RMSD=0.000e+00\RMSF=2.281e-05\Dipole=-1.3025923,0.8400743,0.2118529\PG=C01 [X(C6H12N1Si1)]\\@

8-*endo* product
1\1\GINC-NODE051\FOpt\UBHandHLYP\6-311G(d,p)\C6H12N1Si1(2)\UWILLE\06-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) GEOM=CHECKPOINT GUESS=CHECK OPT=(READFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geom and freq\\0,2\C,0.2998816924,-1.2451635348,1.4340072796\C,-0.1241389687,1.7307439028,0.0200674395\C,1.6584279003,-0.7145633531,1.0824186523\C,1.3269304449,1.4205437028,-0.3418065035\C,1.7793092677,-0.0375850322,-0.287226193\H,1.9729031006,-0.0448302965,1.8804590287\H,-0.3137887824,1.4613443077,1.0566833483\H,1.9691332966,1.9994569243,0.3207324996\H,-0.2403451578,2.8112708669,-0.0265178975\H,2.3329103583,-1.5661453115,1.1410476471\H,1.5184932956,1.7945410343,-1.346641765\H,2.825362597,-0.0672935567,-0.582811168\H,1.2525459599,-0.6333932316,-1.0297061376\H,-2.9810542414,-0.9695709664,-0.472554553\H,-1.051875417,-1.5692122618,-1.7445248479\C,-1.1841378591,1.0897565263,-0.8865026304\H,-0.9189383945,1.2455547274,-1.9315868821\H,-2.1281946663,1.6102190864,-0.7402672534\N,-0.7625649539,-1.2964174957,0.8462478976\Si,-1.5312022955,-0.747100866,-0.6124139693\\Version=AM64L-G03RevC.02\State=2-A\HF=-579.9532649\S2=0.755789\S2-1=0.\S2A=0.750021\RMSD=0.000e+00\RMSF=6.432e-06\Dipole=0.670187,0.7200938,-0.4843217\PG=C01 [X(C6H12N1Si1)]\\@

Cyclization of 16d:
16d
1\1\GINC-AC26\FOpt\UBHandHLYP\6-311G(d,p)\C7H14N1Si1(2)\UXW563\22-Nov-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-2.3163025536,-5.2359020488,0.0754272363\H,-2.9297045019,-4.3794150926,-0.1983873663\H,-2.3048208
775,-5.8901715974,-0.7975168058\C,-0.8945879462,-4.7808355624,0.4014797628\H,-0.9122031604,-4.1158983837,1.2638566432\H,-0.2932125941,-5.6401621139,0.6956458635\C,-0.2116705454,-4.0713376396,-0.7609742813\H,-0.8105868334,-3.2110127791,-1.057897763\H,-0.1870474785,-4.7372105199,-1.6229331982\C,1.2033274036,-3.6136787002,-0.4360542705\H,1.8009368127,-4.4744694257,-

0.136695556\H,1.1775752488,-2.9456497591,0.4246257617\Si,-3.1845131835,-6.1693050646,1.4661812151\H,-4.5523567392,-6.5763863071,1.0721984661\H,-2.4088249741,-7.3612008591,1.8823949855\N,4.4666793874,-1.2559471416,-3.2347386269\C,3.962837336,-1.7819251284,-2.3586051981\C,1.8812672183,-2.9092740674,-1.6017017778\H,1.9223274695,-3.5714128525,-2.4627286341\H,1.2971903844,-2.0435208128,-1.9030874183\C,3.2999580286,-2.4573089189,-1.2510773785\H,3.9091162521,-3.309505379,-0.9620671497\H,3.2830725765,-1.7780177493,-0.4030816765\\Version=IA64L-G03RevD.01\HF=-619.237291\S2=0.751609\S2-1=0.\S2A=0.750001\RMSD=6.386e-09\RMSF=1.414e-06\Thermal=0.\Dipole=-0.740377,-0.5926652,0.9966934\PG=C01 [X(C7H14N1Si1)]\\@

8-*exo* transition state

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET7\FTS\UBHandHLYP\6-311G(d,p)\C7H14N1Si1(2)\UWILLE\18-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) OPT=(TS,NOEIGENTEST,CALCFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geometry & frequency\\0,2\C,0.6152877491.5617613069,0.5314969528\C,0.4148960703,1.6284947929,0.8476340825\C,1.724069498,-1.1554040502,-0.360584359\C,1.6438999813,1.4175988464,-0.0395395776\C,1.6242862607,0.2293593246,-0.9976455442\H,-2.4870766178,-1.9783211245,-0.2821643119\H,2.6318555164,-1.2288622858,0.2341695899\H,0.3117450458,0.8058227021,1.5474845318\H,2.5237575532,1.3381016556,0.5977042503\H,-1.6542296956,-0.6832590835,-2.1484404897\H,0.6202101634,2.5034382046,1.4586739628\H,1.7901749023,-1.9060412304,-1.142630662\H,1.7890318108,2.3153039466,-0.6380760426\H,2.4771599021,0.3170512115,-1.6658546578\H,0.747041414,0.2722221699,-1.637597122\C,-1.9271555514,0.6982828418,0.2424077521\H,-2.0549718877,0.451250461,1.2941477111\H,-2.9034378772,1.0326267168,-0.1090858299\C,-0.9168313574,1.8452558266,0.1035203358\H,-0.7267297625,2.0474164274,-0.9497817414\H,-1.3849803704,2.7474420545,0.4879067276\Si,-1.558622176,-0.9032557979,-0.6797120275\N,0.1529206379,-1.9999383295,1.5008249448\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-619.2123212\S2=0.778227\S2-1=0.\S2A=0.750221\RMSD=0.000e+00\RMSF=1.946e-05\Dipole=0.7458041,0.8442875,-0.7936875\PG=C01 [X(C7H14N1Si1)]\\@

8-*exo* product

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET1\FOpt\UBHandHLYP\6-311G(d,p)\C7H14N1Si1(2)\UWILLE\15-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) GEOM=CHECKPOINT GUESS=CHECK OPT=(READFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geometry & frequency\\0,2\C,0.4791164849,-1.0684553118,1.0038440207\C,-0.3921095233,1.8706305317,0.0406645554\C,1.8214133982,-0.4508452787,0.6236909624\C,1.1112329156,1.8882510921,-0.2411952194\C,1.781095508,0.547385815,-0.5305322635\H,-1.6306664064,-2.6575831503,0.2131127838\H,2.2539205675,0.0008983119,1.5119105337\H,-0.5870627313,1.3645381748,0.9818558767\H,1.6166863273,2.3561905474,0.6023717\H,-0.1133661477,-1.9929640091,-1.5316560004\H,-0.6985303248,2.900951995,0.1993120764\H,2.4661563668,-1.2808595487,0.3417080387\H,1.2902050315,2.5379577401,-1.0966967025\H,2.8099383329,0.74530271,-0.8212940076\H,1.3235548924,0.0799233024,-1.4005946169\C,-1.9330954954,-0.0715814333,-0.6897217071\H,-2.5589824682,0.0833063788,0.1881975583\H,-2.6097375928,-0.3836708979,-1.484865955\C,-1.2610873727,1.2533513494,-1.0713059095\H,-0.669184937,1.1190074008,-1.9747681577\H,-2.0431117717,1.957517343,-1.3417916195\Si,-0.8266962246,-1.5430710959,-0.3154286125\N,0.1549332163,-1.2914202204,2.1737903476\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-619.2465394\S2=0.767665\S2-1=0.\S2A=0.750193\RMSD=0.000e+00\RMSF=6.598e-05\Dipole=0.199059,0.5922152,-1.0391305\PG=C01 [X(C7H14N1Si1)]\\@

9-*endo* transition state

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FTS\UBHandHLYP\6-311G(d,p)\C7H14N1Si1(2)\UWILLE\14-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) OPT=(TS,NOEIGENTEST,CALCFC,MAXCYCLE=500,Z-MATRIX) FREQ=NORAMAN\\geometry & frequency\\0,2\C,-1.8978001006,-1.2745630878,0.299402965\H,-2.2216425401,-1.9587188683,-0.4833773806\H,-2.5045404573,-1.493013216,1.1751385159\C,-0.4187841989,-1.5108471373,0.621516018\H,-0.1027968631,-0.7900270887,1.3729131724\H,-0.2835008583,-2.4897495034,1.0793463976\C,0.4896848689,-1.4206756401,-0.6053161282\H,0.165883408,-0.6080965045,-1.2531882543\H,0.3569081605,-2.3271763453,-1.1907769871\C,1.9742066456,-1.2386892278,-0.2719450942\H,2.5770633873,-1.7895309101,-0.9895585732\H,2.1845354011,-1.6886139376,0.6977158332\Si,-2.2349434334,0.5237709303,-0.2240262975\H,-2.5609852929,0.638397754,-1.660081922\H,-3.3340925086,1.1326126922,0.5553659941\N,-0.497210696,2.0091335114,-0.1631840901\C,0.5981103324,1.80145101,0.1765271632\C,2.4922834625,0.1997428943,-0.2832257128\H,3.5497156948,0.1770945868,-0.0346876716\H,2.4261183227,0.6034472106,-1.2903965286\C,1.8270279972,1.1924762523,0.6885539446\H,2.5278777591,1.9925066433,0.908209071\H,1.6007652831,0.7107695015,1.6389561952\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-619.2062519\S2=0.7713

74\S2-1=0.\S2A=0.750116\RMSD=0.000e+00\RMSF=8.156e-06\Dipole=1.3223463,-0.7529425,0.4165946\PG=C01 [X(C7H14N1Si1)]\\@

9-*endo* product

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET12\FOpt\UBHandHLYP\6-311G(d,p)\C7H14N1Si1(2)\UWILLE\08-Dec-2006\0\\#BHANDHLYP/6-311G** SCF=(QC,DIRECT) GEOM=CHECKPOINT GUESS=CHECK OPT=(Z-MATRIX,READFC,MAXCYCLE=500) FREQ=NORAMAN\\geometry & frequency\\0,2\C,1.6990228982,-1.340009751,-0.032769572\H,2.0891178993,-1.3366752435,-1.0481599656\H,2.3922260473,-1.9418206576,0.5537343076\C,1.6256439612,0.0910591385,0.5186275521\H,0.9312124711,0.1236860197,1.3560090901\H,2.5866227064,0.3788491489,0.9383491824\C,1.2209689495,1.1351598069,-0.5324244576\H,0.6149204645,0.6721707166,-1.3049684495\H,2.1231838898,1.4729147807,-1.0358615176\C,0.4728473287,2.342718079,0.0456313173\H,0.7821556837,3.2466032977,-0.4733806454\H,0.769490219,2.4832926739,1.084280585\Si,0.0416919817,-2.2190293673,0.0459492437\H,0.0433758564,-3.4437927991,-0.7729988983\H,-0.2346329013,-2.5953755992,1.4512769337\N,-1.2167619644,-1.1735250001,-0.5216847601\C,-1.7855311853,-0.1069601416,-0.4150903617\C,-1.0543805267,2.2832395621,-0.0403865246\H,-1.4519479649,3.1580790682,0.4669146445\H,-1.3607626601,2.3706323168,-1.0805108607\C,-1.7345518348,1.0393268252,0.5557849152\H,-2.7636688719,1.2917985134,0.7926582696\H,-1.2517643775,0.7335227921,1.4849240206\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-619.2436161\S2=0.755651\S2-1=0.\S2A=0.75002\RMSD=0.000e+00\RMSF=3.533e-06\Dipole=0.5441989,0.6053408,0.4712357\PG=C01 [X(C7H14N1Si1)]\\@

Gaussian archive entries for Table 5

Cyclization of 17a:

17a

1\1\GINC-AC54\FOpt\UBHandHLYP\6-311G(d,p)\C3H7O1Si1(2)\UXW563\17-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\Si,-2.2030199737,-0.1338906298,0.0000009687\C,-0.3533011386,-0.4927383735,-0.0000013979\C,0.5237274464,0.754453996,-0.0000012142\C,1.9991304175,0.4593101045,0.0000005104\H,2.6470364118,1.351712153,0.0000043459\H,0.3273624411,1.3884653177,-0.8654807855\H,0.327360988,1.3884662967,0.8654772083\H,-0.1117706249,-1.1040634376,0.865138023\H,-0.1117722236,-1.1040622286,-0.8651419929\H,-2.6067871443,0.6224628471,1.2082190673\H,-2.6067904103,0.6224646855,-1.208214961\O,2.4742467005,-0.6322397208,-0.0000007721\\Version=IA64L-G03RevD.01\HF=-483.1244683\S2=0.751642\S2-1=0.\S2A=0.750001\RMSD=5.065e-09\RMSF=9.295e-05\Thermal=0.\Dipole=-0.2827146,0.7344684,0.0000003\PG=C01 [X(C3H7O1Si1)]\\@

4-*exo* transition state

1\1\GINC-AC24\FTS\UBHandHLYP\6-311G(d,p)\C3H7O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.0391404758,1.3177982903,-0.1624396441\C,1.355238885,0.7033682271,0.0541586745\Si,0.7690099228,-1.0738458994,-0.0852843842\C,-1.0200210027,0.2943832887,0.4193061829\H,-0.1673933254,2.292522911,0.3036330826\H,-0.2641325856,1.4186234953,-1.2192485316\H,-0.9125469411,0.1424066423,1.5061029279\H,2.1057720623,1.0423908002,-0.6491881034\H,1.7200894803,0.8989792365,1.0581794641\H,1.3246702283,-2.0915119575,0.8293932589\H,0.6687399323,-1.5865424455,-1.4623845352\O,-2.0848831804,-0.0162745892,-0.1265803922\\Version=IA64L-G03RevD.01\HF=-483.09748\S2=0.783295\S2-1=0.\S2A=0.750133\RMSD=7.636e-09\RMSF=6.823e-06\Thermal=0.\Dipole=1.2991454,0.206612,0.3038797\PG=C01 [X(C3H7O1Si1)]\\@

4-*exo* product

1\1\GINC-AC54\FOpt\UBHandHLYP\6-311G(d,p)\C3H7O1Si1(2)\UXW563\17-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-0.0140795943,1.3197393662,-0.1336533104\C,1.4196120167,0.7486868707,0.0236225062\Si,0.6786640634,-0.9748725579,-0.0594272086\C,-0.8763958501,0.1393019545,0.3898263286\H,-0.190251141,2.2532440958,0.3922696846\H,-0.2595602223,1.4669201188,-1.180722029\H,-0.9255777429,0.1168800643,1.4874800965\H,2.1306078112,1.0644898188,-0.7279816976\H,1.8329905861,0.9659104873,1.0032515162\H,1.0717910389,-2.0250730219,0.900020647\H,0.573048972,-1.536721675,-1.4159609079\O,-1.9854469379,-0.1962055215,-0.2130806246\\Version=IA64L-G03RevD.01\HF=-483.1042467\S2=0.759423\S2-1=0.\S2A=0.750036\RMSD=2.577e-09\RMSF=1.333e-05\Thermal=0.\Dipole=1.107413,0.1752106,0.3085646\PG=C01 [X(C3H7O1Si1)]\\@

5-*endo* transition state

1\1\GINC-AC29\FTS\UBHandHLYP\6-311G(d,p)\C3H7O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm freq=noraman opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.4068199245,-0.5497059332,0.2674374301\C,-0.1320277696,-1.2300264369,-0.2706002686\Si,1.354160644,-0.07006784,-0.0653018235\C,-1.2447171827,0.9182957232,0.057796032\H,0.0337047909,-2.1794046405,0.2267240032\H,-0.2386859597,-1.4489205895,-1.3310645634\H,-2.3199085317,-0.9206471553,-0.1860016352\H,-1.4816244155,-0.7267824907,1.3411096826\H,-2.0357571888,1.5390785041,-0.3561108491\H,2.4359432804,-0.6132705103,-0.9438780804\H,1.8654942643,-0.0065199399,1.3172061004\O,-0.1237790071,1.404063309,0.250531973\\Version=IA64L-G03RevD.01\HF=-483.1077229\S2=0.770344\S2-1=0.\S2A=0.750083\RMSD=8.369e-09\RMSF=4.666e-05\Thermal=0.\Dipole=-1.1150718,-0.3897705,-0.1032104\PG=C01 [X(C3H7O1Si1)]\\@

5-*endo* product

1\1\GINC-AC12\FOpt\UBHandHLYP\6-311G(d,p)\C3H7O1Si1(2)\UXW563\17-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.4196858598,-0.560793396,0.1731947057\C,-0.1507897328,-1.3699566251,-0.1782691052\Si,1.1915257483,-0.0754915929,0.0472609671\C,-1.1453087196,0.8749844502,-0.1549632074\H,-0.0457660767,-2.2554679052,0.4372276502\H,-0.1795805824,-1.6898266694,-1.2160834425\H,-2.2969983048,-0.9212904399,-0.3553202991\H,-1.6314986554,-0.6705093229,1.241372736\H,-1.8571184962,1.6662909512,0.0015101689\H,2.1702000226,0.0090356646,-1.0499643506\H,1.9119044438,-0.1345107005,1.3320063242\O,0.1591012129,1.2436275857,0.0298748528\\Version=IA64L-G03RevD.01\HF=-

483.1656446\S2=0.755358\S2-1=0.\S2A=0.750021\RMSD=3.822e-09\RMSF=2.073e-05\Thermal=0.\Dipole=-0.1588762,-0.69659,0.09043\PG=C01 [X(C3H7O1Si1)]\\@

Cyclization of 18a:

18a

1\1\GINC-AC54\FOpt\UBHandHLYP\6-311G(d,p)\C4H9O1Si1(2)\UXW563\17-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\Si,-2.2002234755,-0.1578389719,0.000083875\C,-0.3450762006,-0.482287155,0.0278663324\C,0.5076522458,0.7806683052,-0.0203582344\C,1.9994486401,0.5043767214,-0.0252992713\H,0.286846374,1.3719394774,-0.9089880923\H,0.2932866704,1.4383696248,0.8212322571\H,-0.0998191012,-1.0519438916,0.9200233627\H,-0.0843797921,-1.1253669482,-0.807741007\H,-2.6317466391,0.637155939,1.1738593922\H,-2.6106400406,0.5431477472,-1.239312039\O,2.4375755193,-0.6077550057,-0.0567141238\C,2.8993527185,1.7130575268,0.0154412631\H,2.6335373171,2.4190731852,-0.7661723551\H,2.781464123,2.2267463239,0.9663543527\H,3.9295182807,1.4040417417,-0.1002710532\\Version=IA64L-G03RevD.01\HF=-522.4333894\S2=0.751649\S2-1=0.\S2A=0.750001\RMSD=5.830e-09\RMSF=1.359e-05\Thermal=0.\Dipole=-0.0721988,0.9081427,0.0409469\PG=C01 [X(C4H9O1Si1)]\\@

4-*exo* transition state

1\1\GINC-AC50\FTS\UBHandHLYP\6-311G(d,p)\C4H9O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.0252086952,1.3106776601,-0.1158732685\C,1.3962358252,0.7212019371,-0.0258735482\Si,0.8182771826,-1.0615748881,-0.1068871891\C,-0.9774300105,0.2349475398,0.4543802021\H,-0.1384030051,2.2551534469,0.4127779647\H,-0.3144341727,1.4638442189,-1.1494661809\H,2.0665643454,1.0659328705,-0.8037560744\H,1.8580906514,0.9307970418,0.9337131422\H,1.4207152299,-2.0459040869,0.8173367196\H,0.6771478679,-1.6193863529,-1.4617980349\C,-1.0567246512,0.163853944,1.9727417838\H,-1.6720287825,0.9960016012,2.3125904777\H,-1.536308932,-0.757614873,2.277880326\H,-0.0900605064,0.2494757602,2.4594882387\O,-1.9558983469,-0.1515798196,-0.2148845586\\Version=IA64L-G03RevD.01\HF=-522.3999899\S2=0.781022\S2-1=0.\S2A=0.750123\RMSD=9.660e-09\RMSF=2.362e-05\Thermal=0.\Dipole=1.1410624,0.2836271,0.4709971\PG=C01 [X(C4H9O1Si1)]\\@

4-*exo* product

1\1\GINC-AC28\FOpt\UBHandHLYP\6-311G(d,p)\C4H9O1Si1(2)\UXW563\17-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,0.006516301,1.3202182272,-0.0922765368\C,1.4527295217,0.7586255308,-0.0651253468\Si,0.7279332751,-0.971885126,-0.0803032022\C,-0.8407844087,0.1209701739,0.4427622394\H,-0.1313758301,2.2269735127,0.4906763179\H,-0.3135673491,1.5144476938,-1.1099100972\H,2.0831249077,1.0745856255,-0.8857300318\H,1.9608599722,0.9854859046,0.8661375336\H,1.1748077622,-1.9770218626,0.9055993036\H,0.5829692656,-1.5862249739,-1.4094287163\C,-1.0406085415,0.1283276965,1.9563751208\H,-1.7231071795,0.9330057958,2.2211270602\H,-1.4762822425,-0.8089785635,2.2828779085\H,-0.1122652776,0.2912206321,2.4974751975\O,-1.8804169692,-0.2539245564,-0.2578848404\\Version=IA64L-G03RevD.01\HF=-522.4050521\S2=0.760017\S2-1=0.\S2A=0.750038\RMSD=6.826e-09\RMSF=1.402e-05\Thermal=0.\Dipole=1.0227661,0.218723,0.386505\PG=C01 [X(C4H9O1Si1)]\\@

5-*endo* transition state

1\1\GINC-AC32\FTS\UBHandHLYP\6-311G(d,p)\C4H9O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm freq=noraman opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.4206220656,-0.5588721923,0.2387616347\C,-0.1313665294,-1.2263272946,-0.277074183\Si,1.3272847836,-0.0333080978,-0.0490213007\C,-1.2615687824,0.9212671039,0.0722611789\H,0.0400375918,-2.1722007768,0.224835585\H,-0.2161863604,-1.4499374725,-1.338504306\H,-2.3200009211,-0.923870872,-0.2473599024\H,-1.5273283095,-0.7598594484,1.3052696222\H,2.414361278,-0.5492600994,-0.9433958941\H,1.8591636954,0.0014112843,1.3270623393\O,-0.1218409262,1.3717495499,0.2981923038\C,-2.3293157272,1.7830745908,-0.4991289229\H,-2.4647294768,1.5511744283,-1.5575341262\H,-3.2804600639,1.5949224519,-0.0092596887\H,-2.0641003663,2.8277566748,-0.4019877205\\Version=IA64L-G03RevD.01\HF=-522.4179805\S2=0.76835\S2-1=0.\S2A=0.750077\RMSD=9.838e-09\RMSF=2.555e-05\Thermal=0.\Dipole=-1.3814475,-0.1882269,-0.17214\PG=C01 [X(C4H9O1Si1)]\\@

5-*endo* product

1\1\GINC-AC27\FOpt\UBHandHLYP\6-311G(d,p)\C4H9O1Si1(2)\UXW563\17-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.4316102673,-0.5750779609,0.1746316499\C,-0.153704869,-1.369217865,-0.1676961677\Si,1.1648804515,-0.0474141289,0.0361758183\C,-1.1980357461,0.8668731637,-0.1744929219\H,-0.0317983377,-2.2432638927,0.4610766892\H,-0.1799020721,-1.7060592788,-1.2001820313\H,-2.3067521212,-0.9620779756,-0.3386008854\H,-1.6361228534,-0.662944026,1.2481577218\H,2.1312169992,0.045328428,-1.0722061691\H,1.9036492297,-0.0869170073,1.3114803215\O,0.1093454778,1.2494948968,0.0261673891\C,-2.2002293129,1.9270654902,0.0765192459\H,-1.9248511087,2.8426467422,-0.436497213\H,-3.181753935,1.6170551448,-0.2679421265\H,-2.2775464046,2.1598537999,1.143243538\\Version=IA64L-G03RevD.01\HF=-522.4723351\S2=0.755391\S2-1=0.\S2A=0.750022\RMSD=2.646e-09\RMSF=1.468e-05\Thermal=0.\Dipole=-0.2062225,-0.6130358,0.0550259\PG=C01 [X(C4H9O1Si1)]\\@

Cyclization of 17b:

<u>17b</u>

1\1\GINC-AC57\FOpt\UBHandHLYP\6-311G(d,p)\C4H9O1Si1(2)\UXW563\17-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\Si,-2.709431051,-0.401148093,-0.0696558789\C,-1.1791419476,0.7022490425,-0.0087095488\C,0.1482616408,-0.0532788718,-0.0326647427\C,1.3501589234,0.8717641201,0.0524635457\C,2.673608517,0.1653357369,0.0277360919\H,3.5547100739,0.8252201766,0.0904567532\H,1.35339185,1.5931851255,-0.766467165\H,1.3226248862,1.4754033715,0.9612944596\H,0.1936260315,-0.7630379561,0.7889300918\H,0.2271383198,-0.6484159918,-0.9381824761\H,-1.2305742778,1.4022482083,-0.8409405149\H,-1.2507923165,1.3052860025,0.8978355605\H,-2.7215920913,-1.3695286235,1.0510266385\H,-3.9503892438,0.406375389,-0.0467575206\O,2.8106420658,-1.0158986269,-0.0526259842\\Version=IA64L-G03RevD.01\HF=-522.4213282\S2=0.751601\S2-1=0.\S2A=0.750001\RMSD=7.599e-09\RMSF=1.959e-06\Thermal=0.\Dipole=-0.0580919,1.1310882,0.0183177\PG=C01 [X(C4H9O1Si1)]\\@

<u>5-*exo* transition state</u>

1\1\GINC-AC46\FTS\UBHandHLYP\6-311G(d,p)\C4H9O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm freq=noraman opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.8815765584,1.2321605242,-0.395291667\C,1.6159236724,-0.0995458948,-0.1917508217\Si,0.3822597226,-1.4854058409,0.1356723256\C,-1.3297668992,0.3594819152,0.4179815508\C,-0.2296848203,1.3838625205,0.6358978259\H,1.5761513371,2.0648503785,-0.332930016\H,0.4311405908,1.2613660983,-1.3821946847\H,0.1616670324,1.2961451876,1.647458679\H,-0.6982985649,2.3639121817,0.5548356293\H,-1.8397831735,-0.0114243735,1.3148011334\H,0.8177502047,-2.4096213245,1.2066480294\H,-0.0583969405,-2.2354806705,-1.0516833062\H,2.2488134594,-0.3334114786,-1.043539284\H,2.2669881841,-0.0332068869,0.6776575218\O,-1.8460793635,0.2128876639,-0.6840199158\\Version=IA64L-G03RevD.01\HF=-522.4086709\S2=0.779305\S2-1=0.\S2A=0.750117\RMSD=8.168e-09\RMSF=5.682e-06\Thermal=0.\Dipole=0.8596026,0.2199922,0.7039238\PG=C01 [X(C4H9O1Si1)]\\@

<u>5-*exo* product</u>

1\1\GINC-AC16\FOpt\UBHandHLYP\6-311G(d,p)\C4H9O1Si1(2)\UXW563\11-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,0.9338325751,1.2820011179,-0.3724813085\C,1.6382227614,-0.0831208832,-0.2627727148\Si,0.2460728715,-1.2955838314,0.1162222841\C,-1.108208428,0.089147524,0.4275430663\C,-0.2120132753,1.3222583716,0.6361259588\H,1.6266599116,2.1035699303,-0.2172034041\H,0.5173639283,1.3961260101,-1.3686449437\H,0.1811649372,1.3032655455,1.6522943297\H,-0.8065746517,2.2262511098,0.5362088211\H,-1.7193663476,-0.1630194675,1.2983054262\H,0.4500779816,-2.0741998723,1.3557333598\H,-0.129319175,-2.2064818406,-0.9762193201\H,2.195664874,-0.3314350885,-1.1593481603\H,2.3440930968,-0.0796586829,0.5644340688\O,-1.7774120601,0.077449057,-0.7206534632\\Version=IA64L-G03RevD.01\HF=-522.4270757\S2=0.75767\S2-1=0.\S2A=0.75003\RMSD=6.750e-09\RMSF=1.163e-05\Thermal=0.\Dipole=0.7990482,0.0494379,0.5643957\PG=C01 [X(C4H9O1Si1)]\\@

<u>6-*endo* transition state</u>

1\1\GINC-AC54\FTS\UBHandHLYP\6-311G(d,p)\C4H9O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,0.0948944997,-0.0132317959,-0.0294539105\C,0.0997364645,0.0529383275,1.503825542\Si,1.8154314436,0.2839090386,2.2794133737\C,2.2087163814,-1.3781072634,-0.2146534081\C,0.7694657611,-1.2661657634,-0.6009727918\H,-0.5342850833,0.8748024918,1.8256163886\H,-0.3496839076,-0.854302259,1.9030677918\H,-0.9285515967,0.0019105994,-0.3948364486\H,0.5743429079,0.872240681,-0.4440920856\H,0.6842953984,-

1.2825872516,-1.6831523071\H,0.2506161451,-2.1507063227,-0.2273345403\H,2.9565186206,-1.5544653287,-0.988168032\H,2.0396163907,-0.5960826616,3.4395337963\H,1.9027141492,1.702130729,2.7543985877\O,2.5901244248,-1.2061672177,0.9434620468\\Version=IA64L-G03RevD.01\HF=-522.4036714\S2=0.771669\S2-1=0.\S2A=0.750089\RMSD=5.645e-09\RMSF=1.036e-05\Thermal=0.\Dipole=-0.5745638,-0.3303826,-1.1700842\PG=C01 [X(C4H9O1Si1)]\\@

6-*endo* product
1\1\GINC-AC43\FOpt\UBHandHLYP\6-311G(d,p)\C4H9O1Si1(2)\UXW563\11-Jul-2007\1\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C\C,1,B1\Si,2,B2,1,A1\C,1,B3,2,A2,3,D1,0\C,4,B4,1,A3,2,D2,0\H,2,B5,1,A4,5,D3,0\H,2,B6,1,A5,5,D4,0\H,1,B7,5,A6,4,D5,0\H,1,B8,5,A7,4,D6,0\H,5,B9,4,A8,1,D7,0\H,5,B10,4,A9,1,D8,0\H,4,B11,1,A10,5,D9,0\H,3,B12,2,A11,1,D10,0\H,3,B13,2,A12,1,D11,0\O,4,B14,1,A13,5,D12,0\\B1=1.53743391\B2=1.86868974\B3=2.53247081\B4=1.49133856\B5=1.08730882\B6=1.08894537\B7=1.08680802\B8=1.08862878\B9=1.08639018\B10=1.09684441\B11=1.0764813\B12=1.47139948\B13=1.47748339\B14=1.36227578\A1=109.45825599\A2=94.50288858\A3=33.64091033\A4=110.75867743\A5=109.53293078\A6=109.26494955\A7=108.83199663\A8=108.22579505\A9=109.98698986\A10=150.94675037\A11=114.19673237\A12=110.73456388\A13=95.87122099\D1=26.11528384\D2=125.54271827\D3=177.30705577\D4=-65.22866146\D5=176.54441734\D6=60.51269361\D7=122.49317865\D8=-121.7502273\D9=36.7210593\D10=-155.44055189\D11=80.42190016\D12=-136.17529493\\Version=IA64L-G03RevD.01\HF=-522.4696453\S2=0.755249\S2-1=0.\S2A=0.75002\RMSD=4.824e-09\RMSF=2.373e-05\Thermal=0.\Dipole=-0.6604412,0.0904567,-0.1568961\PG=C01 [X(C4H9O1Si1)]\\@

Cyclization of 18b:
18b
1\1\GINC-AC59\FOpt\UBHandHLYP\6-311G(d,p)\C5H11O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\Si,-2.7001150079,-0.4215792643,-0.0414710438\C,-1.1812143437,0.6983041576,-0.0296232471\C,0.1534319235,-0.0451523753,-0.0277955062\C,1.3460986525,0.894477241,0.0212373714\C,2.6833096797,0.1880772344,0.0013746482\H,1.3259952696,1.5852158779,-0.8226254728\H,1.3080300581,1.5263069395,0.9088158185\H,0.2056067136,-0.7235588429,0.8195678012\H,0.2377257665,-0.6729252683,-0.9098763118\H,-1.2421824235,1.3640022541,-0.8890184444\H,-1.2570896229,1.3365401348,0.8522649666\H,-2.6992851721,-1.3460591097,1.1159105211\H,-3.95031215,0.3725150367,-0.0441556856\O,2.7693625963,-0.9997588424,-0.1182523437\C,3.9050361822,1.0594105195,0.144592475\H,3.8880957211,1.8704457528,-0.5780170328\H,3.9204872827,1.5106750271,1.13371046\H,4.7965845845,0.4619667265,0.0088640996\\Version=IA64L-G03RevD.01\HF=-561.7302198\S2=0.751603\S2-1=0.\S2A=0.750001\RMSD=7.588e-09\RMSF=3.161e-06\Thermal=0.\Dipole=0.190288,1.234703,0.0617844\PG=C01 [X(C5H11O1Si1)]\\@

5-*exo* transition state
1\1\GINC-AC44\FTS\UBHandHLYP\6-311G(d,p)\C5H11O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm freq=noraman opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.8717527056,1.2394917525,-0.3896549199\C,1.6446105327,-0.0801513064,-0.2547822734\Si,0.442336849,-1.4796660105,0.122173886\C,-1.2823112044,0.2554779667,0.4710754881\C,-0.2087258038,1.3239884106,0.6780025937\H,1.5463215371,2.0878871472,-0.3174976767\H,0.3912292569,1.2886761435,-1.3607870984\H,0.220623588,1.2436768077,1.6742888907\H,-0.723378347,2.2836622003,0.629527683\H,0.9194867094,-2.3687706808,1.2078766773\H,-0.0013660804,-2.2774767762,-1.031718419\H,2.2329522681,-0.2869651599,-1.1442026154\H,2.3412458928,-0.0180517538,0.5788555198\O,-1.7318937509,0.0827009299,-0.6675329552\C,-2.1130748203,-0.1252448793,1.6766695408\H,-2.7707910079,0.7120341628,1.9097230216\H,-2.7316091025,-0.9828238596,1.4447272868\H,-1.5098052526,-0.3285137646,2.55412512\\Version=IA64L-G03RevD.01\HF=-561.7132619\S2=0.777389\S2-1=0.\S2A=0.75011\RMSD=9.629e-09\RMSF=8.924e-06\Thermal=0.\Dipole=0.6483525,0.2557312,0.7947914\PG=C01 [X(C5H11O1Si1)]\\@

5-*exo* product
1\1\GINC-AC50\FOpt\UBHandHLYP\6-311G(d,p)\C5H11O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,0.9228314731,1.2851128997,-0.3731395806\C,1.6483453598,-0.0725208791,-0.3107881356\Si,0.2936928865,-1.3061911939,0.1209222623\C,-1.0923648003,0.0554605577,0.4757470433\C,-0.188761985,1.294530682,0.6711846309\H,1.6106106633,2.1119022507,-0.2225250095\H,0.4747172485,1.4110014656,-1.3530394933\H,0.2359003477,1.273699001,1.6739811783\H,-0.8016189091,2.1903865365,0.5994686306\H,0.5518872627,-2.0589618662,1.3682816739\H,-0.0917619613,-

2.2504693433,-0.9390192178\H,2.168071462,-0.303201194,-
1.2342828753\H,2.3909000671,0.0692365048,0.4836402576\O,-1.6738670051,0.0239267885,-0.7186167571\C,-
2.0231221853,-0.2414609993,1.6432659415\H,-2.7131808011,0.5884403608,1.7800753128\H,-2.6092067937,-
1.1317919753,1.4431760669\H,-1.4778285098,-0.3820118366,2.571376011\\Version=IA64L-G03RevD.01\HF=-
561.727770\S2=0.758483\S2-1=0.\S2A=0.750033\RMSD=5.026e-09\RMSF=5.907e-
06\Thermal=0.\Dipole=0.6941597,0.0767655,0.5994934\PG=C01 [X(C5H11O1Si1)]\\@

6-*endo* transition state
1\1\GINC-AC56\FTS\UBHandHLYP\6-311G(d,p)\C5H11O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-
311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)
freq=noraman\\freq&geom\\0,2\C,0.1059345545,-0.0102706702,-
0.0376367117\C,0.1046690353,0.0623385963,1.4948082506\Si,1.8295776161,0.2378115433,2.2628602052\C,2.2116
669086,-1.4023255731,-0.2171892163\C,0.7667037621,-1.2735519055,-0.601474651\H,-
0.5037960798,0.9053265636,1.8107721512\H,-0.3747021825,-0.8292061122,1.8948200854\H,-
0.9151420828,0.0175539096,-0.4093529328\H,0.599118353,0.8680829306,-0.4522425645\H,0.6699479181,-
1.294540035,-1.6826020581\H,0.2407135034,-2.1493729974,-0.2189291742\H,2.0282454658,-
0.6377892011,3.4312385425\H,1.9496350051,1.6555932798,2.7414349482\O,2.5547262611,-
1.2327995512,0.9622371792\C,3.2450344153,-1.6096819852,-1.2711513501\H,2.9618716974,-2.4185690572,-
1.939111713\H,3.3319416422,-0.7090498542,-1.8823440006\H,4.2052253877,-1.8209190497,-
0.8195129801\\Version=IA64L-G03RevD.01\HF=-561.7136263\S2=0.769773\S2-
1=0.\S2A=0.750084\RMSD=8.544e-09\RMSF=1.399e-05\Thermal=0.\Dipole=-0.3936299,-0.4327856,-
1.3948305\PG=C01 [X(C5H11O1Si1)]\\@

6-*endo* product
1\1\GINC-AC57\FOpt\UBHandHLYP\6-311G(d,p)\C5H11O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-
311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-0.0020504263,-
0.0028774182,0.0053376255\C,0.0001058777,-
0.0109036293,1.5421317483\Si,1.7655272454,0.0060318211,2.1497199697\C,2.2903535544,-1.086821942,-
0.2282621156\C,0.8389508166,-1.1361647503,-0.5903971491\H,-0.561674283,0.8341227117,1.9325281096\H,-
0.4943157548,-0.9113543978,1.9033213642\H,-1.0209335895,-0.0839193719,-
0.3643476373\H,0.3840554087,0.9481829956,-0.3576324597\H,0.7558600359,-1.1196272413,-
1.6732423868\H,0.4141218166,-2.0948404146,-0.2649045295\H,1.9452314198,-
0.5450571948,3.5024976802\H,2.3213850953,1.3746538333,2.0997368871\O,2.5940202442,-
0.9852376312,1.1054364305\C,3.291719162,-1.8710379275,-0.9921850748\H,3.235646132,-2.9358317727,-
0.7454235961\H,3.1341545243,-1.7690430419,-2.061015649\H,4.2963216609,-1.5376025976,-
0.752896078\\Version=IA64L-G03RevD.01\HF=-561.7755865\S2=0.755267\S2-1=0.\S2A=0.750021\RMSD=6.235e-
09\RMSF=5.646e-06\Thermal=0.\Dipole=-0.5794357,0.0729819,-0.2084551\PG=C01 [X(C5H11O1Si1)]\\@

Cyclization of 17c:
17c
1\1\GINC-AC46\FOpt\UBHandHLYP\6-311G(d,p)\C5H11O1Si1(2)\UXW563\17-Jul-2007\0\\# BHandHLYP/6-
311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-
1.6905965645,0.6274968367,-0.0257105418\C,-0.5812670462,-0.4224722919,-
0.0614326834\C,0.813240143,0.1874408455,-0.0077182718\C,1.9140970556,-0.8564170825,-
0.0443496702\C,3.3027749733,-0.2912926478,0.0063788181\H,4.1107459849,-1.0411585769,-
0.0190047505\H,1.8508272459,-1.4714813932,-0.9439500701\H,1.8238068408,-
1.5603456984,0.7850774673\H,0.9198496344,0.7861213801,0.8933646979\H,0.9468646675,0.8760638221,-
0.8382174033\H,-0.6766585527,-1.0233592046,-0.9650731831\H,-0.7038020039,-1.11220257,0.7731139014\H,-
1.5914078696,1.2394082365,0.8719094421\Si,-3.4420664414,-0.0719622164,-0.0408483711\H,-3.6631111325,-
1.0037615296,1.0901717921\H,-4.4563558676,1.0060034473,-0.0036821806\H,-1.5857594303,1.3098291493,-
0.8671939803\O,3.5619313634,0.8703074937,0.069574987\\Version=IA64L-G03RevD.01\HF=-
561.7188757\S2=0.751612\S2-1=0.\S2A=0.750001\RMSD=4.182e-09\RMSF=8.885e-06\Thermal=0.\Dipole=-
0.1193831,-0.8463008,-0.1088521\PG=C01 [X(C5H11O1Si1)]\\@

6-*exo* transition state
1\1\GINC-AC46\FTS\UBHandHLYP\6-311G(d,p)\C5H11O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-
311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-
1.8898499019,0.220258801,0.3189349906\C,-1.4687690851,-1.148339371,-0.2236869998\Si,0.318577973,-
1.6053584019,0.1417368543\C,1.3776404732,0.7243046008,-
0.479321832\C,0.3262260542,1.5668904902,0.2180124978\C,-1.1181499351,1.4084498405,-
0.2541848209\H,1.1458975888,0.461619321,-
1.5244114035\H,0.6449402752,2.5926881664,0.0271455473\H,0.4177989929,1.425005342,1.2915109355\H,-

1.6548393802,2.3142504771,0.0135929072\H,-1.1404626216,1.3636054167,-1.3436464007\H,-2.946507819,0.3664186857,0.1069528781\H,-1.7982390915,0.23019908,1.4043558229\H,-2.115061133,-1.9235183284,0.1868657334\H,-1.6106559224,-1.1758909647,-1.3027862106\H,0.7880436574,-2.7692460234,-0.6375239393\H,0.574787962,-1.800275415,1.5835059087\O,2.5132299131,0.6270592831,-0.061268469\\Version=IA64L-G03RevD.01\HF=-561.7032779\S2=0.775526\S2-1=0.\S2A=0.750103\RMSD=7.849e-09\RMSF=6.161e-06\Thermal=0.\Dipole=-1.4391648,0.0530633,-0.2397197\PG=C01 [X(C5H11O1Si1)]\\@

6-*exo* product
1\1\GINC-AC52\FOpt\UBHandHLYP\6-311G(d,p)\C5H11O1Si1(2)\UXW563\17-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.9325286177,0.2372648967,0.3097341982\C,-1.4274978586,-1.1070698221,-0.2307826775\Si,0.4031000368,-1.3496748106,0.1060807879\C,1.1646127331,0.3599671917,-0.3989673239\C,0.3092721322,1.4837706548,0.1962870606\C,-1.1582335603,1.4409563871,-0.2253149732\H,1.0912307782,0.3428796968,-1.4967485957\H,0.7481881649,2.4315214566,-0.107909995\H,0.390427129,1.4416041118,1.2809673327\H,-1.6435368624,2.350845724,0.1169905664\H,-1.2237499666,1.4554548605,-1.3137466089\H,-2.9849064028,0.3521185248,0.0615935515\H,-1.8758063181,0.2373169629,1.3976778133\H,-1.9932267468,-1.9296591225,0.2008823676\H,-1.5894083804,-1.1545418155,-1.3067405983\H,1.0047874104,-2.4278950702,-0.6980846492\H,0.6644109252,-1.5781468574,1.5391086848\O,2.4174744038,0.2914060306,0.0347580589\\Version=IA64L-G03RevD.01\HF=-561.7291279\S2=0.757496\S2-1=0.\S2A=0.750028\RMSD=7.934e-09\RMSF=4.980e-06\Thermal=0.\Dipole=-1.2081128,-0.0274426,-0.240339\PG=C01 [X(C5H11O1Si1)]\\@

7-*endo* transition state
1\1\GINC-AC8\FTS\UBHandHLYP\6-311G(d,p)\C5H11O1Si1(2)\UXW563\20-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.246808256,-1.4773012079,-0.4599158336\C,-1.4846607033,-1.4467157554,0.44155121\C,-1.2820303613,1.6015428791,0.7398652576\C,-2.5803479997,-0.4754470624,0.0023237872\C,-2.1474476288,0.9697464786,-0.2874731422\H,-0.5421329254,-1.4735582148,-1.5083658169\H,1.8650942147,-0.4012665595,1.0146799941\H,-1.5326522476,2.5913124161,1.122612936\H,-1.190140826,-1.2276871669,1.4636391477\H,-3.3574965314,-0.4599578606,0.7625925983\H,0.2765240179,-2.4208932911,-0.3098633809\H,1.9814025817,-0.2142864811,-1.3680818093\H,-1.9360039613,-2.4363804392,0.4671960237\H,-3.0485051014,-0.8550347642,-0.9035365849\H,-3.0209341103,1.5859837873,-0.4743802095\H,-1.543253708,0.984932581,-1.2036525865\O,-0.2126111989,1.095801828,1.0704900391\Si,1.0586947451,-0.1307601672,-0.1897786288\\Version=IA64L-G03RevD.01\HF=-561.7009994\S2=0.768911\S2-1=0.\S2A=0.750074\RMSD=5.718e-09\RMSF=1.905e-05\Thermal=0.\Dipole=-1.3118674,0.2740485,-0.1666262\PG=C01 [X(C5H11O1Si1)]\\@

7-*endo* product
1\1\GINC-AC42\FOpt\UBHandHLYP\6-311G(d,p)\C5H11O1Si1(2)\UXW563\17-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-0.2616656402,-1.5433501902,-0.3274798379\C,-1.5656067267,-1.4513434869,0.4804155112\C,-1.1428154164,1.5815292653,0.6083235518\C,-2.5740611411,-0.4400055238,-0.0665762767\C,-1.9971018018,0.9433800421,-0.4269658155\H,-0.483426929,-1.6256381441,-1.3900266246\H,2.0380085849,-0.4712667998,0.8322050395\H,-1.5542542925,2.1432851303,1.4287695371\H,-1.3348699775,-1.2046630571,1.5142460356\H,-3.3681737068,-0.3138628387,0.6654712121\H,0.2682155278,-2.4549191206,-0.0585529199\H,1.3915387506,0.4814002045,-1.2792125555\H,-2.0459864046,-2.4264125713,0.5069278811\H,-3.0414222237,-0.8477503245,-0.9618819722\H,-2.8218084235,1.6133218166,-0.6543040625\H,-1.4266149458,0.8560002423,-1.3538940354\O,0.0836193499,1.0610678896,0.872965464\Si,0.8931134163,-0.0907395334,-0.0105281339\\Version=IA64L-G03RevD.01\HF=-561.7633121\S2=0.755359\S2-1=0.\S2A=0.750021\RMSD=3.638e-09\RMSF=5.371e-05\Thermal=0.\Dipole=-0.462172,-0.5003179,-0.3003521\PG=C01 [X(C5H11O1Si1)]\\@

Cyclization of 18c:

18c
1\1\GINC-AC24\FOpt\UBHandHLYP\6-311G(d,p)\C6H13O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.68402512,0.6350021466,0.0002885322\C,-0.5832740664,-0.4213231724,-0.0863316886\C,0.8162251893,0.1739487513,-0.0047777236\C,1.9080513487,-0.8768760266,-0.0884563481\C,3.3097098,-0.3114974918,-0.0401541064\H,1.8215161156,-1.4506935241,-1.0123460387\H,1.8094171751,-1.6099112007,0.7125441666\H,0.9259045707,0.7301728237,0.9230222094\H,0.9574023474,0.8985994661,-0.801975295\H,-0.6842024119,-0.9773093915,-1.0178325921\H,-0.7122794488,-1.1495160896,0.7140362496\H,-

1.5788244984,1.2028486693,0.9257931246\Si,-3.4409164563,-0.0483972208,-0.0454236881\H,-3.6685698395,-1.0321055726,1.0395570593\H,-4.447572802,1.0337352162,0.0458765839\H,-1.5736602258,1.3555791644,-0.8079557695\O,3.5181812603,0.8671437322,-0.0409923876\C,4.43514363,-1.3129974193,0.0155271667\H,4.4215846797,-1.8214658226,0.9767145749\H,4.3193464422,-2.0731621773,-0.7515483823\H,5.3822858502,-0.8045458906,-0.1050810163\\Version=IA64L-G03RevD.01\HF=-601.0277021\S2=0.751614\S2-1=0.\S2A=0.750001\RMSD=8.613e-09\RMSF=1.469e-05\Thermal=0.\Dipole=0.1207017,-0.9740439,-0.0428109\PG=C01 [X(C6H13O1Si1)]\\@

6-*exo* transition state

1\1\GINC-AC59\FTS\UBHandHLYP\6-311G(d,p)\C6H13O1Si1(2)\UXW563\20-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-1.9392102866,0.2170358941,0.4050529916\C,-1.561159652,-1.1705207028,-0.1209710319\Si,0.2449049895,-1.6082759735,0.1683494223\C,1.3406997884,0.6180911795,-0.5384913965\C,0.2933560635,1.5113299742,0.1257327823\C,-1.1869589987,1.3807825756,-0.239244358\H,0.6196374497,2.520054506,-0.1361195121\H,0.4351035614,1.4250660901,1.1990985959\H,-1.6745831065,2.3001069053,0.0748933051\H,-1.308412764,1.3405358128,-1.3200350978\H,-3.0044124517,0.3722900858,0.2490559233\H,-1.7859541119,0.2538998387,1.4830113942\H,-2.1874365363,-1.9282435927,0.34849233\H,-1.7623707475,-1.2299457736,-1.189312182\H,0.6901770339,-2.7813448006,-0.6130538875\H,0.5617345098,-1.7796996054,1.5996545047\O,2.4148131971,0.4549907222,0.0274255488\C,1.2551464441,0.4382681822,-2.0433486222\H,1.4760859325,1.4014619162,-2 .5037024311\H,2.0081716924,-0.2703033833,-2.362252625\H,0.2798479439,0.1250778571,-2.3964903455\\Version=IA64L-G03RevD.01\HF=-601.0057633\S2=0.775993\S2-1=0.\S2A=0.750107\RMSD=3.569e-09\RMSF=1.805e-05\Thermal=0.\Dipole=-1.3322386,0.13822,-0.4689417\PG=C01 [X(C6H13O1Si1)]\\@

6-*exo* product

1\1\GINC-AC3\FOpt\UBHandHLYP\6-311G(d,p)\C6H13O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-1.9616446713,0.2228018729,0.3750109083\C,-1.4733278894,-1.1192618935,-0.1846969829\Si,0.3655225916,-1.3540161541,0.111299201\C,1.1414875583,0.3425755927,-0.4720163705\C,0.2742638223,1.4643291193,0.1355486497\C,-1.2175776763,1.4287326023,-0.1956684184\H,0.6953789558,2.4101708235,-0.2031628697\H,0.4131289296,1.4368572235,1.2140800836\H,-1.6722525604,2.3350195009,0.1960848794\H,-1.361330058,1.4649073476,-1.2742384316\H,-3.0248504986,0.3334928934,0.1755482953\H,-1.8548478728,0.2241267967,1.4593180039\H,-2.0207137689,-1.9435597685,0.2674645922\H,-1.6702865687,-1.1698382483,-1.2542226536\H,0.9454191769,-2.4571412425,-0.6761074264\H,0.6446391316,-1.5442212597,1.5452386535\O,2.3425299474,0.2455728684,0.0926652449\C,1.1990340621,0.3721679171,-2.0028234463\H,1.5905582995,1.3342071246,-2.3264727525\H,1.8672879924,-0.401557496,-2.362634314\H,0.2272500067,0.237470399,-2.4665804461\\Version=IA64L-G03RevD.01\HF=-601.0277266\S2=0.758368\S2-1=0.\S2A=0.750032\RMSD=5.763e-09\RMSF=2.188e-05\Thermal=0.\Dipole=-1.1448604,0.0066257,-0.3344827\PG=C01 [X(C6H13O1Si1)]\\@

7-*endo* transition state

1\1\GINC-AC57\FTS\UBHandHLYP\6-311G(d,p)\C6H13O1Si1(2)\UXW563\20-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.249600755,-1.4734960824,-0.4501662963\C,-1.4963475205,-1.4484077852,0.4381048083\C,-1.2841699105,1.606851707,0.7570246588\C,-2.5809755577,-0.4671415494,-0.0062058605\C,-2.1342746082,0.974012166,-0.2901226176\H,-0.5348387623,-1.4790787569,-1.5014970138\H,1.8545566925,-0.3832505232,1.0221137053\H,-1.2112856608,-1.2383720957,1.4648070972\H,-3.3654706989,-0.4478226629,0.7468909457\H,0.2815034153,-2.4107706942,-0.288992482\H,1.9579254885,-0.1851570624,-1.3526567797\H,-1.9524785664,-2.4362806534,0.4508580599\H,-3.0441521489,-0.8410903876,-0.9171679082\H,-3.0027314789,1.5887844384,-0.5042264946\H,-1.5076379191,0.9820905321,-1.1911045186\O,-0.2136911962,1.0694755857,1.0642531699\Si,1.0333403087,-0.1061271196,-0.1713668492\C,-1.620404663,2.9613589193,1.2827210299\H,-1.5734281933,3.6908684297,0.4726688453\H,-2.6347508608,2.9840876096,1.6711310064\H,-0.9216534946,3.2471751453,2.0575526237\\Version=IA64L-G03RevD.01\HF=-601.0109711\S2=0.76696\S2-1=0.\S2A=0.750068\RMSD=9.003e-09\RMSF=1.281e-05\Thermal=0.\Dipole=-1.4356315,0.5470757,-0.0193626\PG=C01 [X(C6H13O1Si1)]\\@

7-*endo* product

1\1\GINC-AC57\FOpt\UBHandHLYP\6-311G(d,p)\C6H13O1Si1(2)\UXW563\18-Jul-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,maxcycle=500,z-matrix) freq=noraman\\freq&geom\\0,2\C,-0.2616740569,-1.5387979362,-0.2964952629\C,-1.5618624236,-1.4193162009,0.5133492264\C,-1.1469746252,1.6235450312,0.5881960301\C,-2.5672424281,-0.4184497972,-0.0576403621\C,-

1.983108799,0.9527984544,-0.4504626387\H,-0.4891298984,-1.6683141207,-1.3531106815\H,2.0619642413,-0.4144782384,0.7633390582\H,-1.3243830759,-1.1462105574,1.5390454553\H,-3.3636194144,-0.2739327885,0.6688245124\H,0.274056932,-2.4351138509,0.009086437\H,1.3413385812,0.477574179,-1.3478657695\H,-2.0461736015,-2.391362719,0.5684696171\H,-3.0350251866,-0.8457691087,-0.9434418878\H,-2.8040603963,1.6122327004,-0.7185616632\H,-1.3926970316,0.8371918701,-1.3604101338\O,0.0906106007,1.0936138508,0.8326861188\Si,0.8857243297,-0.0652642149,-0.049879418\C,-1.737228239,2.3115438731,1.7631271327\H,-1.0101180099,2.9817852483,2.211252648\H,-2.6107713349,2.8883110786,1.4761044525\H,-2.0442900639,1.6055622068,2.541169008\\Version=IA64L-G03RevD.01\HF=-601.0683309\S2=0.75536\S2-1=0.\S2A=0.750022\RMSD=4.980e-09\RMSF=3.209e-06\Thermal=0.\Dipole=-0.4923907,-0.4407582,-0.2406735\PG=C01 [X(C6H13O1Si1)]\\@

Cyclization of 19a:

19a

1\1\GINC-AC9\FOpt\UBHandHLYP\6-311G(d,p)\C3H7Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.3217314367,-0.5119062006,0.0001009862\C,0.538033434,0.7433558222,-0.0001170886\C,2.0173965722,0.4644320005,-0.0000478977\H,2.6553774557,1.3639187023,-0.0002262452\H,0.3358962423,1.3751176776,-0.8658977324\H,0.3358777734,1.3754538524,0.8654144392\H,-0.0899469723,-1.1195007847,0.8681244562\H,-0.09000166,-1.1197296705,-0.867777851\H,-2.6619324134,0.655088973,1.2530660429\H,-2.6617082507,0.655317991,-1.2528805726\O,2.5039927404,-0.6222224316,0.0001808423\Ge,-2.2558314846,-0.1389849317,0.0000596217\\Version=IA64L-G03RevD.01\HF=-2270.5724199\S2=0.751577\S2-1=0.\S2A=0.750001\RMSD=8.416e-09\RMSF=5.259e-06\Thermal=0.\Dipole=-0.2740882,0.7481435,-0.0001588\PG=C01 [X(C3H7Ge1O1)]\\@

4-*exo* transition state

1\1\GINC-AC19\FTS\UBHandHLYP\6-311G(d,p)\C3H7Ge1O1(2)\UXW563\30-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.0349408018,1.3474147922,-0.1288584979\C,1.3797181564,0.7644639199,0.0280256861\C,-0.9755893061,0.2502801921,0.3958744924\H,-0.1822948158,2.2909605992,0.3922474166\H,-0.2763395429,1.5016740491,-1.1756455925\H,-0.9312294001,0.1150135111,1.4877553688\H,2.0926371695,1.0915788182,-0.716708793\H,1.7949563955,0.9497905348,1.0122951063\H,1.2198661212,-2.1247261796,0.9386899546\H,0.6597963351,-1.6853223309,-1.4893622642\O,-2.0401756008,-0.065427807,-0.1914673453\Ge,0.7489982898,-1.093403099,-0.0871985322\\Version=IA64L-G03RevD.01\HF=-2270.5414314\S2=0.777224\S2-1=0.\S2A=0.750106\RMSD=3.880e-09\RMSF=2.290e-05\Thermal=0.\Dipole=1.2948912,0.1466551,0.3102083\PG=C01 [X(C3H7Ge1O1)]\\@

5-*endo* transition state

1\1\GINC-AC29\FTS\UBHandHLYP\6-311G(d,p)\C3H7Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-1.424053306,-0.5380050334,0.2983191301\C,-0.1759509293,-1.2615080726,-0.2566899246\C,-1.2563093326,0.9199758827,0.0272464443\H,-0.0351899665,-2.2180060237,0.2318838656\H,-0.282510758,-1.4502201151,-1.3208400191\H,-2.3463672132,-0.9212782674,-0.125754814\H,-1.4662077998,-0.6916073909,1.3764866045\H,-1.9781394652,1.474815513,-0.5675036897\H,2.4620633293,-0.3860176269,-1.0689058875\H,1.9810547609,-0.1625576625,1.4064812479\O,-0.1585886374,1.4397755931,0.3075533625\Ge,1.3861823176,-0.0892747961,-0.0004293196\\Version=IA64L-G03RevD.01\HF=-2270.5503704\S2=0.776122\S2-1=0.\S2A=0.750122\RMSD=9.342e-09\RMSF=1.884e-05\Thermal=0.\Dipole=-0.7062243,-0.5950048,-0.2029736\PG=C01 [X(C3H7Ge1O1)]\\@

5-*endo* product

1\1\GINC-AC25\FOpt\UBHandHLYP\6-311G(d,p)\C3H7Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-1.4253104826,-0.5572864535,0.1744928755\C,-0.1872326652,-1.3998921571,-0.186288281\C,-1.1517797921,0.8774662353,-0.165571391\H,-0.0925811998,-2.2855290393,0.4289345988\H,-0.2129324793,-1.70721954,-1.2262424076\H,-2.3142087519,-0.9109066688,-0.3400532998\H,-1.6243834332,-0.6615942913,1.2465861654\H,-1.8995525994,1.643034067,-0.0404327595\H,2.2394363052,0.0516476488,-1.100988133\H,1.9943921297,-0.1251877881,1.3954676721\O,0.1195926633,1.2986694574,0.0643083171\Ge,1.2605443063,-0.107109471,0.0576356431\\Version=IA64L-G03RevD.01\HF=-2270.5834677\S2=0.755582\S2-1=0.\S2A=0.750023\RMSD=7.999e-09\RMSF=2.612e-05\Thermal=0.\Dipole=0.0647123,-0.8778508,0.0802157\PG=C01 [X(C3H7Ge1O1)]\\@

Cyclization of 19b:

19b

1\1\GINC-AC12\FOpt\UBHandHLYP\6-311G(d,p)\C4H9Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.1585200832,0.7271135038,-0.0188103059\C,0.1585718069,-0.0392138972,-0.0363383044\C,1.3676113158,0.8779223612,0.0458740828\C,2.6856198122,0.1607357636,0.0370367145\H,3.5715719464,0.8145189203,0.094946463\H,1.38131111,1.5905830974,-0.7805242756\H,1.3397759897,1.4912748706,0.9482021963\H,0.1971959685,-0.7443450288,0.7894132072\H,0.2347618072,-0.6396576983,-0.9385146626\H,-1.2129918877,1.421082254,-0.8534652607\H,-1.243816196,1.322729083,0.8893199273\H,-2.7407806705,-1.4590098828,1.047316731\H,-4.0421045919,0.4182453251,0.0044347293\O,2.8135983822,-1.0224949576,-0.0260413191\Ge,-2.7595617097,-0.4237267139,-0.0891109247\\Version=IA64L-G03RevD.01\HF=-2309.8695403\S2=0.751547\S2-1=0.\S2A=0.750001\RMSD=6.286e-09\RMSF=7.174e-06\Thermal=0.\Dipole=-0.0382351,1.1534582,0.0258782\PG=C01 [X(C4H9Ge1O1)]\\@

5-*exo* transition state

1\1\GINC-AC22\FTS\UBHandHLYP\6-311G(d,p)\C4H9Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,0.889812719,1.2525802758,-0.3920977632\C,1.6466254367,-0.0658254098,-0.2134332249\C,-1.3152656876,0.3431111325,0.4105345074\C,-0.2243045963,1.3765940119,0.6403683897\H,1.5718824076,2.0952602579,-0.3175245401\H,0.4389259072,1.2909859229,-1.3786818722\H,0.1681484537,1.280103862,1.6508730648\H,-0.7015298864,2.3533704114,0.5715304427\H,-1.8316501342,-0.0278625407,1.3034579467\H,0.7459646522,-2.4174329824,1.3062940771\H,-0.0759930035,-2.3172736588,-1.0793060573\H,2.2526019238,-0.3027547394,-1.0813630743\H,2.3085816605,-0.0130251035,0.6462282633\O,-1.8449188504,0.2228802168,-0.6949378073\Ge,0.3513799978,-1.5041406565,0.1376016474\\Version=IA64L-G03RevD.01\HF=-2309.8555484\S2=0.779879\S2-1=0.\S2A=0.750114\RMSD=9.252e-09\RMSF=5.051e-06\Thermal=0.\Dipole=0.8944645,0.1707768,0.6849034\PG=C01 [X(C4H9Ge1O1)]\\@

5-*exo* product

1\1\GINC-AC25\FOpt\UBHandHLYP\6-311G(d,p)\C4H9Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.9319055765,1.2843410366,-0.3791922897\C,1.6714896084,-0.0547267492,-0.2551179899\C,-1.1375259234,0.1272149313,0.4371883733\C,-0.2110629386,1.334120326,0.632565106\H,1.6093710849,2.1225568765,-0.2418859381\H,0.5091381622,1.3743683204,-1.3755020252\H,0.1842271475,1.3152736729,1.6478988682\H,-0.7895165293,2.2487537767,0.5288912239\H,-1.727335321,-0.1302669862,1.3206986385\H,0.4455949602,-2.1786481188,1.3873391902\H,-0.1478729823,-2.2681391697,-1.0466240789\H,2.2401927543,-0.2990240924,-1.1442780104\H,2.357562805,-0.0443064969,0.5864976048\O,-1.8044034801,0.0957099855,-0.6977623374\Ge,0.2484960756,-1.3606583127,0.1088276655\\Version=IA64L-G03RevD.01\HF=-2309.8646511\S2=0.759101\S2-1=0.\S2A=0.750036\RMSD=3.130e-09\RMSF=8.938e-06\Thermal=0.\Dipole=0.8632981,0.0061909,0.5655605\PG=C01 [X(C4H9Ge1O1)]\\@

6-*endo* transition state

1\1\GINC-AC4\FTS\UBHandHLYP\6-311G(d,p)\C4H9Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,0.0865256396,-0.0350971204,-0.0423226699\C,0.0472332001,0.0531369225,1.4863780688\C,2.2280262961,-1.3304664234,-0.2512130318\C,0.7709773286,-1.3030478079,-0.5801834156\H,-0.5476511712,0.9098780289,1.7883115189\H,-0.4424717509,-0.8288223847,1.8905529999\H,-0.9301443167,-0.0201807172,-0.4280807154\H,0.577618161,0.8435588139,-0.458626758\H,0.6394391467,-1.3647806981,-1.6560059146\H,0.2894104722,-2.1749677731,-0.1378370987\H,2.955520434,-1.217788557,-1.0551589773\H,1.9005631331,-0.6122629358,3.6332699175\H,2.1482198148,1.6867420064,2.6140825278\O,2.6274066191,-1.3170494324,0.9245088845\Ge,1.8232759936,0.1972650795,2.3389796644\\Version=IA64L-G03RevD.01\HF=-2309.8471029\S2=0.779391\S2-1=0.\S2A=0.750137\RMSD=6.933e-09\RMSF=1.385e-05\Thermal=0.\Dipole=-0.6518366,0.0365231,-0.8237331\PG=C01 [X(C4H9Ge1O1)]\\@

6-*endo* product

1\1\GINC-AC19\FOpt\UBHandHLYP\6-311G(d,p)\C4H9Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.0118225996,-0.0069947076,-0.0136911857\C,-0.0525376735,0.0168246706,1.518185474\C,2.2766060398,-1.0997033355,-0.2172280163\C,0.8262288315,-1.164665467,-0.5674236564\H,-0.6012838036,0.8795803036,1.8837553647\H,-

0.5582239525,-0.8694203693,1.8930738225\H,-1.0254644255,-0.0816808562,-0.401001268\H,0.3949725917,0.931053882,-0.3870609641\H,0.7429307411,-1.1849168073,-1.6505003005\H,0.3930922981,-2.1063952454,-0.2077106605\H,2.9999179301,-1.5957300471,-0.8444904824\H,1.9496128708,-0.6150014057,3.5921739132\H,2.4166588625,1.4077250728,2.1638341725\O,2.6565704082,-1.0485230161,1.0831659267\Ge,1.7666948813,0.0239633283,2.2215728597\\Version=IA64L-G03RevD.01\HF=-2309.8849536\S2=0.755431\S2-1=0.\S2A=0.750022\RMSD=5.020e-09\RMSF=3.403e-05\Thermal=0.\Dipole=-0.7793427,0.2735215,0.0827807\PG=C01 [X(C4H9Ge1O1)]\\@

Cyclization of 19c:

19c

1\1\GINC-AC8\FOpt\UBHandHLYP\6-311G(d,p)\C5H11Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.6685523769,0.6400872328,-0.0332580944\C,-0.5679559581,-0.4138683477,-0.0646688652\C,0.8293375636,0.1911524588,-0.0084505629\C,1.9259919858,-0.8571939635,-0.0479130728\C,3.3168904608,-0.2980595144,0.0087532414\H,4.1218855861,-1.0509642276,-0.0199601854\H,1.8619090405,-1.4673836157,-0.9507418586\H,1.8309064193,-1.5648727088,0.777778741\H,0.9380830287,0.78668446,0.894456107\H,0.9661109217,0.8816680842,-0.836882007\H,-0.6637804005,-1.0149793098,-0.9679312819\H,-0.6947132598,-1.1019716939,0.7705037549\H,-1.5844205937,1.249491917,0.865474241\H,-3.7193712826,-1.0433300567,1.1418222735\H,-4.5476690241,1.0276656097,-0.0092693443\H,-1.5737987631,1.316253574,-0.8784425635\O,3.5804645839,0.8620996371,0.0798071967\Ge,-3.4982049315,-0.094263536,-0.04866772\\Version=IA64L-G03RevD.01\HF=-2349.1671022\S2=0.751555\S2-1=0.\S2A=0.750001\RMSD=7.764e-09\RMSF=5.923e-06\Thermal=0.\Dipole=-0.1030368,-0.8262535,-0.0949393\PG=C01 [X(C5H11Ge1O1)]\\@

6-*exo* transition state

1\1\GINC-AC28\FTS\UBHandHLYP\6-311G(d,p)\C5H11Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-1.9082401414,0.2361472476,0.3177189347\C,-1.5184034163,-1.1402503765,-0.2165000988\C,1.3767873739,0.7102364823,-0.4569938093\C,0.320283557,1.564916746,0.2183717616\C,-1.1199910628,1.4078296023,-0.2678087616\H,1.1715002022,0.4677006617,-1.51208992\H,0.6444492161,2.5876780495,0.0199294614\H,0.3982248386,1.4347592759,1.2944569045\H,-1.6523973704,2.3223583708,-0.0220765849\H,-1.13094347,1.3443052826,-1.3565645726\H,-2.9639068197,0.3989647475,0.1094301061\H,-1.8121820086,0.2526305502,1.4026277616\H,-2.144295853,-1.9109568193,0.2272607958\H,-1.6753977212,-1.1856320991,-1.2910402612\H,0.8603680095,-2.7783021187,-0.7220562146\H,0.6489313389,-1.8411330702,1.6116836134\O,2.5093252287,0.6127254643,-0.0170574235\Ge,0.3604960983,-1.6058569969,0.1264943071\\Version=IA64L-G03RevD.01\HF=-2349.1500532\S2=0.77702\S2-1=0.\S2A=0.750103\RMSD=5.437e-09\RMSF=5.595e-06\Thermal=0.\Dipole=-1.4466136,0.0359018,-0.2550405\PG=C01 [X(C5H11Ge1O1)]\\@

6-*exo* product

1\1\GINC-AC29\FOpt\UBHandHLYP\6-311G(d,p)\C5H11Ge1O1(2)\UXW563\31-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-1.941890575,0.246130399,0.310235903\C,-1.4824483828,-1.1117099531,-0.2253313992\C,1.1971392211,0.408083163,-0.4016618313\C,0.307865774,1.4977515839,0.1980002558\C,-1.1547586168,1.4354510389,-0.2398613959\H,1.1280434173,0.3858402996,-1.4983203908\H,0.7290727556,2.4587315391,-0.0919075424\H,0.3804325308,1.4473032797,1.2828628476\H,-1.6462743342,2.3511830098,0.0772025042\H,-1.2077578557,1.4287903035,-1.3292013027\H,-2.9948644683,0.3821190318,0.0723087529\H,-1.8754165451,0.252237362,1.3976352904\H,-2.05305785,-1.9191608998,0.224132038\H,-1.6452080653,-1.1670030111,-1.2989056246\H,1.0482146271,-2.4934852417,-0.7599266071\H,0.7170546911,-1.6534077019,1.5860209448\O,2.4308133114,0.3327447243,0.0540311415\Ge,0.4276483649,-1.403479927,0.1084704152\\Version=IA64L-G03RevD.01\HF=-2349.1646216\S2=0.758515\S2-1=0.\S2A=0.750033\RMSD=4.891e-09\RMSF=6.299e-06\Thermal=0.\Dipole=-1.258508,-0.0858992,-0.2398342\PG=C01 [X(C5H11Ge1O1)]\\@

7-*endo* transition state

1\1\GINC-AC23\FTS\UBHandHLYP\6-311G(d,p)\C5H11Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.2705766875,-1.5400349493,-0.4604012717\C,-1.5040590276,-1.4696217492,0.4435670651\C,-1.2881805064,1.6194236428,0.7422508888\C,-2.5813415403,-0.4765888219,0.0051522502\C,-2.1357861638,0.9634924967,-0.2843085807\H,-0.5571465103,-1.517925625,-1.5091393374\H,1.9729266302,-

0.4797327116,1.0400725957\H,-1.4893355788,2.6534373542,1.0194251971\H,-1.2016922542,-1.2516530767,1.4632073007\H,-3.3559519706,-0.4523744656,0.7678292801\H,0.2407281247,-2.4863957104,-0.3027379987\H,1.9496985828,0.0413464056,-1.4161520939\H,-1.9758616518,-2.4500255748,0.4744842213\H,-3.0571239163,-0.8512553519,-0.8993608934\H,-3.0058507102,1.5768894412,-0.4973676553\H,-1.5208853508,0.9692302109,-1.1964022162\O,-0.2363115481,1.0911629974,1.1350227616\Ge,1.0734400789,-0.1293425123,-0.1452395132\\Version=IA64L-G03RevD.01\HF=-2349.1442109\S2=0.775727\S2-1=0.\S2A=0.750119\RMSD=5.777e-09\RMSF=1.599e-05\Thermal=0.\Dipole=-0.981879,0.0667934,-0.3368027\PG=C01 [X(C5H11Ge1O1)]\\@

7-*endo* product
1\1\GINC-AC4\FOpt\UBHandHLYP\6-311G(d,p)\C5H11Ge1O1(2)\UXW563\29-Dec-2007\0\\# BHandHLYP/6-311G** scf=direct nosymm opt=(calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-0.2899947434,-1.6057181907,-0.3319431581\C,-1.5798325341,-1.4553803493,0.482632374\C,-1.1597686112,1.5903989664,0.6420517339\C,-2.5696362182,-0.4347004284,-0.0779378476\C,-1.976723944,0.9456959537,-0.4211607432\H,-0.5109573762,-1.699648353,-1.392041095\H,2.14318842,-0.4444340722,0.814862306\H,-1.6212935669,2.1366883445,1.4485232565\H,-1.3320103836,-1.188942892,1.5069475957\H,-3.3725183146,-0.3049666411,0.6439620705\H,0.2328252742,-2.5112248895,-0.0381517234\H,1.378654496,0.5747397402,-1.3539947166\H,-2.081186137,-2.419444778,0.5353637435\H,-3.0283614032,-0.8375442465,-0.9804295469\H,-2.7938685383,1.6140717194,-0.6799250808\H,-1.3782077091,0.8560062939,-1.3303751755\O,0.0578423502,1.0944784332,0.9636338664\Ge,0.9385379393,-0.1000426105,-0.0521158594\\Version=IA64L-G03RevD.01\HF=-2349.1792073\S2=0.75553\S2-1=0.\S2A=0.750022\RMSD=2.312e-09\RMSF=2.781e-05\Thermal=0.\Dipole=-0.2541422,-0.7153513,-0.4487157\PG=C01 [X(C5H11Ge1O1)]\\@

Cyclization of 20a:
20a
1\1\GINC-AC24\FOpt\UBHandHLYP\Gen\C3H7O1Sn1(2)\UXW563\07-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.2631006579,-0.5508014423,0.0013838485\C,0.5734361081,0.7188522107,-0.0006561272\C,2.0595337834,0.4725841619,-0.0000926049\H,2.6767889919,1.3868456062,-0.0015161979\H,0.3626809661,1.3476904381,-0.8669499523\H,0.3624838472,1.3506024985,0.8634636499\H,-0.0223480654,-1.1536804039,0.8702462512\H,-0.0220199424,-1.1566722742,-0.8653044006\H,-2.8010117217,0.7472986077,1.3884457781\H,-2.8005387958,0.7424239155,-1.3910946446\O,2.5715910797,-0.6022450998,0.0016997506\Sn,-2.3920725933,-0.1825562184,0.0003726508\\Version=IA64L-G03RevD.01\HF=-196.9687298\S2=0.751625\S2-1=0.\S2A=0.750001\RMSD=4.759e-09\RMSF=1.425e-05\Thermal=0.\Dipole=-0.4285413,0.529903,-0.0008529\PG=C01 [X(C3H7O1Sn1)]\\@

5-*endo* transition state
1\1\GINC-AC30\FTS\UBHandHLYP\Gen\C3H7O1Sn1(2)\UXW563\11-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500) freq=noraman\\freq&geom\\0,2\C,-1.4645756699,-0.558974487,0.2867683934\C,-0.2281299166,-1.3034538488,-0.2664918612\C,-1.3075224381,0.9061791507,0.0405843405\H,-0.0928760054,-2.2540422773,0.2344538174\H,-0.3414427515,-1.5073712959,-1.3271411979\H,-2.392355559,-0.9266000294,-0.1407560831\H,-1.5151696786,-0.7255405996,1.3637037857\H,-2.0359103246,1.4656301057,-0.5383739514\H,2.6576596416,-0.3299075276,-1.2150488487\H,2.1650444094,-0.0932061668,1.5494964456\O,-0.2074550828,1.4472610447,0.3261246325\Sn,1.4687183754,-0.0038830687,-0.0054674722\\Version=IA64L-G03RevD.01\HF=-196.9489827\S2=0.773947\S2-1=0.\S2A=0.750116\RMSD=6.813e-09\RMSF=3.073e-05\Thermal=0.\Dipole=-0.5840263,-0.4832091,-0.2257127\PG=C01 [X(C3H7O1Sn1)]\\@

5-*endo* product
1\1\GINC-AC27\FOpt\UBHandHLYP\Gen\C3H7O1Sn1(2)\UXW563\07-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.4553872094,-0.5579526264,0.174168713\C,-0.2541463787,-1.4513807766,-0.1956788275\C,-1.1875880952,0.8788640605,-0.1738004659\H,-0.2017394999,-2.3460663193,0.4110374337\H,-0.2916163285,-1.7479424088,-1.2385032689\H,-2.3619140313,-0.8957785564,-0.3210836226\H,-1.6391223896,-0.6528786108,1.2508999512\H,-1.9768918046,1.611396852,-0.1148033323\H,2.4391283529,0.1278123402,-1.2274251492\H,2.2176660103,-0.1077773533,1.5500747113\O,0.0450062576,1.3573883226,0.1172810575\Sn,1.3725891165,-0.0995929237,0.0756837996\\Version
=IA64L-G03RevD.01\HF=-196.9707983\S2=0.755713\S2-1=0.\S2A=0.750024\RMSD=6.562e-09\RMSF=4.488e-05\Thermal=0.\Dipole=0.2991429,-0.9447241,0.0539733\PG=C01 [X(C3H7O1Sn1)]\\@

Cyclization of 20b:

20b

1\1\GINC-AC28\FOpt\UBHandHLYP\Gen\C4H9O1Sn1(2)\UXW563\30-Dec-2007\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.118076269,0.7381691005,-0.0415229048\C,0.2005627231,-0.026075124,-0.0527311516\C,1.4099794997,0.8894399982,0.0536923105\C,2.7286475989,0.1738223953,0.0314946629\H,3.6140020715,0.8259550546,0.1135506316\H,1.4249645728,1.619938792,-0.7570398733\H,1.3781069567,1.4830392414,0.9688546028\H,0.2345328606,-0.7414429924,0.7647189478\H,0.2917578418,-0.6159626524,-0.960729087\H,-1.1670333206,1.4386176476,-0.8708933535\H,-1.2170164568,1.3242657194,0.8707012321\H,-2.8817998452,-1.5824964634,1.2133988521\H,-4.2814634523,0.4857938723,-0.0217889445\O,2.8583293645,-1.0069199516,-0.066776495\Sn,-2.8832521455,-0.510388637,-0.1311894324\\Version=IA64L-G03RevD.01\HF=-236.2658315\S2=0.751658\S2-1=0.\S2A=0.750001\RMSD=3.495e-09\RMSF=4.897e-05\Thermal=0.\Dipole=-0.0598286,1.0318809,-0.135767\PG=C01 [X(C4H9O1Sn1)]\\@

5-*exo* transition state

1\1\GINC-AC4\FTS\UBHandHLYP\Gen\C4H9O1Sn1(2)\UXW563\04-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.899149287,1.2909082974,-0.3851040945\C,1.691922456,-0.0118633148,-0.2427012903\C,-1.3184840446,0.3641086458,0.4101090472\C,-0.2179632722,1.3889334422,0.6493748521\H,1.5605013307,2.1492129796,-0.2962078577\H,0.4449873787,1.3407616984,-1.3695909427\H,0.1734239777,1.2813614273,1.6596500821\H,-0.6938827133,2.368166237,0.5962473377\H,-1.9078853865,0.0814023157,1.2890124429\H,0.7704571843,-2.5977002438,1.4645515668\H,-0.1613254897,-2.5429391555,-1.1761896242\H,2.2840083221,-0.2210934245,-1.1263632585\H,2.3719273373,0.0399375275,0.6028660284\O,-1.8118989037,0.2291603685,-0.7240612993\Sn,0.2953225361,-1.5937878009,0.1579500107\\Version=IA64L-G03RevD.01\HF=-236.2484287\S2=0.777465\S2-1=0.\S2A=0.750102\RMSD=6.716e-09\RMSF=2.415e-05\Thermal=0.\Dipole=0.7902878,0.1240762,0.700785\PG=C01 [X(C4H9O1Sn1)]\\@

5-*exo* product

1\1\GINC-AC26\FOpt\UBHandHLYP\Gen\C4H9O1Sn1(2)\UXW563\31-Dec-2007\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.9261549012,1.3068541278,-0.3787816171\C,1.7234297234,-0.0009397667,-0.2724132682\C,-1.206023103,0.2155508967,0.4427193265\C,-0.2067950968,1.3584397859,0.64608497\H,1.5801917532,2.1662750268,-0.2545238043\H,0.4861317282,1.384254449,-1.3683563859\H,0.1945659809,1.3074193506,1.6580665353\H,-0.7452964414,2.301104803,0.5652976553\H,-1.837724163,0.0085615271,1.3112353961\H,0.4959560261,-2.4125962838,1.5331774055\H,-0.2102358218,-2.5192034949,-1.1655572773\H,2.3036288878,-0.1999024216,-1.1653021259\H,2.4093773741,0.0263350352,0.5690103014\O,-1.7745528647,0.1235308143,-0.7223422553\Sn,0.2414531156,-1.4991138494,0.1112301438\\Version=IA64L-G03RevD.01\HF=-236.2512783\S2=0.760685\S2-1=0.\S2A=0.75004\RMSD=7.195e-09\RMSF=5.784e-05\Thermal=0.\Dipole=0.8926829,-0.0891201,0.5951019\PG=C01 [X(C4H9O1Sn1)]\\@

6-*endo* transition state

1\1\GINC-AC11\FTS\UBHandHLYP\Gen\C4H9O1Sn1(2)\UXW563\04-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,0.0553776494,-0.059541494,-0.0953475676\C,-0.0066980281,0.1099743103,1.4252472585\C,2.2373893167,-1.3047342061,-0.3067778805\C,0.767818685,-1.343433805,-0.5606218985\H,-0.5551805332,1.0139814977,1.6716123093\H,-0.5578914272,-0.7186106323,1.8626554595\H,-0.9551240802,-0.0817039279,-0.4986422104\H,0.5384768148,0.8025416696,-0.553902679\H,0.5943159073,-1.492764463,-1.6218568156\H,0.3338153561,-2.1931290137,-0.0332908501\H,2.9191092724,-1.1874730048,-1.1466714211\H,1.9880181852,-0.8485850305,3.7439238737\H,2.1883802152,1.8290309938,2.927432834\O,2.7067001808,-1.2389449315,0.8530172699\Sn,1.9194404874,0.1995090372,2.3998783155\\Version=IA64L-G03RevD.01\HF=-236.2462161\S2=0.77638\S2-1=0.\S2A=0.750129\RMSD=8.038e-09\RMSF=9.688e-06\Thermal=0.\Dipole=-0.55628,0.0058661,-0.8346819\PG=C01 [X(C4H9O1Sn1)]\\@

6-*endo* product

1\1\GINC-AC2\FOpt\UBHandHLYP\Gen\C4H9O1Sn1(2)\UXW563\04-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.0327821225,-0.0289946836,-0.0514938041\C,-0.1316663243,0.059997237,1.4774546002\C,2.2847596692,-1.0912231092,-

0.2934010815\C,0.8170009274,-1.2055883686,-0.5538618055\H,-0.6798354978,0.9456320576,1.782423882\H,-0.6701494166,-0.799622813,1.8677478319\H,-1.0352815419,-0.1184029642,-0.4657743247\H,0.3830137643,0.89428529,-0.4510373185\H,0.6804057528,-1.3029048038,-1.6274595681\H,0.4213398516,-2.1286922185,-0.1107376016\H,2.9782520946,-1.5493629016,-0.9816051615\H,2.0162515715,-0.7926926007,3.7869520551\H,2.5667463797,1.5770030333,2.3924454952\O,2.7525329024,-1.0200399949,0.9718457846\Sn,1.8233649917,0.0467238423,2.3231560152\\Version=IA64L-G03RevD.01\HF=-236.272664\S2=0.75567\S2-1=0.\S2A=0.750024\RMSD=4.205e-09\RMSF=1.079e-05\Thermal=0.\Dipole=-0.8112176,0.3390696,0.3047843\PG=C01 [X(C4H9O1Sn1)]\\@

Cyclization of 20c:

20c

1\1\GINC-AC5\FOpt\UBHandHLYP\Gen\C5H11O1Sn1(2)\UXW563\02-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.6336142615,0.6507059647,-0.0654206772\C,-0.5349376222,-0.4057800478,-0.0890122595\C,0.8646960055,0.1946393711,-0.0198589224\C,1.9589079857,-0.856960728,-0.0411085397\C,3.3512231131,-0.3017975332,0.0199026083\H,4.1537182315,-1.0579400538,0.0077217552\H,1.9000714797,-1.4757815591,-0.9385326809\H,1.8558103484,-1.5564808181,0.7905567957\H,0.9638697714,0.7944120537,0.8813115692\H,1.0123628783,0.8807276213,-0.8500311588\H,-0.6196416472,-1.0068803439,-0.9939413326\H,-0.6672964587,-1.0961558916,0.7436225834\H,-1.5625491962,1.2539432447,0.8377909508\H,-3.8617070317,-1.1929992203,1.2414449611\H,-4.7685876687,1.1646654833,0.0706520501\H,-1.5281027178,1.3318355166,-0.9051233164\O,3.6187488051,0.8581888555,0.0775884376\Sn,-3.6498580147,-0.1301269151,-0.0951538235\\Version=IA64L-G03RevD.01\HF=-275.5632029\S2=0.751672\S2-1=0.\S2A=0.750001\RMSD=7.416e-09\RMSF=4.510e-06\Thermal=0.\Dipole=-0.1582895,-0.92346,-0.2763789\PG=C01 [X(C5H11O1Sn1)]\\@

6-*exo* transition state

1\1\GINC-AC26\FTS\UBHandHLYP\Gen\C5H11O1Sn1(2)\UXW563\07-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.9449069718,0.2740655876,0.3075570083\C,-1.6019717025,-1.1314539507,-0.1837561901\C,1.3989740424,0.7551096944,-0.4370516291\C,0.3038251201,1.5808953941,0.2187686176\C,-1.122127236,1.4078191141,-0.3084383419\H,1.2403647324,0.5591003078,-1.5094277258\H,0.6161946661,2.6112094201,0.0417289156\H,0.3517602523,1.4433376267,1.2960310981\H,-1.6530888401,2.3375014223,-0.1248461239\H,-1.0985182338,1.2934120874,-1.3929693046\H,-2.9950086848,0.4671923176,0.094145467\H,-1.8502202901,0.3226609887,1.3917046645\H,-2.223960017,-1.8711810059,0.312938813\H,-1.800835568,-1.2153991914,-1.2490770281\H,0.9437200321,-2.970333569,-0.884033406\H,0.8059978049,-2.0217258863,1.7482823941\O,2.5335192589,0.7028905344,0.0309769317\Sn,0.460889635,-1.666979892,0.1132518395\\Version=IA64L-G03RevD.01\HF=-275.5416778\S2=0.778824\S2-1=0.\S2A=0.750109\RMSD=6.988e-09\RMSF=1.200e-05\Thermal=0.\Dipole=-1.364561,-0.0014879,-0.2881056\PG=C01 [X(C5H11O1Sn1)]\\@

6-*exo* product

1\1\GINC-AC23\FOpt\UBHandHLYP\Gen\C5H11O1Sn1(2)\UXW563\31-Dec-2007\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-1.9675054683,0.2770356695,0.3070749877\C,-1.5891075823,-1.1215193825,-0.1899392845\C,1.2633730498,0.5162001021,-0.3895245436\C,0.2941730572,1.5417291714,0.1949993672\C,-1.1525063978,1.4272862822,-0.29005293\H,1.2353228032,0.5028340841,-1.4889564736\H,0.6775615257,2.5275078418,-0.066623873\H,0.3355363113,1.481895982,1.2811566109\H,-1.6603777534,2.3573215807,-0.0499138958\H,-1.1674719827,1.3541957888,-1.3783798985\H,-3.0185139104,0.4524687601,0.083770428\H,-1.8845218945,0.3176617285,1.3927778086\H,-2.1854631682,-1.8806874266,0.3069442763\H,-1.7891648679,-1.2078053592,-1.2549522785\H,1.1511759208,-2.6765439632,-0.9583720963\H,0.8751163135,-1.8879746045,1.7209449988\O,2.4505466415,0.4184986495,0.1390867923\Sn,0.4964354026,-1.5219859048,0.1057440043\\Version=IA64L-G03RevD.01\HF=-275.5488956\S2=0.759394\S2-1=0.\S2A=0.750036\RMSD=8.222e-09\RMSF=1.458e-05\Thermal=0.\Dipole=-1.3088736,-0.2219138,-0.2702838\PG=C01 [X(C5H11O1Sn1)]\\@

7-*endo* transition state

1\1\GINC-AC26\FTS\UBHandHLYP\Gen\C5H11O1Sn1(2)\UXW563\07-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(ts,noeigentest,calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-

0.313842331,-1.5988104095,-0.4587965431\C,-1.5452292654,-1.4741321815,0.4431299122\C,-1.3330055622,1.6175754997,0.7836774276\C,-2.6022623179,-0.4708458753,-0.0178129291\C,-2.1448281942,0.973551872,-0.2754932419\H,-0.6025091625,-1.6286524226,-1.5067863356\H,2.1839217124,-0.4258368925,1.134326187\H,-1.5983896776,2.6093941791,1.1424723633\H,-1.242561884,-1.2369819974,1.4593270922\H,-3.3985896652,-0.4496779574,0.7223022265\H,0.190718682,-2.5395958857,-0.2548788417\H,2.1384710284,0.0474507685,-1.6187912771\H,-2.0428937238,-2.4411066554,0.501857743\H,-3.0531564707,-0.8326677201,-0.940198855\H,-3.0105548963,1.5867380286,-0.5059238276\H,-1.5019003671,0.9883669043,-1.1703399838\O,-0.2313757074,1.1400108438,1.1239694898\Sn,1.1646758025,-0.0547510986,-0.1821396048\\Version=IA64L-G03R
evD.01\HF=-275.5444747\S2=0.772964\S2-1=0.\S2A=0.750114\RMSD=5.515e-09\RMSF=1.970e-05\Thermal=0.\Dipole=-1.0317006,0.1737941,-0.2653491\PG=C01 [X(C5H11O1Sn1)]\\@

7-*endo* product
1\1\GINC-AC27\FOpt\UBHandHLYP\Gen\C5H11O1Sn1(2)\UXW563\02-Jan-2008\0\\# BHandHLYP/gen pseudo=read scf=direct freq=noraman nosymm opt=(calcfc,z-matrix,maxcycle=500)\\freq&geom\\0,2\C,-0.3342418008,-1.6843297559,-0.3564892406\C,-1.6028312277,-1.468918778,0.4806679179\C,-1.2188424583,1.6224507591,0.6788766244\C,-2.5807028416,-0.4347369517,-0.0766890792\C,-1.9981580097,0.9554875948,-0.4008661126\H,-0.5765873909,-1.785854638,-1.4108962625\H,2.3707730502,-0.4420462471,0.9265921446\H,-1.7181922221,2.1368480545,1.4849545381\H,-1.3326100713,-1.1904520082,1.4966567421\H,-3.3876485258,-0.3132552545,0.6423243668\H,0.1581822529,-2.6046291798,-0.0571119074\H,1.5728014685,0.6602289687,-1.5258232606\H,-2.1350448007,-2.4148461639,0.5636567467\H,-3.0355554383,-0.8286991209,-0.9854484913\H,-2.8236215978,1.6045904371,-0.6833330365\H,-1.3777461998,0.8799539168,-1.2986784041\O,0.0241917801,1.1988059219,0.9826995572\Sn,1.0525210331,-0.0805655549,-0.081191843\\Version=IA64L-G03RevD.01\HF=-275.5685041\S2=0.755626\S2-1=0.\S2A=0.750023\RMSD=4.994e-09\RMSF=3.607e-05\Thermal=0.\Dipole=-0.095538,-0.8206028,-0.5015229\PG=C01 [X(C5H11O1Sn1)]\\@