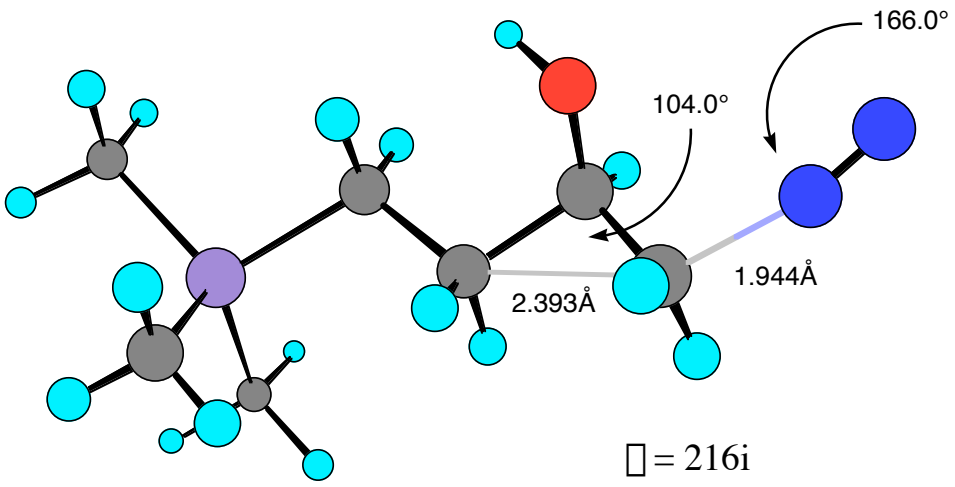


□ = 216i

E(HF/6-31G*) = -747.4071413 H/molecule
(ZPE = 658.8 kJ/mol)

Archive:

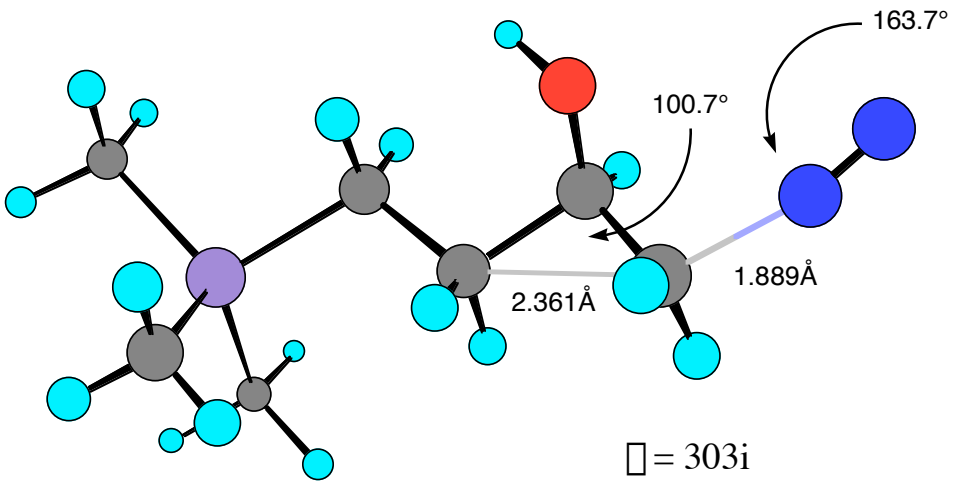
N-N= 6.978994473539D+02 E-N=-3.142130373229D+03 KE= 7.465802949520D+02
1\1\ CHEMCLUSTER-KNET9\FTS\RHF\6-31G(d)\C7H17N2O1Si1(1+)\CARLHS\31-Mar
-2004\1\\#RHF/ 6-31G* OPT=(GRAD,TS,READFC) GEOM=CHECKPOINT GUESS=READ\
\SiMe3butOHN2d-6 stretching C-N bond\\1,1\C\C,1,r1\C,1,r2,2,a1\C,2,r3,
1,a2,3,D1,0\Si,4,r4,2,a3,1,D2,0\C,5,r5,4,a4,2,D3,0\C,5,r6,4,a5,2,D4,0\
C,5,r7,4,a6,2,D5,0\O,1,rA,2,aA,4,DA,0\H,1,r8,2,a7,4,D6,0\H,3,r9,1,a8,2
,D7,0\H,3,r10,1,a9,2,D8,0\N,3,rTS,1,aB,2,DB,0\X,13,1.,3,90.,1,180.,0\N
,13,r11,14,a10,3,D9,0\H,2,r12,1,a11,3,D10,0\H,2,r13,1,a12,3,D11,0\H,4,
r14,2,a13,1,D12,0\H,4,r15,2,a14,1,D13,0\H,6,r16,5,a15,4,D14,0\H,6,r17,
5,a16,4,D15,0\H,6,r18,5,a17,4,D16,0\H,7,r19,5,a18,6,D17,0\H,7,r20,5,a1
9,6,D18,0\H,7,r21,5,a20,6,D19,0\H,8,r22,5,a21,6,D20,0\H,8,r23,5,a22,6,
D21,0\H,8,r24,5,a23,6,D22,0\H,9,r25,1,a24,2,D23,0\\rTS=1.94421482\r1=1
.55842506\r2=1.48043971\r3=1.53668605\r4=1.92657135\r5=1.88379135\r6=1
.88831084\r7=1.88884928\r8=1.08487049\rA=1.38315302\r9=1.0746174\r10=1
.07489418\r11=1.0752295\r12=1.08568801\r13=1.08546782\r14=1.0891809\r1
5=1.08809472\r16=1.08687608\r17=1.08687555\r18=1.0866807\r19=1.0867347
6\r20=1.0871297\r21=1.08740624\r22=1.08715817\r23=1.08675658\r24=1.087
45623\r25=0.94964618\a1=103.85189544\a2=111.03356782\a3=115.15905898\a
4=106.62854249\a5=108.78344297\a6=108.74788171\aA=114.45731506\a7=108.
924878\a8=120.1204827\a9=117.66110633\aB=103.97295145\a10=92.22843406\
a11=109.24165077\a12=108.54068476\a13=109.71086167\a14=109.72157573\a1
5=111.85076694\a16=111.8404926\a17=110.82587825\a18=110.4573196\a19=11
1.87215029\a20=112.56376768\a21=111.86841146\a22=110.40145578\a23=112.
66805936\a24=111.03479423\D1=175.83837825\D2=175.22803679\D3=178.61239
299\D4=58.77678805\D5=-61.70520121\DA=60.64498466\D6=-66.33756714\D7=7
2.32275984\D8=-81.8629887\DB=177.20992144\D9=177.80814\D10=54.6247139\
D11=-62.97630197\D12=53.31925128\D13=-63.98238836\D14=60.12120819\D15=
-60.73705882\D16=179.70209795\D17=59.10546062\D18=-60.06437521\D19=178
.41933669\D20=59.6090341\D21=-59.49371429\D22=181.24209006\D23=-63.026
54792\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-747.4071413\RMSD=7.0
71e-09\RMSF=1.338e-05\Dipole=2.2562161,-0.4890261,-3.1715364\PG=C01 [X
(C7H17N2O1Si1)]\\@

GS = 747.4116961 H/molecule
GS_{ZPE} = 666.3 kJ/mol

□$E^{‡}$ = 12.0 kJ/mol (2.85 kcal/mol)
□$E^{‡}_{ZPE}$ = 4.5 kJ/mol (1.08 kcal/mol)

10.1071/CH04077_AC

Accessory Publication: Aust. J. Chem., 2004, 57(9), 869–876.



□ = 303i

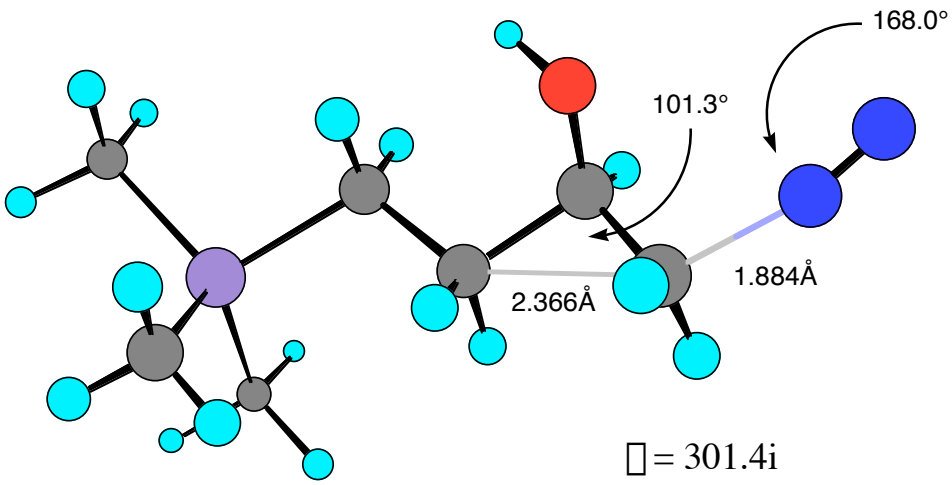
E(b3lyp/6-31G*) = -750.923753856 H/molecule
(ZPE = 617.1 kJ/mol)

Archive:

N-N= 6.976943740072D+02 E-N=-3.141876538122D+03 KE= 7.452566532347D+02
1\1\ CHEMCLUSTER-KNET9\FTS\RB3LYP\6-31G(d)\C7H17N2O1Si1(1+)\CARLHS\30-
Mar-2004\1\\#B3LYP/ 6-31G* OPT=(GRAD,TS,READFC) GEOM=CHECKPOINT GUESS=
READ\\SiMe3butOHN2d-6 stretching C-N bond\\1,1\C\C,1,r1\C,1,r2,2,a1\C,
2,r3,1,a2,3,D1,0\Si,4,r4,2,a3,1,D2,0\C,5,r5,4,a4,2,D3,0\C,5,r6,4,a5,2,
D4,0\C,5,r7,4,a6,2,D5,0\O,1,rA,2,aA,4,DA,0\H,1,r8,2,a7,4,D6,0\H,3,r9,1
,a8,2,D7,0\H,3,r10,1,a9,2,D8,0\N,3,rTS,1,aB,2,DB,0\X,13,1.,3,90.,1,180
.,0\N,13,r11,14,a10,3,D9,0\H,2,r12,1,a11,3,D10,0\H,2,r13,1,a12,3,D11,0
\H,4,r14,2,a13,1,D12,0\H,4,r15,2,a14,1,D13,0\H,6,r16,5,a15,4,D14,0\H,6
,r17,5,a16,4,D15,0\H,6,r18,5,a17,4,D16,0\H,7,r19,5,a18,6,D17,0\H,7,r20
,5,a19,6,D18,0\H,7,r21,5,a20,6,D19,0\H,8,r22,5,a21,6,D20,0\H,8,r23,5,a
22,6,D21,0\H,8,r24,5,a23,6,D22,0\H,9,r25,1,a24,2,D23,0\\rTS=1.88874298
\r1=1.60601616\r2=1.45903237\r3=1.53423171\r4=1.94231884\r5=1.88536594
\r6=1.88797467\r7=1.88821097\r8=1.09841136\rA=1.39510243\r9=1.08743999
\r10=1.08851591\r11=1.10413874\r12=1.09507817\r13=1.09422684\r14=1.098
77436\r15=1.09796529\r16=1.09612727\r17=1.09616168\r18=1.09666007\r19=
1.09658023\r20=1.09653298\r21=1.09675514\r22=1.096529\r23=1.09661549\r
24=1.09679291\r25=0.97201098\a1=100.70528792\a2=108.98427066\a3=113.68
20767\a4=105.65577414\a5=108.58450658\a6=108.47194793\aA=114.21449033\
a7=106.71190064\a8=119.27877286\a9=117.05675461\aB=106.32646198\a10=10
3.97830309\a11=109.83923224\a12=108.088261\a13=110.52373514\a14=110.31
668221\a15=111.91295853\a16=111.89376575\a17=110.23229023\a18=110.0609
8418\a19=111.9496105\a20=112.64912246\a21=111.92328261\a22=110.0219693
7\a23=112.75968954\a24=109.02509784\D1=171.1776357\D2=175.22145711\D3=
178.35100935\D4=58.71932228\D5=-62.13688474\DA=55.31146307\D6=-71.0072
16\D7=70.5604273\D8=-78.4185113\DB=178.62668204\D9=176.28937291\D10=50
.51331675\D11=-67.97100022\D12=54.02316697\D13=-65.04971389\D14=60.501
0371\D15=-60.79911039\D16=179.86953674\D17=60.61781409\D18=-58.3692938
2\D19=179.72513137\D20=58.18958265\D21=-60.73220686\D22=180.18007233\D
23=-60.72416056\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-750.923753
9\RMSD=2.418e-09\RMSF=4.607e-06\Dipole=1.8636636,-0.5100101,-2.6190277
\PG=C01 [X(C7H17N2O1Si1)]\\@

GS = 750.9323265 H/molecule
GS_{ZPE} = 623.6 kJ/mol

$\Delta E^{\ddagger}$ = 22.5 kJ/mol (5.4 kcal/mol)
$\Delta E^{\ddagger}_{ZPE}$ = 16.0 kJ/mol (3.8 kcal/mol)



□ = 301.4i

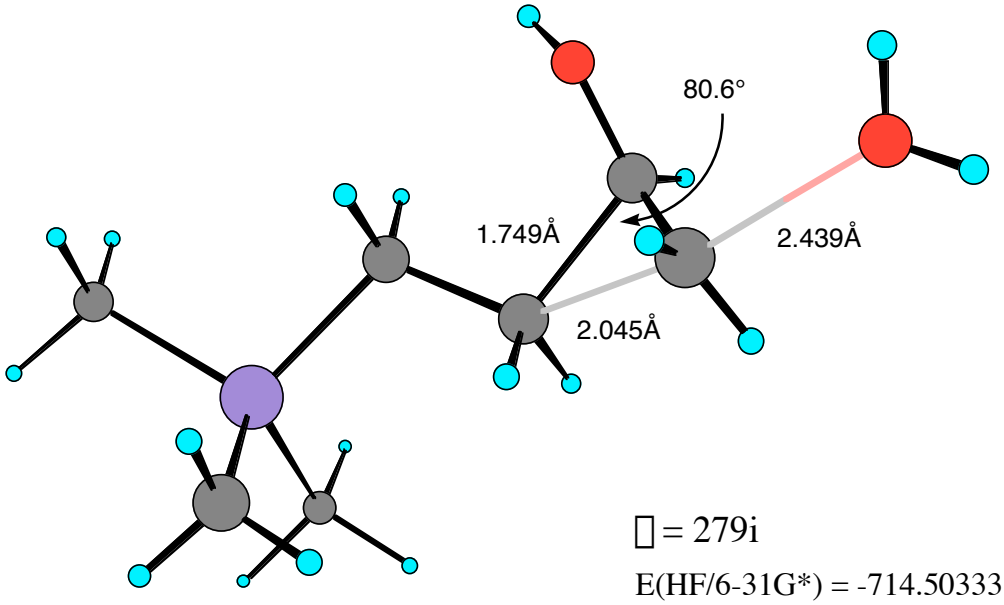
E(b3lyp/6-311G**) = -751.0868442 H/molecule
(ZPE = 612.1 kJ/mol)

Archive:

N-N= 6.986510688242D+02 E-N=-3.147615815998D+03 KE= 7.486453363496D+02
1\1\ CHEMCLUSTER-KNET8\FTS\RB3LYP\6-311G(d,p)\C7H17N2O1Si1(1+)\CARLHS\
04-Apr-2004\1\\#B3LYP/ 6-311G** OPT=(GRAD,TS,READFC,NOEIGENTEST) GEOM=
CHECKPOINT GUESS=READ\\SiMe3butOHN2d-6 stretching C-N bond\\1,1\C\C,1,
r1\C,1,r2,2,a1\C,2,r3,1,a2,3,D1,0\Si,4,r4,2,a3,1,D2,0\C,5,r5,4,a4,2,D3
,0\C,5,r6,4,a5,2,D4,0\C,5,r7,4,a6,2,D5,0\O,1,rA,2,aA,4,DA,0\H,1,r8,2,a
7,4,D6,0\H,3,r9,1,a8,2,D7,0\H,3,r10,1,a9,2,D8,0\N,3,rTS,1,aB,2,DB,0\X,
13,1.,3,90.,1,180.,0\N,13,r11,14,a10,3,D9,0\H,2,r12,1,a11,3,D10,0\H,2,
r13,1,a12,3,D11,0\H,4,r14,2,a13,1,D12,0\H,4,r15,2,a14,1,D13,0\H,6,r16,
5,a15,4,D14,0\H,6,r17,5,a16,4,D15,0\H,6,r18,5,a17,4,D16,0\H,7,r19,5,a1
8,6,D17,0\H,7,r20,5,a19,6,D18,0\H,7,r21,5,a20,6,D19,0\H,8,r22,5,a21,6,
D20,0\H,8,r23,5,a22,6,D21,0\H,8,r24,5,a23,6,D22,0\H,9,r25,1,a24,2,D23,
0\\rTS=1.88375759\r1=1.60022772\r2=1.45800381\r3=1.5332459\r4=1.937544
91\r5=1.87972717\r6=1.88293741\r7=1.88318886\r8=1.09614681\rA=1.396340
24\r9=1.08555188\r10=1.08668389\r11=1.09495494\r12=1.09310507\r13=1.09
22696\r14=1.09641828\r15=1.09547532\r16=1.09366615\r17=1.09368722\r18=
1.09418314\r19=1.0941355\r20=1.09405388\r21=1.09424473\r22=1.09406805\
r23=1.09416039\r24=1.09425378\r25=0.96489723\a1=101.28172689\a2=109.30
840174\a3=114.0945846\a4=105.91923391\a5=108.5583447\a6=108.45863019\a
A=114.19571606\a7=106.83569822\a8=119.27041889\a9=116.86724181\aB=106.
36586924\a10=101.43189822\a11=109.69172212\a12=108.09083996\a13=110.51
063762\a14=110.35903803\a15=111.88751089\a16=111.86447912\a17=110.2019
2184\a18=110.07114367\a19=111.90232227\a20=112.58346166\a21=111.857242
\a22=110.02143588\a23=112.70427668\a24=109.43352352\D1=171.26643109\D2
=175.57274111\D3=178.49675309\D4=58.747507\D5=-61.91354729\DA=55.38319
689\D6=-70.73524107\D7=69.85783698\D8=-79.20070986\DB=177.94652749\D9=
176.48438439\D10=50.55751788\D11=-67.81004311\D12=54.38805799\D13=-64.
63577883\D14=60.48261972\D15=-60.84247745\D16=179.83520098\D17=60.4053
4943\D18=-58.60363557\D19=179.47373018\D20=58.55190734\D21=-60.3648077
7\D22=180.57959086\D23=-61.48431458\\Version=x86-Linux-G03RevB.04\Stat
e=1-A\HF=-751.0868442\RMSD=6.336e-09\RMSF=9.533e-06\Dipole=1.9201363,-
0.5382973,-2.7241479\PG=C01 [X(C7H17N2O1Si1)]\\@

GS = -751.094888 H/molecule
GS_{ZPE} = 618.7 kJ/mol

□$E^{‡}$ = 21.1 kJ/mol (5.0 kcal/mol)
□$E^{‡}_{ZPE}$ = 14.5 kJ/mol (3.5 kcal/mol)



□ = 279i

E(HF/6-31G*) = -714.503331 H/molecule
(ZPE = 701.8 kJ/mol)

Archive:

N-N= 6.506492656442D+02 E-N=-2.9735624959 61D+03 KE= 7.138933872086D+02
1\1\ CHEMCLUSTER-KNET9\FTS\RHF\6-31G(d)\C7H19O2Si1(1+)\CARLHS\02-Apr-2
004\1\\#RHF/ 6-31G* OPT=(GRAD,TS,READFC,NOEIGENTEST,NOFREEZE) GEOM=CHE
CKPOINT GUESS=READ\\Finding TS with OH and OH2 leaving group\\1,1\C\C,
1,r1\C,1,r2,2,a1\C,2,r3,1,a2,3,D1,0\Si,4,r4,2,a3,1,D2,0\C,5,r5,4,a4,2,
D3,0\C,5,r6,4,a5,2,D4,0\C,5,r7,4,a6,2,D5,0\O,1,rA,2,aA,4,DA,0\H,1,r8,2
,a7,4,D6,0\H,3,r9,1,a8,2,D7,0\H,3,r10,1,a9,2,D8,0\O,3,rTS,1,aB,2,DB,0\
H,13,r11,3,a10,1,D9,0\H,2,r12,1,a11,3,D10,0\H,2,r13,1,a12,3,D11,0\H,4,
r14,2,a13,1,D12,0\H,4,r15,2,a14,1,D13,0\H,6,r16,5,a15,4,D14,0\H,6,r17,
5,a16,4,D15,0\H,6,r18,5,a17,4,D16,0\H,7,r19,5,a18,6,D17,0\H,7,r20,5,a1
9,6,D18,0\H,7,r21,5,a20,6,D19,0\H,8,r22,5,a21,6,D20,0\H,8,r23,5,a22,6,
D21,0\H,8,r24,5,a23,6,D22,0\H,9,r25,1,a24,2,D23,0\H,13,r26,3,a25,1,D24
,0\\rTS=2.438725\r1=1.74853908\r2=1.38187231\r3=1.52823326\r4=1.936400
39\r5=1.88226199\r6=1.88733453\r7=1.88685891\r8=1.07633037\r9=1.069999
4\r10=1.07132574\r11=0.95003678\r12=1.08502901\r13=1.0786503\r14=1.087
76222\r15=1.0844099\r16=1.08675072\r17=1.08666527\r18=1.08667002\r19=1
.08672176\r20=1.08706683\r21=1.08750246\r22=1.08707169\r23=1.08670655\
r24=1.08738407\r25=0.94949769\r26=0.95017093\a1=80.61438746\a2=105.363
64772\a3=113.45389954\a4=105.89122945\a5=108.43672845\a6=108.72949479\
a7=103.44168554\a8=120.88730225\a9=119.65209213\a10=120.9509644\a11=11
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748282\a16=111.8936156\a17=110.65886201\a18=110.21203778\a19=111.99061
755\a20=112.79718258\a21=111.94218426\a22=110.30423239\a23=112.7371927
9\a24=112.04109001\a25=132.91624984\D1=147.11521185\D2=172.98275289\D3
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D12=52.14280307\D13=-66.048139\D14=60.59141375\D15=-60.43442479\D16=18
0.04783595\D17=59.00810502\D18=-59.97499415\D19=178.06592669\D20=59.37
556614\D21=-59.65339643\D22=181.14441467\D23=-81.09931691\D24=-135.225
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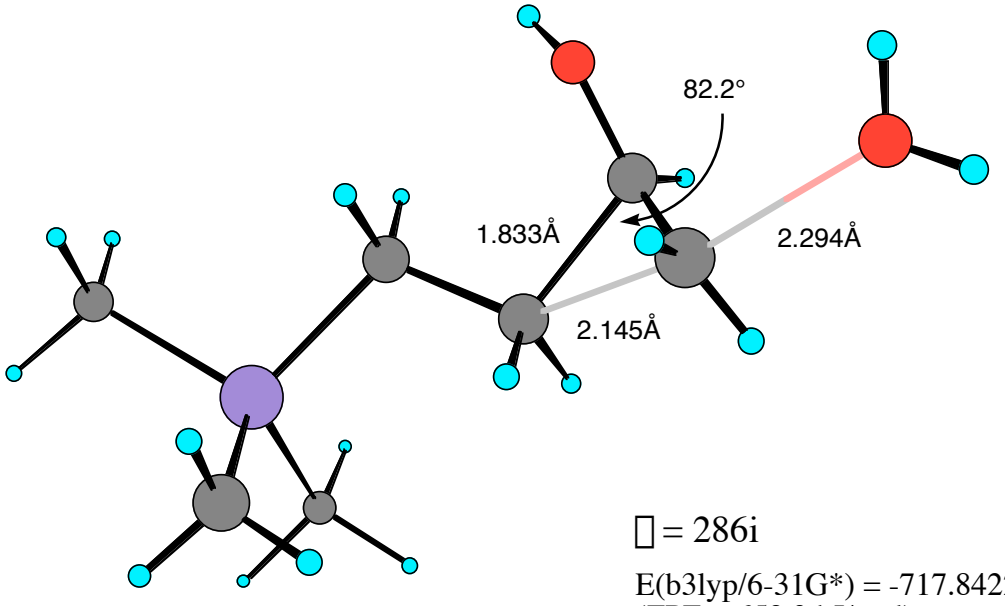
175.18903551\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-714.5033316\R
MSD=1.743e-09\RMSF=1.397e-06\Dipole=1.803057,-0.9851112,-2.8343405\PG=
C01 [X(C7H19O2Si1)]\\@

GS = -714.5424432 H/molecule
GS_{ZPE} = 720.7 kJ/mol

□$E^{‡}$ = 102.7 kJ/mol (24.5 kcal/mol)
□$E^{‡}_{ZPE}$ = 83.3 kJ/mol (20.0 kcal/mol)



□ = 286i

E(b3lyp/6-31G*) = -717.8422785 H/molecule
(ZPE = 659.3 kJ/mol)

Archive:

N-N= 6.490653166092D+02 E-N=-2.970527934694D+03 KE= 7.126033475604D+02
1\1\ CHEMCLUSTER-KNET3\FTS\RB3LYP\6-31G(d)\C7H19O2Si1(1+)\CARLHS\02-Ap
r-2004\1\\#B3LYP/ 6-31G* GEOM=CHECKPOINT GUESS=READ OPT=(GRAD,TS,READF
C,NOEIGENTEST,NOFREEZE)\\Finding TS with OH and OH2 leaving group\\1,1
\C\C,1,r1\C,1,r2,2,a1\C,2,r3,1,a2,3,D1,0\Si,4,r4,2,a3,1,D2,0\C,5,r5,4,
a4,2,D3,0\C,5,r6,4,a5,2,D4,0\C,5,r7,4,a6,2,D5,0\O,1,rA,2,aA,4,DA,0\H,1
,r8,2,a7,4,D6,0\H,3,r9,1,a8,2,D7,0\H,3,r10,1,a9,2,D8,0\O,3,rTS,1,aB,2,
DB,0\H,13,r11,3,a10,1,D9,0\H,2,r12,1,a11,3,D10,0\H,2,r13,1,a12,3,D11,0
\H,4,r14,2,a13,1,D12,0\H,4,r15,2,a14,1,D13,0\H,6,r16,5,a15,4,D14,0\H,6
,r17,5,a16,4,D15,0\H,6,r18,5,a17,4,D16,0\H,7,r19,5,a18,6,D17,0\H,7,r20
,5,a19,6,D18,0\H,7,r21,5,a20,6,D19,0\H,8,r22,5,a21,6,D20,0\H,8,r23,5,a
22,6,D21,0\H,8,r24,5,a23,6,D22,0\H,9,r25,1,a24,2,D23,0\H,13,r26,3,a25,
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.95386723\r5=1.88460074\r6=1.88684942\r7=1.88624705\r8=1.08985621\r9=1
.08178403\r10=1.08367398\r11=0.97143974\r12=1.09320942\r13=1.08979634\
r14=1.09803213\r15=1.09524108\r16=1.09610513\r17=1.09603084\r18=1.0966
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09656934\r24=1.09666093\r25=0.97155407\r26=0.97189197\a1=82.18858094\a
2=103.45534832\a3=112.18123689\a4=104.86828077\a5=108.26770373\a6=108.
70187639\a7=100.964169\a8=120.34527036\a9=119.53566908\a10=113.0283112
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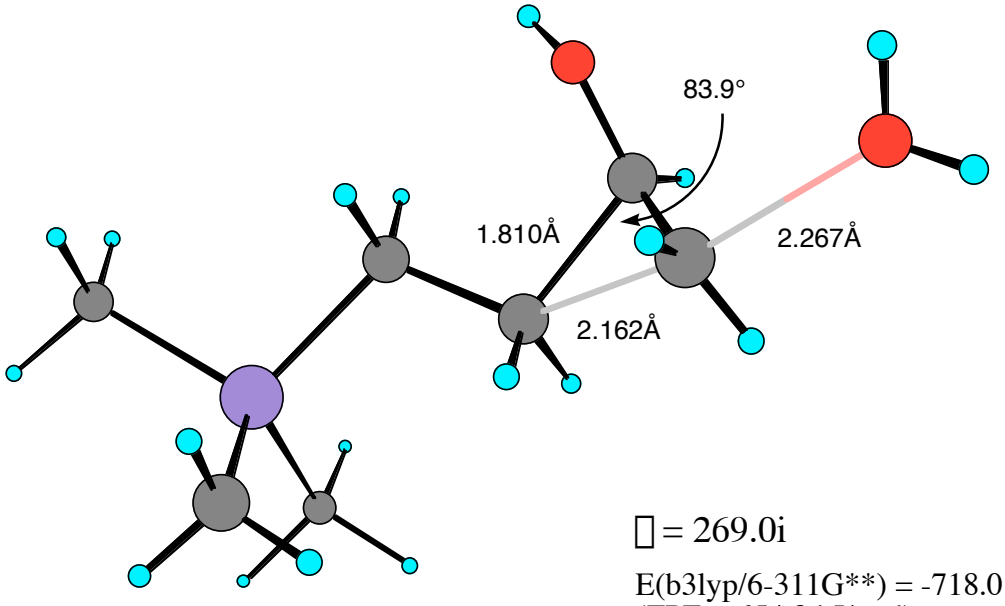
45459\PG=C01 [X(C7H19O2Si1)]\\@

GS = -717.8778967 H/molecule
GS_{ZPE} = 627.8 kJ/mol

□$E^{‡}$ = 93.5 kJ/mol (22.3 kcal/mol)
□$E^{‡}_{ZPE}$ = 62.0 kJ/mol (14.8 kcal/mol)



ν = 269.0i

E(b3lyp/6-311G**) = -718.013317 H/molecule
(ZPE = 654.8 kJ/mol)

Archive:

1\1\ CHEMCLUSTER-KNET8\FTS\RB3LYP\6-311G(d,p)\C7H19O2Si1(1+)\CARLHS\05
-Apr-2004\1\\#B3LYP/ 6-311G** GEOM=CHECKPOINT GUESS=READ OPT=(GRAD,TS,
READFC,NOEIGENTEST,NOFREEZE)\\Finding TS with OH and OH2 leaving group
\\1,1\C\C,1,r1\C,1,r2,2,a1\C,2,r3,1,a2,3,D1,0\Si,4,r4,2,a3,1,D2,0\C,5,
r5,4,a4,2,D3,0\C,5,r6,4,a5,2,D4,0\C,5,r7,4,a6,2,D5,0\O,1,rA,2,aA,4,DA,
0\H,1,r8,2,a7,4,D6,0\H,3,r9,1,a8,2,D7,0\H,3,r10,1,a9,2,D8,0\O,3,rTS,1,
aB,2,DB,0\H,13,r11,3,a10,1,D9,0\H,2,r12,1,a11,3,D10,0\H,2,r13,1,a12,3,
D11,0\H,4,r14,2,a13,1,D12,0\H,4,r15,2,a14,1,D13,0\H,6,r16,5,a15,4,D14,
0\H,6,r17,5,a16,4,D15,0\H,6,r18,5,a17,4,D16,0\H,7,r19,5,a18,6,D17,0\H,
7,r20,5,a19,6,D18,0\H,7,r21,5,a20,6,D19,0\H,8,r22,5,a21,6,D20,0\H,8,r2
3,5,a22,6,D21,0\H,8,r24,5,a23,6,D22,0\H,9,r25,1,a24,2,D23,0\H,13,r26,3
,a25,1,D24,0\\rTS=2.26736953\r1=1.81006487\r2=1.39033617\r3=1.50975637
\r4=1.94980243\r5=1.87895352\r6=1.88163768\r7=1.88094168\r8=1.08772007
\r9=1.07983169\r10=1.08154049\r11=0.96508061\r12=1.09137447\r13=1.0873
9445\r14=1.09555684\r15=1.09277798\r16=1.09360875\r17=1.0935247\r18=1.
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23=1.09412917\r24=1.09412511\r25=0.96462157\r26=0.96536495\a1=83.87546
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108.67956638\a7=101.47209225\a8=120.21496737\a9=119.33874417\a10=113.6
8109883\a11=114.34885553\a12=102.35621899\a13=111.47078577\a14=110.944
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656\a19=111.93562775\a20=112.7293258\a21=111.84788343\a22=109.95644192
\a23=112.7410055\a24=110.71743654\a25=122.94299162\D1=149.71419956\D2=
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6678927\D20=58.29551582\D21=-60.55056215\D22=180.34190539\D23=-80.5738
5741\D24=-172.23983532\rA=1.36106098\aA=113.71049616\aB=104.54296587\D
A=34.58233483\DB=172.79933442\\Version=x86-Linux-G03RevB.04\State=1-A\
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7,-2.6735194\PG=C01 [X(C7H19O2Si1)]\\@

GS = -718.0449254 H/molecule
GS_{ZPE} = 668.2 kJ/mol

$\Delta E^{\ddagger}$ = 83.0 kJ/mol (19.8 kcal/mol)
$\Delta E^{\ddagger}_{ZPE}$ = 60.6 kJ/mol (14.5 kcal/mol)