Reactant Strucures:

Structure: s-trans isoprene
Atoms: 13 Charge: 0 Multiplicity: 1

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	0.012244	2.628704	0.000000
6	0.585248	1.717352	0.000000
6	0.000000	0.524325	0.000000
1	1.658054	1.814603	0.000000
6	-1.492135	0.378049	-0.000000
6	0.822329	-0.686666	0.000000
1	-1.829367	-0.171846	0.875027
1	-1.829367	-0.171846	-0.875027
1	-1.976414	1.347172	-0.000000
6	0.369677	-1.932310	0.000000
1	1.889163	-0.520237	0.000000
1	1.046930	-2.768458	0.000000
1	-0.681956	-2.162597	-0.000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.116957 (Hartree/Particle)
Thermal correction to Energy= 0.122669
Thermal correction to Enthalpy= 0.123613
Thermal correction to Gibbs Free Energy= 0.088566
Sum of electronic and zero-point Energies= -195.111889
Sum of electronic and thermal Energies= -195.106177
Sum of electronic and thermal Enthalpies= -195.105232
Sum of electronic and thermal Free Energies= -195.140280

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz -194.7703694
UCCSD(T)/aug-cc-pVTZ -194.9524706
BD(T)/aug-cc-pVDZ -194.7702383

Structure: s-gauche isoprene
Atoms: 13 Charge: 0 Multiplicity: 1

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.603455	1.429147	-0.092527
1	0.224613	2.085329	-0.297440
6	-0.453290	0.112107	-0.065320
6	0.855700	-0.531253	-0.271102
1	0.841167	-1.449462	-0.842164
6	2.009527	-0.098946	0.209924
1	2.068663	0.782200	0.826786
1	2.929585	-0.620373	0.008998
6	-1.608011	-0.822073	0.153394
1	-1.718700	-1.499137	-0.691307
1	-1.445899	-1.438431	1.034570
1	-2.538510	-0.280835	0.278600

```
   1    -1.563748      1.886819    0.075742
 ---------------------------------------------------------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 ---------------------------------------------------------------------
 Zero-point correction=                           0.116517 (Hartree/Particle)
 Thermal correction to Energy=                    0.122397
 Thermal correction to Enthalpy=                  0.123341
 Thermal correction to Gibbs Free Energy=         0.087792
 Sum of electronic and zero-point Energies=           -195.107640
 Sum of electronic and thermal Energies=              -195.101760
 Sum of electronic and thermal Enthalpies=            -195.100816
 Sum of electronic and thermal Free Energies=         -195.136365
 ---------------------------------------------------------------------
 Single Point Energy Calculations (Hartrees)
 ---------------------------------------------------------------------
 UCCSD(T)/aug-cc-pvdz                         -194.7657579
 UCCSD(T)/aug-cc-pVTZ                             -194.9477931
 BD(T)/auc-cc-pVDZ                                -194.7656093
 =+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=
 Structure: OHradical
 Atoms: 2 Charge: 0 Multiplicity: 2
-----------------------------------------------------
   Atomic          Coordinates (Angstroms)
   Number         X         Y       Z
-----------------------------------------------------
      8             0.000000  0.000000    0.106940
      1             0.000000  0.000000   -0.855517
 ---------------------------------------------------------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 ---------------------------------------------------------------------
 Zero-point correction=                           0.008840 (Hartree/Particle)
 Thermal correction to Energy=                    0.011201
 Thermal correction to Enthalpy=                  0.012145
 Thermal correction to Gibbs Free Energy=        -0.008062
 Sum of electronic and zero-point Energies=           -75.714615
 Sum of electronic and thermal Energies=              -75.712255
 Sum of electronic and thermal Enthalpies=            -75.711311
 Sum of electronic and thermal Free Energies=         -75.731518
 ---------------------------------------------------------------------
 Single Point Energy Calculations (Hartrees)
 ---------------------------------------------------------------------
 UCCSD(T)/aug-cc-pvdz                         -75.5838141
 UCCSD(T)/aug-cc-pVTZ                             -75.6454799
 BD(T)/aug-cc-pVDZ                                -75.5837091
=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=
 Structure: ts_rotationalbarrier for isoprene trans to gauche
 Atoms: 13 Charge: 0 Multiplicity: 1
 -------------------------------------------------
   Atomic                Coordinates (Angstroms)
   Number               X       Y         Z
 -------------------------------------------------
      1            -2.222553   -1.192693   -0.429392
      6            -1.180215   -1.232084   -0.159275
      6            -0.489553   -0.130278    0.081374
      1            -0.725723   -2.206373   -0.098185
      6            -1.097424    1.239996    0.005326
      6             0.943192   -0.188669    0.473626
      1            -0.578558    1.847300   -0.732321
```

```
      1            -1.002313    1.756894    0.957797
      1            -2.148031    1.193271   -0.259285
      6             1.951376    0.088077   -0.331786
      1             1.148054   -0.463393    1.499075
      1             2.971710    0.037810    0.008419
      1             1.793163    0.364933   -1.361696
 ---------------------------------------------------------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 ---------------------------------------------------------------------
 Zero-point correction=                           0.116043 (Hartree/Particle)
 Thermal correction to Energy=                    0.121260
 Thermal correction to Enthalpy=                  0.122204
 Thermal correction to Gibbs Free Energy=         0.088078
 Sum of electronic and zero-point Energies=           -195.103155
 Sum of electronic and thermal Energies=              -195.097938
 Sum of electronic and thermal Enthalpies=            -195.096994
 Sum of electronic and thermal Free Energies=         -195.131120
 ---------------------------------------------------------------------
 Single Point Energy Calculations (Hartrees)
 ---------------------------------------------------------------------
 UCCSD(T)/aug-cc-pvdz                          -194.7615017
 UCCSD(T)/aug-cc-pVTZ                          -194.9431109
 BD(T)/aug-cc-pVDZ                                    -194.7613411
 =+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=
Structure: ts_rotationalbarrier for isoprene gauche to gauche
 Atoms: 13 Charge: 0 Multiplicity: 1
----------------------------------------
 Atomic        Coordinates (Angstroms)
 Number       X     Y         Z
----------------------------------------
    1   1.495000    1.934738    0.000000
    6   1.258451    0.884754    0.000000
    6   0.000000    0.466390    0.000000
    1   2.091460    0.203350    0.000000
    6  -1.146919    1.435681    0.000000
    6  -0.391614   -0.956835    0.000000
    1  -1.777031    1.286942    0.874431
    1  -1.777031    1.286942   -0.874431
    1  -0.801450    2.462549    0.000000
    6   0.404912   -2.013703    0.000000
    1  -1.457805   -1.131334    0.000000
    1  -0.000802   -3.010246    0.000000
    1   1.478680   -1.930663    0.000000
 ---------------------------------------------------------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 ---------------------------------------------------------------------
 Zero-point correction=                           0.116304 (Hartree/Particle)
 Thermal correction to Energy=                    0.121448
 Thermal correction to Enthalpy=                  0.122392
 Thermal correction to Gibbs Free Energy=         0.088429
 Sum of electronic and zero-point Energies=           -195.106368
 Sum of electronic and thermal Energies=              -195.101224
 Sum of electronic and thermal Enthalpies=            -195.100279
 Sum of electronic and thermal Free Energies=         -195.134243
 ---------------------------------------------------------------------
 Single Point Energy Calculations (Hartrees)
 ---------------------------------------------------------------------
 UCCSD(T)/aug-cc-pvdz                          -194.7643774
```

UCCSD(T)/aug-cc-pVTZ -194.9464664
BD(T)/aug-cc-pVDZ -194.7642296

Prereactive Complex Structures:

Pathway: s-trans carbon 1
Atoms: 15 Charge: 0 Multiplicity: 2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.954713	-0.153348	1.227820
1	-0.973604	-1.121223	1.699863
6	0.075066	0.227249	0.469306
6	1.193897	-0.691112	0.259343
1	1.121164	-1.636214	0.776824
6	2.258430	-0.456635	-0.496443
1	2.389894	0.466804	-1.033757
1	3.039894	-1.189424	-0.596742
6	0.109102	1.571824	-0.190632
1	0.978780	2.139709	0.130098
1	0.165267	1.471287	-1.271127
1	-0.781991	2.139055	0.045557
8	-2.332271	-0.582395	-0.940991
1	-1.579559	-1.093199	-1.249141
1	-1.792368	0.494498	1.409993

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.127621 (Hartree/Particle)
Thermal correction to Energy= 0.136684
Thermal correction to Enthalpy= 0.137628
Thermal correction to Gibbs Free Energy= 0.092546
Sum of electronic and zero-point Energies= -270.829775
Sum of electronic and thermal Energies= -270.820711
Sum of electronic and thermal Enthalpies= -270.819767
Sum of electronic and thermal Free Energies= -270.864850

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pVDZ -270.3610001
BD(T)/aug-cc-pVDZ -270.3609645

Pathway: s-gauche carbon 1
Atoms: 15 Charge: 0 Multiplicity: 2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.178707	-0.882481	1.149730
1	0.498576	-0.400649	1.833752
6	-0.821817	-0.193434	0.212082
6	-0.605220	1.250531	0.012558
1	-1.494514	1.830046	-0.192319
6	0.570102	1.858029	0.025152
1	1.490648	1.315588	0.159399

```
    1      0.645519      2.921113   -0.126371
    6     -1.842676     -0.828017   -0.686904
    1     -2.810492     -0.348814   -0.555858
    1     -1.568745     -0.705956   -1.731938
    1     -1.955905     -1.885332   -0.478599
    8      2.639407     -0.879088   -0.517467
    1      1.697725     -0.983073   -0.327516
    1     -0.348166     -1.937987    1.283479
 ---------------------------------------------------------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 ---------------------------------------------------------------------
 Zero-point correction=                           0.127580 (Hartree/Particle)
 Thermal correction to Energy=                    0.136462
 Thermal correction to Enthalpy=                  0.137406
 Thermal correction to Gibbs Free Energy=         0.093136
 Sum of electronic and zero-point Energies=           -270.827304
 Sum of electronic and thermal Energies=              -270.818422
 Sum of electronic and thermal Enthalpies=            -270.817478
 Sum of electronic and thermal Free Energies=         -270.861748
 ---------------------------------------------------------------------
 Single Point Energy Calculations (Hartrees)
 ---------------------------------------------------------------------
 UCCSD(T)/aug-cc-pVDZ                          -270.3562301
 BD(T)/aug-cc-pVDZ                             -270.3562146
=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=
 Pathway: s-trans carbon 2
 Atoms: 15 Charge: 0 Multiplicity: 2
---------------------------------------------
 Atomic        Coordinates (Angstroms)
 Number       X         Y       Z
---------------------------------------------
    1      -1.336577    2.130063   -0.340636
    6      -0.565484    1.514551   -0.771767
    6       0.173207    0.697148   -0.023351
    1      -0.408213    1.599260   -1.834248
    6      -0.043396    0.573773    1.455352
    6       1.207439   -0.127018   -0.653793
    1       0.873038    0.783680    1.999080
    1      -0.360774   -0.432834    1.711900
    1      -0.808543    1.263058    1.791632
    6       1.950038   -1.034581   -0.037061
    1       1.344594    0.030153   -1.712979
    1       2.683002   -1.609526   -0.575459
    1       1.855901   -1.237163    1.015854
    1      -1.777216   -0.711339   -0.516513
    8      -2.299504   -1.444824   -0.169364
 ---------------------------------------------------------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 ---------------------------------------------------------------------
 Zero-point correction=                           0.127752 (Hartree/Particle)
 Thermal correction to Energy=                    0.136647
 Thermal correction to Enthalpy=                  0.137591
 Thermal correction to Gibbs Free Energy=         0.092769
 Sum of electronic and zero-point Energies=           -270.830903
 Sum of electronic and thermal Energies=              -270.822008
 Sum of electronic and thermal Enthalpies=            -270.821064
 Sum of electronic and thermal Free Energies=         -270.865886
 ---------------------------------------------------------------------
```

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pVDZ	-270.3611798
BD(T)/aug-cc-pVDZ	-270.3609402

Pathway: s-gauche carbon 2
Atoms: 15 Charge: 0 Multiplicity: 2

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1.063257	0.622780	2.016902
6	0.273033	0.151827	1.458246
6	0.011384	0.501919	0.202443
1	-0.292495	-0.615974	1.958613
6	0.815825	1.536155	-0.526689
6	-1.076076	-0.122628	-0.571283
1	0.179805	2.352759	-0.859862
1	1.276770	1.096902	-1.406597
1	1.600667	1.940988	0.100897
6	-2.268860	-0.446221	-0.098937
1	-0.861184	-0.292241	-1.616626
1	-3.012527	-0.905463	-0.727323
1	-2.544707	-0.249277	0.923680
1	1.158747	-2.014423	-0.047112
8	1.862479	-1.457796	-0.390657

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction=	0.127156 (Hartree/Particle)
Thermal correction to Energy=	0.136409
Thermal correction to Enthalpy=	0.137354
Thermal correction to Gibbs Free Energy=	0.091965
Sum of electronic and zero-point Energies=	-270.825895
Sum of electronic and thermal Energies=	-270.816641
Sum of electronic and thermal Enthalpies=	-270.815697
Sum of electronic and thermal Free Energies=	-270.861086

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pVDZ	-270.3566089
BD(T)/aug-cc-pVDZ	-270.3564147

Pathway: s-gauche carbon 3
Atoms: 15 Charge: 0 Multiplicity: 2

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	2.537842	-0.522485	-1.228245
6	1.890646	0.199694	-0.760162
6	0.929290	-0.176213	0.071795
1	2.069583	1.237231	-0.983432
6	0.696850	-1.610121	0.450678
6	0.027802	0.802635	0.705562
1	-0.317735	-1.909909	0.203190
1	0.819965	-1.746318	1.523435
1	1.390682	-2.269886	-0.056507

```
     6       -0.493652    1.870362    0.116910
     1       -0.238185    0.595695    1.733265
     1       -1.130363    2.550785    0.656081
     1       -0.290955    2.100009   -0.916323
     1       -2.069505   -0.047194   -0.348246
     8       -2.634617   -0.813258   -0.511490
 ---------------------------------------------------------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 ---------------------------------------------------------------------
 Zero-point correction=                           0.127558 (Hartree/Particle)
 Thermal correction to Energy=                    0.136438
 Thermal correction to Enthalpy=                  0.137383
 Thermal correction to Gibbs Free Energy=         0.093118
 Sum of electronic and zero-point Energies=           -270.827355
 Sum of electronic and thermal Energies=              -270.818475
 Sum of electronic and thermal Enthalpies=            -270.817531
 Sum of electronic and thermal Free Energies=         -270.861796
 ---------------------------------------------------------------------
 Single Point Energy Calculations (Hartrees)
 ---------------------------------------------------------------------
 UCCSD(T)/aug-cc-pVDZ                            -270.3562349
 BD(T)/aug-cc-pVDZ                               -270.3563176
=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=
 Pathway: s-trans carbon 3 and carbon 4
 Atoms: 15 Charge: 0 Multiplicity: 2
-----------------------------------------------
 Atomic               Coordinates (Angstroms)
 Number              X         Y       Z
-----------------------------------------------
    6       -1.948277   -0.365592   -0.836205
    1       -2.172873    0.232912   -1.703219
    1       -2.562472   -1.233763   -0.670301
    6       -0.958004   -0.044136   -0.010383
    6       -0.156039    1.149948   -0.287269
    1       -0.437357    1.700598   -1.172509
    6        0.858415    1.595887    0.445228
    1        1.178574    1.100878    1.346326
    6       -0.625002   -0.870262    1.195513
    1        0.388854   -1.254148    1.125956
    1       -0.692967   -0.278802    2.104968
    1       -1.302022   -1.710984    1.285709
    8        2.409644   -1.184754   -0.604160
    1        1.908116   -0.364936   -0.695405
    1        1.388429    2.491208    0.170452
 ---------------------------------------------------------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 ---------------------------------------------------------------------
 Zero-point correction=                           0.127998 (Hartree/Particle)
 Thermal correction to Energy=                    0.136741
 Thermal correction to Enthalpy=                  0.137685
 Thermal correction to Gibbs Free Energy=         0.093789
 Sum of electronic and zero-point Energies=           -270.831295
 Sum of electronic and thermal Energies=              -270.822552
 Sum of electronic and thermal Enthalpies=            -270.821608
 Sum of electronic and thermal Free Energies=         -270.865505
 ---------------------------------------------------------------------
 Single Point Energy Calculations (Hartrees)
 ---------------------------------------------------------------------
```

UCCSD(T)/aug-cc-pVDZ -270.3602278
BD(T)/aug-cc-pVDZ -270.3608253

=+=

Pathway: s-gauche carbon 4
Atoms: 15 Charge: 0 Multiplicity: 2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.648174	-0.957666	-0.601707
1	-1.357290	-1.990801	-0.682686
1	-2.563257	-0.665048	-1.088221
6	-0.924654	-0.084914	0.087117
6	0.341159	-0.458588	0.739225
1	0.548579	0.031275	1.678764
6	1.253091	-1.286080	0.242332
1	1.118292	-1.768172	-0.712181
6	-1.342584	1.344585	0.274476
1	-1.511785	1.556142	1.328365
1	-0.555462	2.014671	-0.059461
1	-2.254396	1.567247	-0.267278
8	2.087720	1.078035	-0.513698
1	1.642431	0.792842	-1.315266
1	2.158103	-1.506451	0.778892

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.127764 (Hartree/Particle)
Thermal correction to Energy= 0.136680
Thermal correction to Enthalpy= 0.137624
Thermal correction to Gibbs Free Energy= 0.093075
Sum of electronic and zero-point Energies= -270.824794
Sum of electronic and thermal Energies= -270.815878
Sum of electronic and thermal Enthalpies= -270.814934
Sum of electronic and thermal Free Energies= -270.859482

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pVDZ -270.3562874
BD(T)/aug-cc-pVDZ -270.356075

=+=

TS_structures:

=+=

Pathway: s-trans carbon 1 TS
Atoms: 15 Charge: 0 Multiplicity: 2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.079932	-0.102973	1.042534
1	-1.188738	-1.074208	1.492071
6	0.054027	0.246517	0.407366
6	1.125653	-0.728521	0.264657
1	0.947919	-1.686762	0.729845
6	2.274733	-0.531909	-0.374312
1	2.512174	0.401203	-0.855505

1	3.018337	-1.307459	-0.429363
6	0.216511	1.607984	-0.194135
1	1.081624	2.117930	0.222247
1	0.364906	1.541449	-1.268812
1	-0.662146	2.214384	-0.015652
8	-2.275355	-0.589691	-0.837086
1	-1.550093	-1.040694	-1.273856
1	-1.867093	0.605096	1.219054

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction=	0.127832	(Hartree/Particle)
Thermal correction to Energy=	0.135824	
Thermal correction to Enthalpy=	0.136768	
Thermal correction to Gibbs Free Energy=	0.094969	
Sum of electronic and zero-point Energies=	-270.829274	
Sum of electronic and thermal Energies=	-270.821282	
Sum of electronic and thermal Enthalpies=	-270.820338	
Sum of electronic and thermal Free Energies=	-270.862137	

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz	-270.3614852
BD(T)/aug-cc-pVDZ	-270.3624000

=+=

Pathway: s-gauche carbon 1 TS

Atoms: 15 Charge: 0 Multiplicity: 2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.300275	-0.818688	0.981991
1	1.028201	-0.281520	1.558597
6	-0.623976	-0.171563	0.246128
6	-0.565556	1.276953	0.032649
1	-1.517144	1.776158	-0.084842
6	0.552291	1.984395	-0.068536
1	1.517096	1.507960	-0.026664
1	0.524981	3.049904	-0.218442
6	-1.763189	-0.896807	-0.406829
1	-2.714235	-0.514695	-0.040805
1	-1.760809	-0.748148	-1.484631
1	-1.726208	-1.960869	-0.205845
8	1.950755	-1.039136	-0.508483
1	1.406810	-0.881859	-1.282381
1	0.236186	-1.879577	1.140466

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction=	0.127863	(Hartree/Particle)
Thermal correction to Energy=	0.135817	
Thermal correction to Enthalpy=	0.136761	
Thermal correction to Gibbs Free Energy=	0.095283	
Sum of electronic and zero-point Energies=	-270.825330	
Sum of electronic and thermal Energies=	-270.817376	
Sum of electronic and thermal Enthalpies=	-270.816432	
Sum of electronic and thermal Free Energies=	-270.857910	

```
---------------------------------------------------------------------
Single Point Energy Calculations (Hartrees)
---------------------------------------------------------------------
UCCSD(T)/aug-cc-pvdz                                   -270.3575308
BD(T)/aug-cc-pVDZ                                      -270.3582223
=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=
Pathway: s-trans carbon 2 TS
Atoms: 15 Charge: 0 Multiplicity: 2
-----------------------------------------------
 Atomic               Coordinates (Angstroms)
 Number              X        Y         Z
-----------------------------------------------
    1         -2.150224    0.271145   -1.324411
    6         -1.258112   -0.309529   -1.164089
    6         -0.265731    0.132998   -0.330214
    1         -1.194814   -1.273363   -1.636954
    6         -0.286590    1.541001     0.185629
    6            1.004530   -0.607382   -0.308749
    1            0.301602    2.186957   -0.461952
    1            0.123524    1.585484    1.185919
    1         -1.300475    1.922127     0.214154
    6            2.171553   -0.113220    0.067206
    1            0.942679   -1.629829   -0.644996
    1            3.061999   -0.716489    0.038081
    1            2.284150    0.897884    0.418221
    1         -1.980064   -0.728893     1.149539
    8         -1.035284   -0.797279     1.295463
---------------------------------------------------------------------
Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
---------------------------------------------------------------------
Zero-point correction=                             0.127896 (Hartree/Particle)
Thermal correction to Energy=                      0.135562
Thermal correction to Enthalpy=                    0.136506
Thermal correction to Gibbs Free Energy=           0.096268
Sum of electronic and zero-point Energies=             -270.821569
Sum of electronic and thermal Energies=                -270.813903
Sum of electronic and thermal Enthalpies=              -270.812959
Sum of electronic and thermal Free Energies=           -270.853197
---------------------------------------------------------------------
Single Point Energy Calculations (Hartrees)
---------------------------------------------------------------------
UCCSD(T)/aug-cc-pvdz                                   -270.3597772
BD(T)/aug-cc-pVDZ                                      -270.3604148
=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=
Pathway: s-gauche Carbon 2 TS
Atoms: 15 Charge: 0 Multiplicity: 2
--------------------------------------------
Atomic      Coordinates (Angstroms)
Number     X          Y        Z
--------------------------------------------
   1     1.214560   -0.280653    2.026146
   6     0.346020   -0.429412    1.410359
   6     0.204964      0.236532    0.232694
   1    -0.369628   -1.169802    1.722447
   6     1.131804      1.356388   -0.139790
   6    -1.037556      0.143538   -0.558934
   1     0.684411      2.309554    0.132394
   1     1.310719      1.357450   -1.208255
```

```
    1     2.083935      1.257035    0.366359
    6    -2.252639      0.000585   -0.057796
    1    -0.903930      0.235203   -1.624879
    1    -3.115555   -0.050100   -0.699257
    1    -2.428621   -0.058537    1.003252
    1     0.816929   -1.980936   -0.576447
    8     1.293953   -1.183125   -0.807620
-----------------------------------------
 ---------------------------------------------------------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 ---------------------------------------------------------------------
 Zero-point correction=                           0.128093 (Hartree/Particle)
 Thermal correction to Energy=                    0.135709
 Thermal correction to Enthalpy=                  0.136653
 Thermal correction to Gibbs Free Energy=         0.096493
 Sum of electronic and zero-point Energies=           -270.821156
 Sum of electronic and thermal Energies=              -270.813540
 Sum of electronic and thermal Enthalpies=            -270.812596
 Sum of electronic and thermal Free Energies=         -270.852756
 ---------------------------------------------------------------------
 Single Point Energy Calculations (Hartrees)
 ---------------------------------------------------------------------
 UCCSD(T)/aug-cc-pvdz                        -270.3586171
 BD(T)/aug-cc-pVDZ                           -270.3591754
 =+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=
 Pathway: s-trans carbon 3 TS
 Atoms: 15 Charge: 0 Multiplicity: 2
-----------------------------------------
  Atomic       Coordinates (Angstroms)
  Number      X         Y       Z
-----------------------------------------
     1       -2.764241   -0.800604   -0.043666
     6       -1.747381   -0.953277   -0.362373
     6       -0.808791   -0.041724   -0.147931
     1       -1.525364   -1.882661   -0.858972
     6       -1.079545    1.245426    0.566228
     6        0.560378   -0.300076   -0.616591
     1       -0.915720    2.104199   -0.080372
     1       -0.411689    1.335191    1.417391
     1       -2.102888    1.283381    0.919617
     6        1.462145    0.678009   -0.921419
     1        0.729808   -1.284345   -1.016275
     1        2.388690    0.435034   -1.411071
     1        1.304862    1.703248   -0.638609
     1        2.219211   -0.392478    1.151546
     8        1.344562   -0.783889    1.181616
 ---------------------------------------------------------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 ---------------------------------------------------------------------
 Zero-point correction=                           0.127985 (Hartree/Particle)
 Thermal correction to Energy=                    0.135720
 Thermal correction to Enthalpy=                  0.136664
 Thermal correction to Gibbs Free Energy=         0.095833
 Sum of electronic and zero-point Energies=           -270.822205
 Sum of electronic and thermal Energies=              -270.814471
 Sum of electronic and thermal Enthalpies=            -270.813526
 Sum of electronic and thermal Free Energies=         -270.854357
 ---------------------------------------------------------------------
```

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz	-270.3590966
BD(T)/aug-cc-pVDZ	-270.3596958

Pathway: s-gauche Carbon 3 TS
Atoms: 15 Charge: 0 Multiplicity: 2

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	2.377664	1.257447	-0.773049
6	1.359654	1.276357	-0.423121
6	0.791283	0.190907	0.085350
1	0.840696	2.216595	-0.490006
6	1.534271	-1.101253	0.245523
6	-0.601083	0.200181	0.580112
1	1.020487	-1.895582	-0.283268
1	1.572864	-1.388203	1.294619
1	2.550891	-1.018605	-0.120602
6	-1.552075	1.100331	0.219102
1	-0.784325	-0.402083	1.453556
1	-2.506679	1.114808	0.711740
1	-1.408204	1.770397	-0.611168
1	-1.482316	-0.902843	-1.357049
8	-1.421672	-1.343884	-0.508321

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction=	0.128190 (Hartree/Particle)
Thermal correction to Energy=	0.135795
Thermal correction to Enthalpy=	0.136739
Thermal correction to Gibbs Free Energy=	0.096196
Sum of electronic and zero-point Energies=	-270.820999
Sum of electronic and thermal Energies=	-270.813395
Sum of electronic and thermal Enthalpies=	-270.812451
Sum of electronic and thermal Free Energies=	-270.852994

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz	-270.3569632
BD(T)/aug-cc-pVDZ	-270.3576818

Pathway: s-trans carbon 4 TS
Atoms: 15 Charge: 0 Multiplicity: 2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.093039	-0.622094	-0.526610
1	2.137364	-1.676856	-0.740785
1	2.960485	-0.035953	-0.776354
6	1.011701	-0.071354	0.027555
6	-0.137373	-0.904435	0.340822
1	-0.061114	-1.943064	0.055915
6	-1.278189	-0.472916	0.910754
1	-1.382079	0.523644	1.294682
6	0.930061	1.397031	0.321013

1	0.065179	1.829488	-0.173563
1	0.818401	1.576782	1.387438
1	1.822031	1.910744	-0.016431
8	-2.274373	0.393602	-0.883478
1	-1.805740	-0.132213	-1.534796
1	-2.074972	-1.158776	1.130516

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction=	0.128119 (Hartree/Particle)
Thermal correction to Energy=	0.135869
Thermal correction to Enthalpy=	0.136814
Thermal correction to Gibbs Free Energy=	0.095721
Sum of electronic and zero-point Energies=	-270.829326
Sum of electronic and thermal Energies=	-270.821576
Sum of electronic and thermal Enthalpies=	-270.820631
Sum of electronic and thermal Free Energies=	-270.861724

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz	-270.36142
BD(T)/aug-cc-pVDZ	-270.3623016

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Pathway: s-gauche carbon 4 TS

Atoms: 15 Charge: 0 Multiplicity: 2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.349262	1.235653	-0.575085
1	0.750040	2.128371	-0.529873
1	2.263297	1.291861	-1.140658
6	0.994901	0.117138	0.053037
6	-0.247656	-0.003977	0.819768
1	-0.272423	-0.796964	1.551598
6	-1.363345	0.723350	0.647783
1	-1.415556	1.526513	-0.065003
6	1.867979	-1.105427	0.039766
1	2.160357	-1.376512	1.051833
1	1.336605	-1.958882	-0.374988
1	2.767805	-0.945707	-0.542111
8	-2.416235	-0.685569	-0.731323
1	-1.662472	-0.788849	-1.315122
1	-2.204630	0.604303	1.303288

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction=	0.127636 (Hartree/Particle)
Thermal correction to Energy=	0.135646
Thermal correction to Enthalpy=	0.136590
Thermal correction to Gibbs Free Energy=	0.094316
Sum of electronic and zero-point Energies=	-270.823460
Sum of electronic and thermal Energies=	-270.815451
Sum of electronic and thermal Enthalpies=	-270.814506
Sum of electronic and thermal Free Energies=	-270.856780

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz -270.3556477
BD(T)/aug-cc-pVDZ -270.3565181

Adduct Structures

Pathway: s-trans carbon 1
Atoms: 15 Charge: 0 Multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.223085	-0.624315	0.408460
2	1	0	-1.103842	-1.704772	0.342867
3	6	0	0.081900	0.049338	0.137636
4	6	0	1.230425	-0.710553	-0.006560
5	1	0	1.097466	-1.782785	0.020866
6	6	0	2.515943	-0.255192	-0.176204
7	1	0	2.757464	0.791770	-0.208526
8	1	0	3.330480	-0.948172	-0.284876
9	6	0	0.052796	1.540453	0.097147
10	1	0	-0.113925	1.950875	1.094122
11	1	0	0.970918	1.964702	-0.287986
12	1	0	-0.770796	1.873631	-0.525537
13	8	0	-2.190165	-0.166409	-0.516368
14	1	0	-3.050701	-0.426487	-0.210553
15	1	0	-1.543626	-0.385872	1.427690

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.131667 (Hartree/Particle)
Thermal correction to Energy= 0.139346
Thermal correction to Enthalpy= 0.140290
Thermal correction to Gibbs Free Energy= 0.099111
Sum of electronic and zero-point Energies= -270.881828
Sum of electronic and thermal Energies= -270.874149
Sum of electronic and thermal Enthalpies= -270.873205
Sum of electronic and thermal Free Energies= -270.914384

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz -270.4146273
BD(T)/aug-cc-pVDZ -270.4147371

Pathway: s-gauche carbon 1
Atoms: 15 Charge: 0 Multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.712826	-0.844001	0.348145
2	1	0	-0.145931	-1.729890	0.074600
3	6	0	0.074297	0.395064	0.071327
4	6	0	1.450727	0.380266	-0.090930
5	1	0	1.913346	1.344362	-0.245451
6	6	0	2.294201	-0.704853	-0.072730
7	1	0	1.947464	-1.711800	0.073578

8	1	0	3.351543	-0.572863	-0.214446
9	6	0	-0.694874	1.673678	0.046144
10	1	0	-0.044244	2.522873	-0.130138
11	1	0	-1.458651	1.648134	-0.725224
12	1	0	-1.217104	1.833939	0.989849
13	8	0	-1.927609	-0.790885	-0.371296
14	1	0	-2.479491	-1.509193	-0.087065
15	1	0	-0.915209	-0.899399	1.422932

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.131782 (Hartree/Particle)
Thermal correction to Energy= 0.139342
Thermal correction to Enthalpy= 0.140286
Thermal correction to Gibbs Free Energy= 0.099629
Sum of electronic and zero-point Energies= -270.880944
Sum of electronic and thermal Energies= -270.873385
Sum of electronic and thermal Enthalpies= -270.872441
Sum of electronic and thermal Free Energies= -270.913098

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz -270.4138014
BD(T)/aug-cc-pVDZ -270.4139097

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Pathway: s-trans carbon 2
Atoms: 15 Charge: 0 Multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.783703	-0.033798	2.209792
2	6	0	0.942695	-0.559517	1.284802
3	6	0	0.392288	-0.024079	0.002532
4	1	0	1.269618	-1.584471	1.319233
5	6	0	0.402840	1.498043	-0.014570
6	6	0	-0.981964	-0.619712	-0.180715
7	1	0	-0.172204	1.913594	0.806466
8	1	0	-0.003968	1.859563	-0.951675
9	1	0	1.423583	1.857002	0.082333
10	6	0	-2.140831	-0.013296	-0.002583
11	1	0	-0.952826	-1.660836	-0.462493
12	1	0	-3.067245	-0.545343	-0.134067
13	1	0	-2.216319	1.024431	0.273768
14	1	0	2.062857	-0.314641	-0.938261
15	8	0	1.147829	-0.525516	-1.092736

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.130182 (Hartree/Particle)
Thermal correction to Energy= 0.137655
Thermal correction to Enthalpy= 0.138599
Thermal correction to Gibbs Free Energy= 0.099128
Sum of electronic and zero-point Energies= -270.857463
Sum of electronic and thermal Energies= -270.849991
Sum of electronic and thermal Enthalpies= -270.849047
Sum of electronic and thermal Free Energies= -270.888518

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz	-270.3956366
BD(T)/aug-cc-pVDZ	-270.3955066

Pathway: s-gauche carbon 2
Atoms: 15 Charge: 0 Multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.199120	1.827402	-0.999888
2	6	0	0.336435	1.437847	-0.488800
3	6	0	0.362518	0.035444	0.014533
4	1	0	-0.399418	2.136075	-0.129129
5	6	0	1.123168	-0.879401	-0.934894
6	6	0	-1.005246	-0.533697	0.291939
7	1	0	0.640013	-0.912712	-1.904832
8	1	0	1.166313	-1.883383	-0.526421
9	1	0	2.139017	-0.516026	-1.051304
10	6	0	-2.164255	-0.056153	-0.119039
11	1	0	-0.975813	-1.437395	0.883201
12	1	0	-3.087431	-0.553864	0.124271
13	1	0	-2.237780	0.834528	-0.720121
14	1	0	0.688097	0.553481	1.869553
15	8	0	1.119021	-0.009043	1.234030

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction=	0.130200 (Hartree/Particle)
Thermal correction to Energy=	0.137729
Thermal correction to Enthalpy=	0.138673
Thermal correction to Gibbs Free Energy=	0.099008
Sum of electronic and zero-point Energies=	-270.857799
Sum of electronic and thermal Energies=	-270.850271
Sum of electronic and thermal Enthalpies=	-270.849327
Sum of electronic and thermal Free Energies=	-270.888992

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz	-270.39626
BD(T)/aug-cc-pVDZ	-270.3960187

Pathway: s-trans carbon 3
Atoms: 15 Charge: 0 Multiplicity: 2
Geometry and frequencies from c3_180_reverse.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.737554	-0.790731	-0.181562
2	6	0	1.691462	-0.989342	-0.343816
3	6	0	0.764856	-0.092340	-0.052942
4	1	0	1.436860	-1.952040	-0.755287
5	6	0	1.081659	1.266547	0.490727
6	6	0	-0.701747	-0.415967	-0.249548
7	1	0	0.615881	1.420093	1.461064
8	1	0	0.695945	2.032786	-0.173217

9	1	0	2.151584	1.399891	0.601293
10	6	0	-1.386877	-0.637017	1.053646
11	1	0	-0.761232	-1.329953	-0.841177
12	1	0	-1.357550	-1.603278	1.524598
13	1	0	-1.730810	0.209430	1.622963
14	1	0	-2.223770	0.529257	-0.979168
15	8	0	-1.282574	0.661658	-0.958488

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.130614 (Hartree/Particle)
Thermal correction to Energy= 0.138232
Thermal correction to Enthalpy= 0.139176
Thermal correction to Gibbs Free Energy= 0.098994
Sum of electronic and zero-point Energies= -270.858703
Sum of electronic and thermal Energies= -270.851085
Sum of electronic and thermal Enthalpies= -270.850141
Sum of electronic and thermal Free Energies= -270.890322

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz -270.3954019
BD(T)/aug-cc-pVDZ -270.395191

=+=

Pathway: s-gauche carbon 3
Atoms: 15 Charge: 0 Multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.088023	1.760780	-0.396960
2	6	0	1.059844	1.497794	-0.212155
3	6	0	0.714355	0.249908	0.058574
4	1	0	0.344256	2.300210	-0.241023
5	6	0	1.722025	-0.858436	0.130801
6	6	0	-0.708342	-0.163679	0.365788
7	1	0	1.492812	-1.641579	-0.583660
8	1	0	1.705812	-1.324085	1.114312
9	1	0	2.723771	-0.490153	-0.057543
10	6	0	-1.747712	0.870872	0.129948
11	1	0	-0.742054	-0.472628	1.407999
12	1	0	-2.686641	0.799182	0.648714
13	1	0	-1.692675	1.517548	-0.728818
14	1	0	-1.101694	-1.143512	-1.267360
15	8	0	-1.046580	-1.360564	-0.341675

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.130802 (Hartree/Particle)
Thermal correction to Energy= 0.138410
Thermal correction to Enthalpy= 0.139354
Thermal correction to Gibbs Free Energy= 0.098896
Sum of electronic and zero-point Energies= -270.857053
Sum of electronic and thermal Energies= -270.849446
Sum of electronic and thermal Enthalpies= -270.848502
Sum of electronic and thermal Free Energies= -270.888959

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz	-270.3937281
BD(T)/aug-cc-pVDZ	-270.3934871

Pathway: s-trans carbon 4
Atoms: 15 Charge: 0 Multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.217025	-0.618133	-0.276110
2	1	0	2.337377	-1.681839	-0.389023
3	1	0	3.087248	-0.002106	-0.417738
4	6	0	0.993811	-0.074121	0.031882
5	6	0	-0.118902	-0.891560	0.202060
6	1	0	0.004147	-1.953166	0.066044
7	6	0	-1.488571	-0.382751	0.490115
8	1	0	-1.453670	0.343876	1.303904
9	6	0	0.854523	1.418582	0.186923
10	1	0	0.026097	1.787098	-0.407019
11	1	0	0.661616	1.685216	1.223712
12	1	0	1.759568	1.928012	-0.121947
13	8	0	-2.022179	0.224189	-0.677400
14	1	0	-2.870329	0.594849	-0.459733
15	1	0	-2.121940	-1.207559	0.811776

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction=	0.131773 (Hartree/Particle)
Thermal correction to Energy=	0.139221
Thermal correction to Enthalpy=	0.140165
Thermal correction to Gibbs Free Energy=	0.099905
Sum of electronic and zero-point Energies=	-270.877459
Sum of electronic and thermal Energies=	-270.870011
Sum of electronic and thermal Enthalpies=	-270.869067
Sum of electronic and thermal Free Energies=	-270.909327

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz	-270.4114012
BD(T)/aug-cc-pVDZ	-270.4115132

Pathway: s-gauche carbon 4
Atoms: 15 Charge: 0 Multiplicity: 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.336558	1.393173	-0.004116
2	1	0	0.560203	2.137856	-0.002233
3	1	0	2.351308	1.749483	-0.008320
4	6	0	1.055626	0.050886	-0.001651
5	6	0	-0.246713	-0.439108	0.002751
6	1	0	-0.421499	-1.502200	0.004566
7	6	0	-1.473258	0.402245	0.009338
8	1	0	-1.478775	1.066560	-0.859342
9	6	0	2.184946	-0.949600	0.000389
10	1	0	2.108903	-1.624288	-0.847363

11	1	0	3.148638	-0.455919	-0.049481
12	1	0	2.165204	-1.555772	0.901744
13	8	0	-2.588632	-0.458280	-0.009548
14	1	0	-3.380067	0.065651	-0.001829
15	1	0	-1.487819	1.039293	0.898368

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction=	0.130796 (Hartree/Particle)
Thermal correction to Energy=	0.138715
Thermal correction to Enthalpy=	0.139659
Thermal correction to Gibbs Free Energy=	0.096335
Sum of electronic and zero-point Energies=	-270.878613
Sum of electronic and thermal Energies=	-270.870694
Sum of electronic and thermal Enthalpies=	-270.869750
Sum of electronic and thermal Free Energies=	-270.913074

Single Point Energy Calculations (Hartrees)

UCCSD(T)/aug-cc-pvdz	-270.4114564
BD(T)/aug-cc-pVDZ	-270.4115621