Supporting Information: Mechanical manipulation of chemical reactions: Reactivity switching of Bergman cyclizations

Martin Krupička, Wolfram Sander and Dominik Marx

January 29, 2014

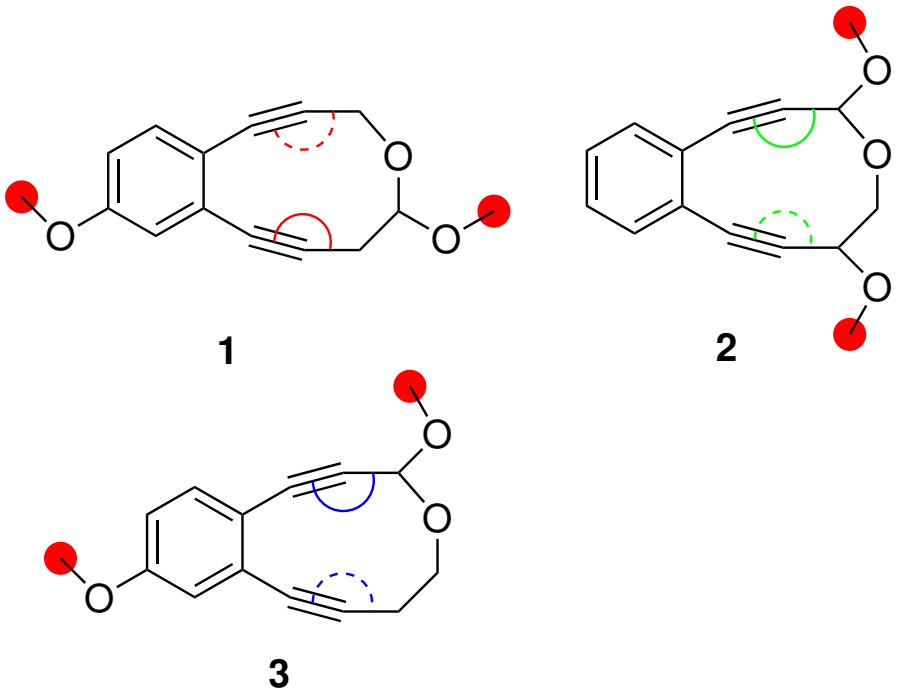

Figure 1: Definition of the two angles (solid and dashed lines) to be analyzed as a function of force for the three species **1**, **2**, and **3** considered in this study keeping the same color coding as in the main text.

1 Analysis of Force–induced Deformations

In order to analyze in more detail the structural distortion of the three species as a function of constant force we chose the angles around the reactive carbons, see Fig 1, to describe the force-induced deformation of the transition state (TS) structures. In the reactant state (RS), the optimum dihedral angles for the carbon-carbon triple bonds, i.e. 180°, are distorted to about 170° due to their inclusion in 10-membered rings. In the biradical product, this angle should be ideally 120° (we observed 122–128° in all three product configurations). At intermediate structures, including the TS being a well-defined a stationary point, the precise value of this angle depends on both the particular substitution pattern and, of course, on the magnitude of the external force as shown in Fig 2. The data reveal most clearly that the TS of species **3** becomes very asymmetric, which is the very reason for the strong increase of the reaction barrier in the absence of any change in reaction mechanism.

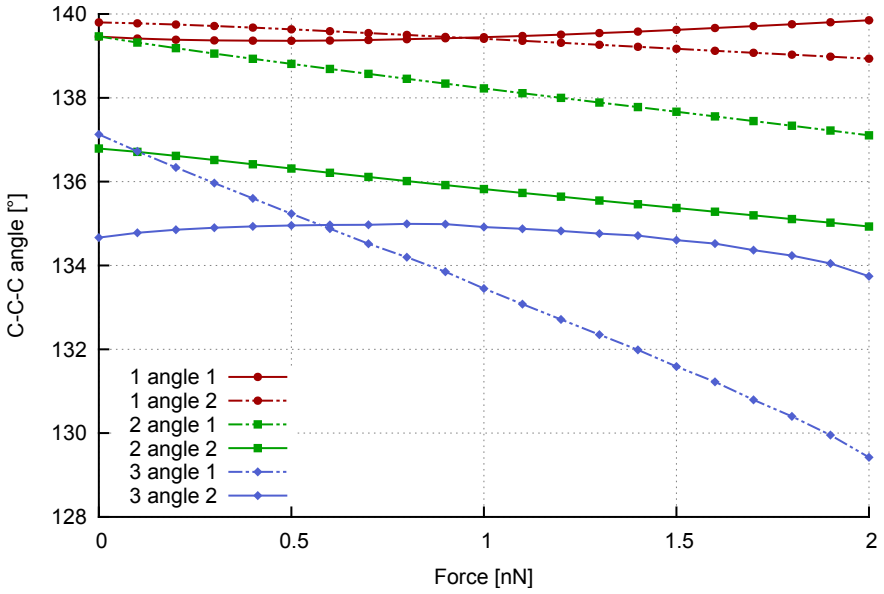

Figure 2: C–C–C angles at both reactive carbons (solid and dashed lines) for species **1** (red circles), **2** (green squares), and **3** (blue diamonds) at the TS as a function of force, see Fig. 1 for species and angle labeling.

2 Decomposition of Isotensional Energies into Structural Distortion and Mechanical Work Contributions

Within the applied EFEI mechanochemical framework, the total energy $E_{\text{total}}(\mathbf{F}_0)$ is defined as: $E_{\text{total}}(\mathbf{F}_0) = E_{\text{ES}} - \mathbf{F}_0\mathbf{q}$, where E_{ES} is the electronic structure energy, $\mathbf{F}_0$ is the constant external force that acts on $\mathbf{q}$ being the mechanical coordinate. The EFEI energy, $E_{\text{total}}(\mathbf{F}_0)$, is optimized with respect to all degrees of freedom to find stationary points at any given $\mathbf{F}_0$. As $E_{\text{total}}(F_0)$ depends on the magnitude of external force, $F_0 = |\mathbf{F}_0|$, the results obtained at different forces cannot be directly compared. On the other hand, the change in electronic energy E_{ES} of stationary points at different values of F_0 can be used as a measure of the deformation that is caused as a response of the molecule to applying the external force.

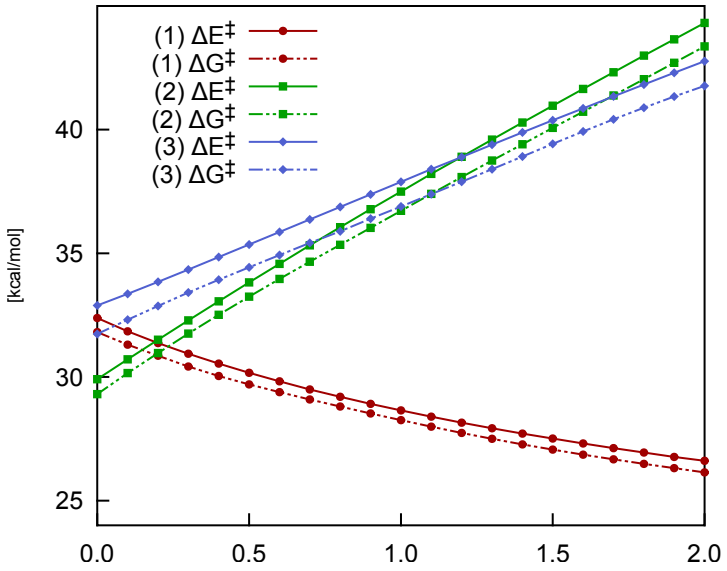

Figure 3: Activation energy $\Delta E^{\ddagger}$ and activation free energy $\Delta G^{\ddagger}$ for species **1** (red circles), **2** (green squares), and **3** (blue diamonds) as a function of force.

3 Activation Energy and Free Energy as a Function of Force

The activation energies and activation free energies are shown in Fig. 3 from the thermal (zero-force) limit up to 2 nN for the three species undergoing Bergman cyclization. The Gibbs free energy was calculated with Gaussian 09[35] using the standard rigid rotor and harmonic oscillator approximations at 300 K as implemented therein.

4 Force-transformed Structures

Optimized stationary point structures at reactant, transition and product states of species **1**, **2** and **3** at representative values of the external force, namely zero force (i.e. thermal limit), 1 and 2 nN.

1 Reactant 0 nN

32

```
C -2.397865 1.636197 -0.193293
C -1.205605 0.917366 -0.209221
C -1.266036 -0.510740 -0.214455
C -2.502379 -1.145064 -0.204747
C -3.684790 -0.401310 -0.189648
C -3.632167 0.993760 -0.182414
H -2.361011 2.717940 -0.190526
H -2.564037 -2.224744 -0.209529
H -4.535112 1.586668 -0.170319
C -0.026880 -1.211718 -0.224764
C 0.086570 1.510059 -0.229935
C 1.267016 1.755213 -0.260109
C 1.131966 -1.543333 -0.233298
C 2.725649 1.779559 -0.328195
H 3.070770 2.487557 -1.083964
H 3.147607 2.094584 0.634531
C 2.568543 -1.766558 -0.201560
H 2.822943 -2.580407 0.481699
H 2.944871 -2.042955 -1.190313
C 3.337818 -0.513387 0.255643
H 2.928895 -0.132753 1.203438
O 3.269832 0.512318 -0.724757
O 4.663391 -0.931102 0.430219
C 5.537785 0.061767 0.947231
H 6.500145 -0.421818 1.103907
H 5.662670 0.889738 0.244682
H 5.172817 0.450263 1.906857
O -4.835454 -1.130188 -0.182274
C -6.079234 -0.442467 -0.174375
H -6.844739 -1.214885 -0.171980
H -6.188998 0.177178 0.720761
H -6.197997 0.180792 -1.065839
```

1 TS Bergman 0 nN

32

```
C -2.087998 -0.739883 -0.190265
```

```
C -0.704991 -0.534399 -0.208112
C -0.232736 0.887835 -0.309525
C -1.197520 1.894533 -0.364734
C -2.559024 1.618267 -0.333242
C -3.005337 0.295253 -0.246241
H -2.446253 -1.758231 -0.126603
H -0.882500 2.925981 -0.432213
H -4.060183 0.062880 -0.223599
C 1.144928 1.070995 -0.335737
C 0.284445 -1.507159 -0.164087
C 1.558801 -1.420841 -0.183322
C 2.120411 0.248157 -0.265356
C 2.763450 -2.306706 -0.224690
H 3.290781 -2.307666 0.735565
H 2.444073 -3.323289 -0.440574
C 3.605603 0.260108 -0.138374
H 3.970441 1.267664 -0.327515
H 3.886420 0.007000 0.888192
C 4.345023 -0.717438 -1.061215
H 4.483465 -0.297536 -2.063652
O 3.644135 -1.927198 -1.279162
O 5.596877 -0.933254 -0.457371
C 6.528541 -1.629712 -1.279304
H 7.455462 -1.695493 -0.712639
H 6.174393 -2.634884 -1.519078
H 6.715415 -1.082922 -2.211313
O -3.380890 2.703999 -0.393122
C -4.786928 2.500003 -0.362528
H -5.230856 3.491164 -0.419167
H -5.125139 1.904502 -1.215918
H -5.102303 2.016524 0.567062
```

1 TS C1–C5 0 nN

```
32

C -2.115839 1.479862 0.027686
C -1.113365 0.532812 -0.085282
C -1.447020 -0.851087 -0.109814
C -2.763338 -1.261154 -0.026201
C -3.769786 -0.291547 0.082862
C -3.448799 1.068563 0.109152
H -1.880690 2.535965 0.048493
H -3.036291 -2.307434 -0.044267
H -4.223502 1.816813 0.191714
C -0.220659 -1.595594 -0.228891
C 0.330297 0.699295 -0.172926
```

```
C 1.220751 1.600421 -0.141639
C 0.911201 -0.986208 -0.302327
C 2.639268 1.948277 -0.122566
H 2.851236 2.782499 -0.793599
H 2.924316 2.260422 0.892953
C 2.349325 -1.290277 -0.509385
H 2.537920 -2.295168 -0.129184
H 2.585940 -1.294588 -1.577580
C 3.350147 -0.344599 0.156731
H 3.056666 -0.110606 1.193601
O 3.479344 0.880461 -0.569091
O 4.580638 -0.994854 0.133064
C 5.625359 -0.316270 0.822016
H 6.493484 -0.971449 0.787520
H 5.866621 0.634558 0.342824
H 5.352110 -0.137265 1.869465
O -5.040723 -0.779925 0.157392
C -6.120776 0.136562 0.263080
H -7.022118 -0.470699 0.304057
H -6.049339 0.738048 1.174532
H -6.171006 0.799124 -0.606426
```

1 Product 0 nN

32

```
C -2.528402 1.679952 -0.034920
C -1.303041 0.986630 -0.104844
C -1.343497 -0.475703 -0.088424
C -2.591628 -1.119960 -0.008516
C -3.764556 -0.395103 0.056106
C -3.730856 1.017222 0.042727
H -2.511081 2.762281 -0.043108
H -2.639631 -2.200428 0.002072
H -4.645719 1.589811 0.093909
C -0.104402 -1.117960 -0.158392
C -0.036245 1.566465 -0.177824
C 1.138385 0.922023 -0.247598
C 1.104151 -0.537756 -0.248905
C 2.524869 1.511346 -0.256040
H 2.971478 1.458017 -1.256429
H 2.511593 2.551980 0.059401
C 2.436199 -1.222272 -0.406732
H 2.368825 -2.273815 -0.133141
H 2.731058 -1.185572 -1.460100
C 3.570226 -0.554734 0.391830
```

```
H 3.695628 -1.021103 1.375483
O 3.340343 0.811722 0.688216
O 4.741437 -0.738514 -0.368616
C 5.941280 -0.398873 0.318353
H 6.763023 -0.623536 -0.359308
H 5.964173 0.660975 0.582062
H 6.054622 -0.997385 1.230476
O -4.916676 -1.122433 0.131277
C -6.161264 -0.439868 0.194178
H -6.921020 -1.216431 0.245186
H -6.231542 0.189787 1.086331
H -6.331879 0.170881 -0.697586
```

1 Reactant 1 nN

```
32

C -2.492856 1.702850 -0.307069
C -1.302210 0.994434 -0.152940
C -1.371325 -0.421189 0.053760
C -2.620952 -1.043895 0.090114
C -3.807821 -0.309124 -0.072690
C -3.734783 1.071132 -0.268038
H -2.449545 2.772866 -0.464877
H -2.689850 -2.113011 0.239888
H -4.631583 1.661773 -0.394706
C -0.114788 -1.096554 0.189076
C -0.001357 1.575275 -0.202423
C 1.189006 1.777683 -0.203984
C 1.067352 -1.349439 0.231804
C 2.652314 1.825301 -0.207594
H 3.008786 2.552792 -0.939454
H 3.020055 2.142653 0.776968
C 2.503491 -1.627364 0.215533
H 2.757142 -2.358055 0.988029
H 2.778372 -2.075377 -0.743780
C 3.449614 -0.411615 0.413741
H 3.301130 0.046733 1.404162
O 3.267284 0.583181 -0.584380
O 4.739111 -0.962769 0.305432
C 5.874409 -0.127197 0.578210
H 6.746255 -0.769086 0.476380
H 5.938325 0.696604 -0.136296
H 5.833434 0.272869 1.598287
O -4.972035 -1.027815 -0.025754
C -6.250088 -0.391640 -0.201381
H -6.980254 -1.192737 -0.124746
```

```
H -6.433747 0.350278 0.580705
H -6.324047 0.082256 -1.184072
```

1 TS Bergman 1 nN

```
32

C -2.111589 -0.751429 -0.224288
C -0.730543 -0.537418 -0.318454
C -0.277726 0.884219 -0.505530
C -1.268833 1.877653 -0.554577
C -2.631930 1.595952 -0.430248
C -3.047275 0.269535 -0.269303
H -2.453720 -1.769587 -0.098179
H -0.968875 2.908443 -0.681208
H -4.096491 0.024784 -0.177384
C 1.104859 1.061806 -0.605278
C 0.269014 -1.502457 -0.268392
C 1.543329 -1.411983 -0.331707
C 2.094726 0.248479 -0.536291
C 2.752961 -2.293633 -0.245735
H 3.228171 -2.205368 0.737592
H 2.440740 -3.326048 -0.382774
C 3.591795 0.279639 -0.389163
H 3.951713 1.259677 -0.696856
H 3.838087 0.173253 0.671656
C 4.402190 -0.803543 -1.139754
H 4.624742 -0.498336 -2.167558
O 3.697367 -2.020967 -1.278775
O 5.610519 -0.952104 -0.416038
C 6.680156 -1.668250 -1.062401
H 7.524571 -1.627150 -0.378193
H 6.403302 -2.708551 -1.247590
H 6.953167 -1.189593 -2.009330
O -3.480855 2.670048 -0.477887
C -4.902363 2.504350 -0.331528
H -5.313753 3.508174 -0.394595
H -5.314666 1.887117 -1.134512
H -5.151992 2.064137 0.637828
```

1 TS C1–C5 1 nN

```
32

C -2.178464 1.496469 0.028538
C -1.152021 0.563704 0.014594
C -1.473312 -0.823786 0.025464
```

```
C -2.795219 -1.243897 0.041640
C -3.829541 -0.288931 0.042994
C -3.514755 1.073490 0.039983
H -1.960711 2.556704 0.020287
H -3.051327 -2.294842 0.042999
H -4.300154 1.817115 0.042083
C -0.227032 -1.555524 -0.009519
C 0.300906 0.734134 -0.013359
C 1.207795 1.620987 0.010356
C 0.907647 -0.939681 -0.062587
C 2.636198 1.943506 0.021220
H 2.839544 2.819041 -0.597864
H 2.945902 2.187981 1.047932
C 2.348371 -1.272864 -0.300625
H 2.536308 -2.251321 0.144368
H 2.514884 -1.375979 -1.377177
C 3.459476 -0.327015 0.197365
H 3.362835 -0.110596 1.274964
O 3.468884 0.909610 -0.514635
O 4.660007 -0.996477 -0.073313
C 5.893922 -0.389203 0.349846
H 6.673050 -1.107779 0.107053
H 6.073534 0.547706 -0.180120
H 5.889894 -0.205956 1.430602
O -5.100433 -0.801623 0.045661
C -6.260367 0.044058 0.010428
H -7.109324 -0.634403 0.007436
H -6.308155 0.689438 0.892342
H -6.275565 0.658134 -0.894644
```

1 Product 1 nN

32

```
C -2.543958 1.674043 -0.038745
C -1.317192 0.974543 -0.053289
C -1.363953 -0.487488 -0.005996
C -2.630881 -1.118300 0.043460
C -3.810476 -0.387402 0.043658
C -3.756514 1.024121 0.005644
H -2.518760 2.755942 -0.068368
H -2.686004 -2.198388 0.074028
H -4.667873 1.606256 0.009951
C -0.112072 -1.125838 -0.029689
C -0.046000 1.550765 -0.115003
C 1.134275 0.909594 -0.157241
C 1.106455 -0.549235 -0.116825
```

```
C 2.516140 1.513135 -0.240960
H 2.903657 1.448097 -1.265117
H 2.503076 2.559884 0.053849
C 2.453574 -1.230318 -0.288347
H 2.408800 -2.263189 0.053563
H 2.686727 -1.262864 -1.357265
C 3.648516 -0.516323 0.397117
H 3.854094 -0.945880 1.383427
O 3.406923 0.853165 0.663830
O 4.773638 -0.716267 -0.441983
C 6.067555 -0.436829 0.124637
H 6.794130 -0.702768 -0.639921
H 6.168156 0.620697 0.379371
H 6.240425 -1.044579 1.019968
O -4.980785 -1.101458 0.082541
C -6.262390 -0.449181 0.058699
H -6.991151 -1.254911 0.085929
H -6.397367 0.196178 0.931122
H -6.394855 0.134526 -0.856479
```

1 Reactant 2 nN

32

```
C -2.523879 1.684889 -0.382677
C -1.332038 0.985854 -0.185682
C -1.402435 -0.423406 0.073852
C -2.664622 -1.039235 0.116406
C -3.860125 -0.310951 -0.087566
C -3.770830 1.059864 -0.335384
H -2.477886 2.748252 -0.580409
H -2.736580 -2.102008 0.306770
H -4.663011 1.650509 -0.496374
C -0.124458 -1.072852 0.250395
C -0.029412 1.571349 -0.230020
C 1.163022 1.767097 -0.198545
C 1.074323 -1.258852 0.309925
C 2.626067 1.864862 -0.130620
H 2.982366 2.636930 -0.815326
H 2.928065 2.160606 0.882818
C 2.524161 -1.533666 0.294379
H 2.768474 -2.256864 1.077070
H 2.780387 -2.007828 -0.657492
C 3.534205 -0.344909 0.454371
H 3.458326 0.103331 1.457512
O 3.329952 0.672581 -0.518913
O 4.801317 -0.942760 0.261437
```

```
C 6.045686 -0.238088 0.539991
H 6.829707 -0.962376 0.336682
H 6.156078 0.629004 -0.113981
H 6.090370 0.075352 1.588140
O -5.039006 -1.020479 -0.025195
C -6.358860 -0.428338 -0.220876
H -7.048538 -1.259338 -0.107897
H -6.559950 0.334116 0.535478
H -6.447929 0.002607 -1.220939
```

1 TS Bergman 2 nN

32

```
C -2.120539 -0.745814 -0.240042
C -0.738335 -0.529103 -0.345521
C -0.290222 0.896853 -0.524935
C -1.299967 1.885674 -0.557555
C -2.670281 1.601742 -0.421812
C -3.066159 0.268176 -0.267223
H -2.456465 -1.766501 -0.117139
H -1.004940 2.918695 -0.680758
H -4.112700 0.012677 -0.165928
C 1.101137 1.063026 -0.638786
C 0.262174 -1.496476 -0.312663
C 1.538279 -1.407808 -0.383339
C 2.095442 0.244943 -0.594247
C 2.744680 -2.294700 -0.253675
H 3.195207 -2.183451 0.738874
H 2.426475 -3.327777 -0.369729
C 3.609533 0.262304 -0.455094
H 3.972980 1.229949 -0.796328
H 3.850558 0.196187 0.610117
C 4.441275 -0.854119 -1.161597
H 4.674318 -0.580959 -2.195590
O 3.722559 -2.066485 -1.267763
O 5.655478 -0.987172 -0.424205
C 6.799203 -1.675725 -1.018723
H 7.604030 -1.567401 -0.296525
H 6.576636 -2.732136 -1.180557
H 7.082342 -1.206483 -1.966036
O -3.539421 2.670566 -0.452472
C -4.986973 2.547790 -0.306402
H -5.352535 3.568466 -0.366320
H -5.411510 1.947957 -1.114885
H -5.245687 2.111052 0.661091
```

1 TS C1–C5 2 nN

32

C -2.210180 1.507333 0.004562
C -1.171296 0.584097 0.014728
C -1.489031 -0.804205 0.040240
C -2.817792 -1.226653 0.047022
C -3.869920 -0.280910 0.026030
C -3.549089 1.080933 0.007498
H -2.001084 2.569350 -0.015312
H -3.065272 -2.279860 0.060760
H -4.334505 1.825649 -0.008652
C -0.227381 -1.526304 0.033046
C 0.288875 0.754503 0.007178
C 1.207339 1.631981 0.035514
C 0.910980 -0.906163 -0.006299
C 2.641413 1.942184 0.074855
H 2.853585 2.835862 -0.514508
H 2.932763 2.158356 1.113247
C 2.367559 -1.251558 -0.231372
H 2.543083 -2.220763 0.238325
H 2.521596 -1.390084 -1.305600
C 3.525809 -0.313375 0.218681
H 3.490204 -0.111823 1.302566
O 3.496326 0.931477 -0.476759
O 4.713382 -0.989107 -0.129911
C 6.025734 -0.462159 0.231605
H 6.731934 -1.210720 -0.116737
H 6.209381 0.492244 -0.263561
H 6.111654 -0.344163 1.316641
O -5.144399 -0.807378 0.025137
C -6.376026 -0.031609 -0.016173
H -7.166837 -0.775795 -0.011053
H -6.461441 0.614404 0.861267
H -6.429494 0.568837 -0.927808

1 Product 2 nN

32

C -2.556133 1.667778 -0.033992
C -1.329168 0.963580 -0.038313
C -1.380908 -0.498617 0.007188
C -2.665243 -1.117872 0.045040
C -3.851009 -0.381662 0.035096
C -3.776541 1.029395 -0.001311
H -2.523915 2.749614 -0.062846
H -2.726398 -2.197975 0.075334

```
H -4.682445 1.621377 -0.005092
C -0.115833 -1.131676 -0.005279
C -0.055169 1.539519 -0.091638
C 1.130588 0.904108 -0.128143
C 1.111355 -0.554634 -0.081969
C 2.508913 1.518412 -0.247341
H 2.865729 1.447742 -1.282232
H 2.491120 2.568297 0.035864
C 2.483265 -1.218727 -0.258897
H 2.457325 -2.247956 0.095901
H 2.697246 -1.263129 -1.331431
C 3.700188 -0.485623 0.398166
H 3.912292 -0.894409 1.391472
O 3.442413 0.886210 0.635699
O 4.834739 -0.701515 -0.441851
C 6.178346 -0.476582 0.085313
H 6.852911 -0.790462 -0.707024
H 6.334828 0.578571 0.318052
H 6.348021 -1.082659 0.980955
O -5.038606 -1.083246 0.063090
C -6.360433 -0.464532 0.039284
H -7.050900 -1.302306 0.062472
H -6.511859 0.170634 0.915305
H -6.504882 0.115947 -0.875029
```

2 Reactant 0 nN

```
32

C -2.396049 1.531839 0.061343
C -1.172351 0.877578 -0.099316
C -1.136499 -0.547909 -0.098733
C -2.329010 -1.258583 0.059861
C -3.534860 -0.587747 0.218445
C -3.568722 0.804417 0.219140
H -2.418206 2.613850 0.060241
H -2.300037 -2.340403 0.057465
H -4.510513 1.324326 0.342020
C 0.133420 -1.169266 -0.256785
C 0.066172 1.554782 -0.274380
C 1.210685 1.881350 -0.468934
C 1.299897 -1.449847 -0.379382
C 2.671880 1.981704 -0.665994
H 3.145223 2.245332 0.295725
C 2.753129 -1.572456 -0.523746
H 2.991240 -1.806375 -1.571335
C 3.458999 -0.248986 -0.160764
```

```
H 3.147780 0.055967 0.840754
O 3.184623 0.752973 -1.132950
H -4.450620 -1.152460 0.340812
H 4.533768 -0.445873 -0.151779
O 3.043178 2.914105 -1.644673
C 2.697768 4.252304 -1.318393
H 3.073368 4.872115 -2.129687
H 1.613598 4.381500 -1.236428
H 3.167047 4.568735 -0.378095
O 3.328242 -2.551091 0.332757
C 2.939742 -3.882606 0.032736
H 3.212731 -4.153679 -0.994813
H 3.475196 -4.528203 0.726686
H 1.862127 -4.026069 0.164171
```

2 TS Bergman 0 nN

```
32

C -2.121380 1.541625 0.127712
C -0.882407 0.912869 -0.059729
C -0.848576 -0.563800 -0.069440
C -2.058361 -1.249524 0.111624
C -3.254074 -0.578873 0.296381
C -3.285921 0.816050 0.303865
H -2.149667 2.622836 0.133201
H -2.038487 -2.330896 0.105456
H -4.224538 1.336448 0.447527
C 0.402002 -1.154622 -0.267051
C 0.342875 1.557880 -0.249752
C 1.531059 1.166529 -0.461847
C 1.585019 -0.724383 -0.426669
C 2.885986 1.813760 -0.683967
H 3.200057 2.257501 0.278195
C 2.982657 -1.254880 -0.573659
H 3.100500 -1.598445 -1.610953
C 4.047651 -0.198550 -0.296669
H 4.025903 0.076623 0.764399
O 3.871290 0.928291 -1.134609
H -4.168044 -1.142910 0.434353
H 5.027567 -0.613031 -0.525678
O 2.828457 2.800279 -1.666506
C 2.249944 4.027949 -1.252929
H 2.368443 4.716344 -2.087093
H 1.185032 3.909783 -1.024557
H 2.764042 4.431457 -0.372242
O 3.253607 -2.316984 0.321326
```

```
C 2.608416 -3.544728 0.022633
H 2.979681 -4.271607 0.743080
H 1.521081 -3.457293 0.119747
H 2.851322 -3.881732 -0.992477
```

2 TS C1–C5 0 nN

```
32

C 2.402315 -1.952925 0.141990
C 1.669468 -0.778315 0.045567
C 2.328077 0.474673 -0.075619
C 3.714434 0.535830 -0.102175
C 4.442147 -0.649718 -0.006402
C 3.795262 -1.877969 0.114099
H 1.905741 -2.909487 0.236457
H 4.218752 1.488873 -0.195407
H 4.379462 -2.786797 0.187442
C 1.317706 1.495686 -0.158195
C 0.223331 -0.586844 0.051576
C -0.843311 -1.263183 0.149872
C 0.069318 1.188652 -0.106260
C -2.317214 -1.265503 0.255105
H -2.591880 -1.445691 1.311041
C -1.272375 1.850667 -0.175112
H -1.564845 1.934287 -1.232396
C -2.410436 1.109479 0.544595
H -2.116967 0.856843 1.568128
O -2.859719 -0.034674 -0.171125
H 5.524410 -0.615017 -0.026147
H -3.252236 1.799150 0.588237
O -2.930532 -2.218121 -0.565502
C -2.753324 -3.555007 -0.120909
H -3.316844 -4.183557 -0.807028
H -1.699577 -3.853295 -0.142309
H -3.142583 -3.691924 0.895642
O -1.251370 3.139603 0.419044
C -0.527129 4.128096 -0.296131
H -0.886202 4.209462 -1.329531
H -0.699733 5.070994 0.220429
H 0.545849 3.909976 -0.305900
```

2 Product 0 nN

```
32

C 3.016866 -1.832453 0.261924
```

```
C 1.879319 -0.998492 0.139151
C 2.080229 0.420523 -0.136728
C 3.406046 0.900631 -0.268146
C 4.477207 0.052758 -0.140016
C 4.282164 -1.319458 0.125984
H 2.864738 -2.884795 0.464536
H 3.556877 1.952985 -0.472311
H 5.141047 -1.971847 0.223165
C 0.923102 1.184867 -0.253398
C 0.555233 -1.407582 0.256900
C -0.549190 -0.647596 0.128612
C -0.355212 0.773345 -0.127308
C -1.955417 -1.198943 0.266020
H -2.212433 -1.290389 1.338130
C -1.571595 1.688527 -0.260697
H -1.679838 1.961664 -1.319120
C -2.841327 0.977417 0.202629
H -2.857873 0.959017 1.300195
O -2.910285 -0.333049 -0.333851
H 5.483877 0.438339 -0.244042
H -3.722217 1.514296 -0.144501
O -2.019624 -2.440345 -0.346170
C -3.235673 -3.145305 -0.105327
H -3.110475 -4.130478 -0.550028
H -3.416839 -3.254975 0.970689
H -4.086649 -2.639994 -0.565692
O -1.483400 2.864621 0.526719
C -0.658509 3.887769 -0.001845
H -0.972999 4.168549 -1.014821
H -0.762478 4.747179 0.659105
H 0.393997 3.581060 -0.030370
```

2 Reactant 1 nN

```
32

C -2.395440 1.532780 0.074482
C -1.171679 0.879791 -0.093688
C -1.136931 -0.545548 -0.108104
C -2.330667 -1.256365 0.043834
C -3.536010 -0.586832 0.210199
C -3.568763 0.805238 0.225400
H -2.416502 2.614775 0.084652
H -2.302352 -2.338124 0.029943
H -4.509941 1.324844 0.354178
C 0.128990 -1.173957 -0.273088
C 0.063932 1.564603 -0.261866
```

```
C 1.202075 1.916025 -0.451837
C 1.287707 -1.484178 -0.400277
C 2.661388 2.015653 -0.648825
H 3.142161 2.253677 0.314773
C 2.739212 -1.611343 -0.549713
H 2.977280 -1.842031 -1.597369
C 3.433633 -0.262886 -0.182439
H 3.122726 0.020589 0.825236
O 3.151958 0.770140 -1.134436
H -4.452007 -1.152315 0.327173
H 4.510337 -0.448093 -0.181497
O 3.042976 2.967476 -1.616691
C 2.711611 4.336087 -1.329577
H 3.104859 4.913863 -2.162222
H 1.628910 4.478319 -1.260665
H 3.181729 4.671089 -0.397521
O 3.324376 -2.595249 0.309690
C 2.963831 -3.963707 0.065967
H 3.236824 -4.268257 -0.951053
H 3.526728 -4.553890 0.785774
H 1.891886 -4.124792 0.216134
```

2 TS Bergman 1 nN

32

```
C -2.202512 1.513196 0.032056
C -0.957348 0.886182 -0.120464
C -0.911671 -0.586674 -0.071383
C -2.117318 -1.276054 0.126142
C -3.319558 -0.608537 0.274475
C -3.362531 0.785780 0.226945
H -2.238526 2.593572 -0.005792
H -2.088357 -2.356673 0.162578
H -4.306526 1.303496 0.342306
C 0.345068 -1.176675 -0.236204
C 0.263702 1.536378 -0.324162
C 1.461264 1.145905 -0.508472
C 1.528299 -0.738651 -0.407537
C 2.808473 1.819804 -0.713439
H 3.112806 2.258996 0.252655
C 2.922608 -1.292563 -0.543557
H 3.038187 -1.659130 -1.572286
C 3.977842 -0.208156 -0.296225
H 3.956562 0.080638 0.761187
O 3.794866 0.915003 -1.147943
H -4.230355 -1.174048 0.426753
```

```
H 4.962905 -0.611431 -0.523259
O 2.767315 2.814308 -1.698448
C 2.413679 4.144768 -1.294440
H 2.567425 4.768720 -2.171520
H 1.364782 4.197315 -0.984848
H 3.055513 4.492547 -0.477590
O 3.209610 -2.336863 0.380877
C 2.715778 -3.652195 0.092212
H 3.061574 -3.995070 -0.889503
H 3.118885 -4.298519 0.868906
H 1.621621 -3.678504 0.121842
```

2 TS C1–C5 1 nN

```
32

C 2.273181 -2.099468 0.170613
C 1.623961 -0.878913 0.047012
C 2.369990 0.320292 -0.107768
C 3.757281 0.282502 -0.136746
C 4.399948 -0.948399 -0.011002
C 3.667789 -2.124227 0.140430
H 1.710292 -3.015992 0.287369
H 4.327127 1.194951 -0.255373
H 4.186254 -3.070184 0.235695
C 1.435348 1.408078 -0.218988
C 0.193034 -0.590495 0.045643
C -0.902841 -1.223462 0.155226
C 0.166880 1.192449 -0.156731
C -2.375887 -1.146531 0.223858
H -2.694820 -1.254141 1.275362
C -1.113104 1.968245 -0.224103
H -1.367123 2.132139 -1.281121
C -2.321171 1.263460 0.438263
H -2.076895 1.015299 1.475403
O -2.798987 0.117846 -0.273867
H 5.481920 -0.990794 -0.032246
H -3.138246 1.983715 0.441757
O -3.032651 -2.098559 -0.575139
C -3.251918 -3.395509 0.003154
H -3.844697 -3.944800 -0.724008
H -2.308964 -3.922943 0.177909
H -3.806643 -3.318360 0.945029
O -1.019057 3.225598 0.450581
C -0.199572 4.250347 -0.129987
H -0.511858 4.467589 -1.157954
H -0.344568 5.131874 0.491065
```

```
H 0.856253 3.962353 -0.124729
```

2 Product 1 nN

```
32

C 3.009992 -1.808313 0.228535
C 1.869313 -0.976956 0.119282
C 2.065044 0.449967 -0.112244
C 3.388942 0.941383 -0.216136
C 4.463666 0.095705 -0.102572
C 4.273815 -1.284797 0.120364
H 2.861922 -2.867089 0.398144
H 3.535618 2.000193 -0.387209
H 5.135363 -1.935234 0.206465
C 0.903329 1.208748 -0.219418
C 0.546090 -1.395922 0.213021
C -0.566423 -0.645065 0.097470
C -0.374467 0.789127 -0.121991
C -1.967470 -1.233849 0.227981
H -2.203011 -1.378539 1.297311
C -1.587398 1.710281 -0.253894
H -1.715425 1.962051 -1.314828
C -2.840955 0.972520 0.237418
H -2.821631 0.936944 1.334286
O -2.932303 -0.338317 -0.318059
H 5.469131 0.489579 -0.184998
H -3.737549 1.506066 -0.072200
O -2.014385 -2.455818 -0.440423
C -2.995841 -3.421963 -0.020420
H -2.779004 -4.325675 -0.584888
H -2.904021 -3.628419 1.051241
H -4.009930 -3.082189 -0.244256
O -1.496960 2.908679 0.514630
C -0.773571 4.015045 -0.040560
H -1.160968 4.282895 -1.030431
H -0.921354 4.845960 0.646496
H 0.295783 3.791840 -0.120396
```

2 Reactant 2 nN

```
32

C -2.395558 1.525912 0.083728
C -1.170533 0.875272 -0.087099
C -1.133557 -0.550010 -0.101011
C -2.326532 -1.262055 0.054428
```

```
C -3.532591 -0.594840 0.223558
C -3.567508 0.797167 0.238020
H -2.418094 2.607885 0.093335
H -2.296429 -2.343770 0.040855
H -4.509031 1.315637 0.368809
C 0.129657 -1.183499 -0.269220
C 0.060325 1.568413 -0.257759
C 1.191400 1.942457 -0.448117
C 1.281629 -1.517146 -0.401061
C 2.647119 2.052694 -0.647317
H 3.134286 2.279822 0.314290
C 2.730734 -1.647638 -0.558926
H 2.965938 -1.875507 -1.606968
C 3.414896 -0.269222 -0.195519
H 3.103175 0.003081 0.814610
O 3.129839 0.788470 -1.138181
H -4.447251 -1.161933 0.343138
H 4.492960 -0.443668 -0.200222
O 3.027209 3.020621 -1.614370
C 2.700873 4.422219 -1.378238
H 3.105362 4.949931 -2.237240
H 1.619171 4.569308 -1.320968
H 3.173331 4.785753 -0.459852
O 3.327152 -2.640478 0.301399
C 2.997675 -4.046877 0.109488
H 3.272462 -4.378594 -0.897084
H 3.588470 -4.579538 0.850181
H 1.932575 -4.226342 0.278950
```

2 TS Bergman 2 nN

```
32

C -2.300825 1.478465 0.155848
C -1.062935 0.850420 -0.046698
C -1.019281 -0.620299 -0.026805
C -2.219414 -1.312375 0.195528
C -3.414714 -0.645564 0.393500
C -3.455919 0.749844 0.372906
H -2.334702 2.559483 0.138564
H -2.191384 -2.393580 0.211122
H -4.394768 1.266868 0.526922
C 0.230456 -1.210609 -0.242301
C 0.152507 1.504106 -0.274068
C 1.347562 1.118959 -0.503576
C 1.411620 -0.768662 -0.442016
C 2.678307 1.822123 -0.735987
```

```
H 3.015774 2.240320 0.226846
C 2.792833 -1.349234 -0.631562
H 2.874154 -1.695225 -1.669705
C 3.851619 -0.251421 -0.396963
H 3.859238 0.009255 0.667628
O 3.646943 0.903959 -1.214164
H -4.321798 -1.212033 0.563489
H 4.833233 -0.638567 -0.663568
O 2.596004 2.843847 -1.702595
C 2.505347 4.244538 -1.312831
H 1.527910 4.464055 -0.874908
H 3.299761 4.507391 -0.607947
H 2.631218 4.800142 -2.238064
O 3.109424 -2.421393 0.269010
C 2.711892 -3.791406 -0.016731
H 3.080274 -4.108158 -0.997716
H 3.174009 -4.388409 0.765422
H 1.624152 -3.899154 0.022560
```

2 TS C1–C5 2 nN

```
32

C 2.169414 -2.196111 0.178730
C 1.582143 -0.945429 0.045160
C 2.389241 0.212597 -0.117919
C 3.772825 0.103948 -0.143918
C 4.352398 -1.156735 -0.007073
C 3.561018 -2.292404 0.151733
H 1.560859 -3.082260 0.300901
H 4.388250 0.985494 -0.268562
H 4.030212 -3.262938 0.255112
C 1.513048 1.346592 -0.239965
C 0.165616 -0.586499 0.039656
C -0.948058 -1.192770 0.158717
C 0.233930 1.194725 -0.177302
C -2.418219 -1.074595 0.232694
H -2.742085 -1.154068 1.283782
C -0.999112 2.042348 -0.246503
H -1.244684 2.222291 -1.302112
C -2.240383 1.366761 0.416471
H -2.000347 1.120753 1.454623
O -2.770670 0.220475 -0.279589
H 5.430881 -1.254036 -0.025718
H -3.037116 2.109290 0.415062
O -3.116636 -2.015042 -0.559133
C -3.535388 -3.290388 0.010789
```

```
H -4.161119 -3.743886 -0.752743
H -2.675533 -3.932598 0.217900
H -4.115359 -3.137394 0.926330
O -0.846982 3.301781 0.437768
C 0.026067 4.342584 -0.085252
H -0.262378 4.616927 -1.105181
H -0.114843 5.188340 0.583152
H 1.070319 4.018630 -0.071011
```

2 Product 2 nN

```
32

C 3.038673 -1.737126 0.208808
C 1.880065 -0.930490 0.106009
C 2.044094 0.503266 -0.101264
C 3.356286 1.027302 -0.189246
C 4.449910 0.204953 -0.082389
C 4.290857 -1.182865 0.116921
H 2.914516 -2.801728 0.360329
H 3.478954 2.091913 -0.342209
H 5.166734 -1.814562 0.197830
C 0.864629 1.235005 -0.204502
C 0.565555 -1.379907 0.186848
C -0.567789 -0.660052 0.078603
C -0.405008 0.789867 -0.122743
C -1.953545 -1.305618 0.208923
H -2.168466 -1.489541 1.274834
C -1.628450 1.702428 -0.251752
H -1.775479 1.939087 -1.312638
C -2.853687 0.917080 0.261776
H -2.806330 0.875532 1.357174
O -2.935387 -0.400860 -0.299853
H 5.446395 0.623338 -0.152114
H -3.773901 1.423790 -0.022401
O -1.991334 -2.516020 -0.504566
C -2.678281 -3.694392 0.016468
H -2.422598 -4.493190 -0.674245
H -2.318864 -3.940350 1.019571
H -3.760256 -3.544684 0.031578
O -1.551698 2.920157 0.509216
C -1.010962 4.141203 -0.067707
H -1.514432 4.386320 -1.008658
H -1.207183 4.915644 0.669916
H 0.065875 4.053775 -0.238763
```

3 Reactant 0 nN

32

```
C -3.287050 1.480476 -0.213877
C -2.039913 0.852976 -0.322432
C -1.993809 -0.566261 -0.380590
C -3.180408 -1.306398 -0.332965
C -4.407365 -0.654688 -0.229291
C -4.454579 0.743135 -0.168387
H -3.329938 2.560890 -0.168963
H -3.117743 -2.383259 -0.379040
H -5.419183 1.226508 -0.087508
C -0.709162 -1.171506 -0.476389
C -0.804747 1.552912 -0.384717
C 0.339220 1.918900 -0.483664
C 0.471378 -1.408182 -0.541301
C 1.791731 2.079794 -0.562490
H 2.202815 2.297083 0.439027
C 1.924396 -1.488763 -0.579867
H 2.267276 -1.708634 -1.595401
C 2.595490 -0.184430 -0.106121
H 2.207978 0.088446 0.879509
O 2.407407 0.873778 -1.041315
H 2.281912 -2.304897 0.057685
H 3.671767 -0.365244 -0.013550
O 2.103153 3.110708 -1.440751
C 3.482919 3.466399 -1.452457
H 3.567943 4.335684 -2.101154
H 3.827327 3.733686 -0.445569
H 4.099405 2.654775 -1.843401
O -5.610642 -1.289204 -0.178985
C -5.638407 -2.709420 -0.244564
H -5.211736 -3.074789 -1.183373
H -5.104555 -3.159476 0.597776
H -6.688472 -2.987535 -0.194392
```

3 TS Bergman 0 nN

32

```
C -3.174543 1.521532 -0.383726
C -1.924285 0.880446 -0.420553
C -1.919862 -0.609267 -0.371926
C -3.157224 -1.271838 -0.296594
C -4.355424 -0.575460 -0.265148
C -4.358588 0.826485 -0.308234
H -3.190411 2.602163 -0.417689
H -3.140320 -2.349843 -0.265013
```

```
H -5.308288 1.344198 -0.282307
C -0.675662 -1.226018 -0.413299
C -0.680167 1.479387 -0.497281
C 0.513704 1.040675 -0.559170
C 0.516639 -0.771266 -0.493733
C 1.881785 1.680541 -0.550122
H 2.089683 2.023725 0.480473
C 1.899529 -1.332466 -0.591644
H 2.086805 -1.629926 -1.627621
C 2.994426 -0.368590 -0.163567
H 2.916487 -0.134601 0.906776
O 2.935538 0.819081 -0.938029
H 1.942807 -2.235000 0.022013
H 3.975661 -0.807286 -0.344385
O 1.860171 2.764074 -1.417559
C 3.007326 3.605906 -1.313702
H 2.814072 4.460856 -1.958391
H 3.143965 3.955390 -0.283017
H 3.911804 3.092321 -1.644570
O -5.582536 -1.161149 -0.192768
C -5.662384 -2.580245 -0.154896
H -5.233130 -3.028828 -1.055705
H -5.160254 -2.985846 0.728551
H -6.722917 -2.815688 -0.105678
```

3 TS C1–C5 0 nN

```
32

C 1.496838 -1.701595 0.098279
C 0.854998 -0.470450 0.016625
C 1.617615 0.719935 -0.056910
C 3.006825 0.681377 -0.056601
C 3.637594 -0.564760 0.018785
C 2.883850 -1.743567 0.095135
H 0.927682 -2.619932 0.157425
H 3.569206 1.601356 -0.114485
H 3.412391 -2.685968 0.151593
C 0.704638 1.833677 -0.125076
C -0.565154 -0.153715 0.012039
C -1.692637 -0.720293 0.119467
C -0.567736 1.626293 -0.122278
C -3.142729 -0.600162 0.304053
H -3.375275 -0.692569 1.381684
C -1.845192 2.369927 -0.249063
H -2.125397 2.445544 -1.304971
C -3.055631 1.807219 0.503200
```

```
H -2.800461 1.575916 1.543973
O -3.627515 0.669371 -0.141559
H -1.667555 3.389239 0.104814
H -3.840959 2.564360 0.509851
O -3.792686 -1.595433 -0.413447
C -5.188187 -1.694851 -0.134221
H -5.544378 -2.570089 -0.673297
H -5.362160 -1.836731 0.939378
H -5.726255 -0.808512 -0.474518
O 4.990049 -0.733999 0.024327
C 5.822789 0.415116 -0.051176
H 5.656773 0.970097 -0.979435
H 5.665970 1.080480 0.803233
H 6.844350 0.042394 -0.033364
```

3 Product 0 nN

32

```
C 1.795268 -1.965186 0.221168
C 0.840488 -0.918272 0.148624
C 1.329723 0.444387 -0.005185
C 2.727320 0.675521 -0.072547
C 3.608649 -0.378722 0.003840
C 3.134408 -1.707069 0.151989
H 1.440389 -2.981626 0.332895
H 3.069156 1.693437 -0.186734
H 3.864053 -2.504390 0.206669
C 0.348282 1.427915 -0.077331
C -0.538567 -1.066952 0.215079
C -1.471174 -0.095199 0.132319
C -0.992589 1.266803 -0.020509
C -2.960295 -0.363710 0.263367
H -3.207806 -0.524047 1.329903
C -1.997293 2.392715 -0.134557
H -2.096521 2.678815 -1.185784
C -3.360323 1.961705 0.391271
H -3.343215 1.867864 1.486378
O -3.746442 0.726208 -0.200694
H -1.638698 3.269817 0.408979
H -4.131982 2.684083 0.126578
O -3.283281 -1.496601 -0.469485
C -4.608033 -1.974343 -0.248772
H -4.690300 -2.911303 -0.796115
H -4.782795 -2.162842 0.817580
H -5.353672 -1.267243 -0.617085
O 4.964508 -0.265677 -0.052333
```

```
C 5.530453 1.028804 -0.207830
H 5.205797 1.495797 -1.142559
H 5.272384 1.680424 0.632512
H 6.607616 0.881575 -0.232731
```

3 Reactant 1 nN

```
32

C -3.246768 1.401702 -0.380952
C -2.002717 0.761566 -0.474621
C -1.987658 -0.662573 -0.450071
C -3.187780 -1.389948 -0.330234
C -4.410334 -0.721877 -0.236226
C -4.421873 0.681296 -0.266504
H -3.284334 2.483266 -0.398332
H -3.137908 -2.470142 -0.312044
H -5.375328 1.187960 -0.195113
C -0.699284 -1.267067 -0.539230
C -0.758907 1.464687 -0.574666
C 0.366396 1.899418 -0.668856
C 0.494043 -1.428806 -0.622193
C 1.829320 2.104433 -0.622223
H 2.130686 2.275071 0.426002
C 1.949210 -1.458870 -0.691011
H 2.276707 -1.632557 -1.720520
C 2.622825 -0.166807 -0.177142
H 2.214644 0.094505 0.803327
O 2.502332 0.924077 -1.088286
H 2.337875 -2.291569 -0.094154
H 3.691203 -0.373498 -0.057923
O 2.226642 3.185436 -1.409716
C 3.595638 3.611696 -1.249449
H 3.697184 4.507313 -1.857234
H 3.806335 3.853261 -0.201280
H 4.288148 2.843414 -1.597516
O -5.646056 -1.295713 -0.113299
C -5.851287 -2.711957 -0.035801
H -5.505024 -3.214160 -0.943866
H -5.344081 -3.139150 0.834226
H -6.925440 -2.840946 0.066389
```

3 TS Bergman 1 nN

```
32

C -1.834478 1.965458 0.101090
```

```
C -0.855245 0.954364 0.049723
C -1.367947 -0.455020 -0.033214
C -2.767523 -0.667468 -0.057037
C -3.670936 0.384228 0.004804
C -3.184780 1.702780 0.081402
H -1.497051 2.990924 0.164486
H -3.111580 -1.689507 -0.123090
H -3.902154 2.511578 0.126878
C -0.387810 -1.433809 -0.090585
C 0.521988 1.106425 0.072042
C 1.507806 0.283982 0.026461
C 0.898891 -1.361680 -0.092271
C 3.020053 0.389218 0.272467
H 3.162635 0.479037 1.365729
C 1.990400 -2.386472 -0.206040
H 2.165882 -2.598881 -1.264811
C 3.303640 -1.955641 0.420794
H 3.203188 -1.842253 1.508796
O 3.746195 -0.741826 -0.165311
H 1.639683 -3.308657 0.260430
H 4.081111 -2.694417 0.226016
O 3.550632 1.507069 -0.367440
C 4.953152 1.745679 -0.098283
H 5.175090 2.707119 -0.554969
H 5.135810 1.800019 0.980776
H 5.574319 0.965592 -0.537535
O -5.035525 0.287963 -0.001227
C -5.732867 -0.963503 -0.050199
H -5.504065 -1.509744 -0.969945
H -5.489712 -1.586809 0.815252
H -6.788109 -0.704663 -0.031008
```

3 TS C1–C5 1 nN

```
32

C 1.547351 -1.711599 0.042519
C 0.865724 -0.498627 -0.021295
C 1.622312 0.702485 -0.056520
C 3.018410 0.696533 -0.038167
C 3.685760 -0.532471 0.018233
C 2.939112 -1.722053 0.057222
H 1.007433 -2.649140 0.074548
H 3.558613 1.632819 -0.067462
H 3.478491 -2.659174 0.100342
C 0.695467 1.804271 -0.110549
C -0.575393 -0.198940 -0.034559
```

```
C -1.716567 -0.762973 0.047356
C -0.575735 1.582550 -0.130481
C -3.175684 -0.607277 0.290831
H -3.342588 -0.671964 1.382719
C -1.843561 2.341603 -0.262529
H -2.124555 2.413581 -1.318508
C -3.057643 1.798048 0.494240
H -2.802303 1.562784 1.534216
O -3.643094 0.667346 -0.148995
H -1.651487 3.360581 0.084143
H -3.834392 2.564077 0.502761
O -3.921887 -1.587241 -0.362935
C -5.335778 -1.591741 -0.059794
H -5.736341 -2.473593 -0.553464
H -5.498894 -1.669138 1.021098
H -5.820263 -0.692991 -0.441749
O 5.044764 -0.699948 0.040720
C 5.958387 0.405825 0.006199
H 5.842121 0.987989 -0.912536
H 5.823843 1.059153 0.873202
H 6.949082 -0.040041 0.034144
```

3 Product 1 nN

32

```
C 1.835885 -1.965715 0.134052
C 0.861212 -0.935087 0.059146
C 1.352024 0.431883 -0.062029
C 2.756541 0.687155 -0.087777
C 3.655924 -0.354195 0.000561
C 3.174767 -1.688408 0.107067
H 1.499043 -2.991038 0.219208
H 3.087307 1.713155 -0.175762
H 3.906551 -2.483328 0.169240
C 0.346814 1.392353 -0.136538
C -0.524759 -1.106913 0.111714
C -1.484942 -0.155805 0.046847
C -0.993670 1.213860 -0.092335
C -2.992975 -0.379959 0.274371
H -3.155828 -0.498011 1.363044
C -1.981125 2.358172 -0.182893
H -2.129408 2.622716 -1.234151
C -3.321560 1.964129 0.417047
H -3.249182 1.871060 1.509935
O -3.759464 0.737837 -0.152808
H -1.576599 3.238446 0.321236
```

H -4.090893 2.701991 0.190051
O -3.469579 -1.505593 -0.392471
C -4.862736 -1.807157 -0.143811
H -5.043327 -2.768304 -0.619353
H -5.053989 -1.887113 0.932271
H -5.510201 -1.044374 -0.575594
O 5.021305 -0.266460 -0.001969
C 5.719769 0.982971 -0.073175
H 5.496105 1.509259 -1.005824
H 5.469839 1.624528 0.776985
H 6.774991 0.725222 -0.041530

3 Reactant 2 nN

32

C -3.214004 1.330921 -0.399504
C -1.963539 0.699080 -0.497156
C -1.966107 -0.728065 -0.458165
C -3.172858 -1.458591 -0.324201
C -4.402797 -0.796446 -0.227785
C -4.391268 0.610615 -0.271215
H -3.260357 2.412196 -0.425104
H -3.117370 -2.539280 -0.297842
H -5.338905 1.128228 -0.199058
C -0.672760 -1.326291 -0.549304
C -0.712875 1.415965 -0.612379
C 0.397052 1.900793 -0.715320
C 0.526734 -1.437088 -0.640515
C 1.871265 2.142612 -0.637673
H 2.133268 2.308630 0.421304
C 1.982666 -1.425494 -0.719671
H 2.307362 -1.570503 -1.754514
C 2.643013 -0.133829 -0.181104
H 2.208460 0.124373 0.788599
O 2.562619 0.967298 -1.086793
H 2.393248 -2.262785 -0.144236
H 3.706114 -0.346940 -0.032292
O 2.301423 3.235726 -1.404593
C 3.679567 3.697986 -1.227707
H 3.753224 4.594809 -1.836199
H 3.870986 3.940480 -0.177340
H 4.385601 2.942475 -1.573911
O -5.666349 -1.328961 -0.093109
C -6.060855 -2.722167 0.005251
H -5.782540 -3.274335 -0.896068
H -5.613963 -3.196163 0.882997

```
H -7.141647 -2.691788 0.106089
```

3 TS Bergman 2 nN

```
32

C 1.855146 -1.945088 0.118266
C 0.847376 -0.957317 0.047967
C 1.367396 0.465403 -0.065239
C 2.776592 0.691271 -0.083685
C 3.698195 -0.344848 0.006378
C 3.202403 -1.665302 0.102772
H 1.538625 -2.976129 0.199487
H 3.104573 1.718251 -0.167739
H 3.921414 -2.471400 0.168442
C 0.365503 1.410745 -0.151789
C -0.528131 -1.123073 0.070925
C -1.521005 -0.285967 -0.005949
C -0.930732 1.286902 -0.141013
C -3.061226 -0.399737 0.276843
H -3.153995 -0.519656 1.371757
C -1.995584 2.352969 -0.214159
H -2.216534 2.563840 -1.264596
C -3.284115 1.954780 0.475867
H -3.133361 1.830122 1.556736
O -3.777926 0.755758 -0.099017
H -1.596616 3.266324 0.228321
H -4.055196 2.710291 0.324010
O -3.671284 -1.482826 -0.368670
C -5.113289 -1.646485 -0.120921
H -5.363615 -2.597546 -0.582653
H -5.313737 -1.685925 0.954220
H -5.674597 -0.833545 -0.577476
O 5.074444 -0.286411 0.011816
C 5.934546 0.881707 -0.036038
H 5.787840 1.439845 -0.964309
H 5.755858 1.535556 0.821452
H 6.942201 0.478877 0.003196
```

3 TS C1–C5 2 nN

```
32

C 1.594906 -1.711075 0.034309
C 0.873529 -0.518317 -0.023924
C 1.623527 0.691893 -0.050980
C 3.026269 0.717155 -0.032072
```

```
C 3.732225 -0.492990 0.017386
C 2.991190 -1.691211 0.049703
H 1.084988 -2.665796 0.061284
H 3.540102 1.669461 -0.056275
H 3.540592 -2.622856 0.088152
C 0.682713 1.781326 -0.101225
C -0.589850 -0.234194 -0.041457
C -1.745306 -0.791141 0.022458
C -0.587301 1.546456 -0.128291
C -3.222000 -0.612251 0.284356
H -3.357007 -0.666080 1.380797
C -1.848523 2.315900 -0.268308
H -2.128289 2.381655 -1.325062
C -3.067510 1.790421 0.490872
H -2.814200 1.551170 1.530428
O -3.667792 0.667545 -0.152245
H -1.646544 3.335802 0.069537
H -3.834853 2.565876 0.500118
O -4.029086 -1.575011 -0.339378
C -5.467402 -1.527477 -0.047569
H -5.876578 -2.409593 -0.531755
H -5.640179 -1.577133 1.032220
H -5.911345 -0.621271 -0.457416
O 5.099514 -0.665260 0.040085
C 6.116938 0.372044 0.011893
H 6.049218 0.963628 -0.904728
H 6.034520 1.026834 0.883255
H 7.058052 -0.169135 0.038842
```

3 Product 2 nN

32

```
C 1.871807 -1.947702 0.128835
C 0.875560 -0.936245 0.039125
C 1.364585 0.432187 -0.083611
C 2.775217 0.709783 -0.096697
C 3.696996 -0.315729 0.006598
C 3.209538 -1.652505 0.115010
H 1.555463 -2.979601 0.215921
H 3.088006 1.742116 -0.187888
H 3.943424 -2.444502 0.189598
C 0.335421 1.368593 -0.169509
C -0.516912 -1.130023 0.081870
C -1.505914 -0.202669 0.007511
C -1.005074 1.172630 -0.131565
C -3.040250 -0.402720 0.279043
```

```
H -3.149193 -0.532703 1.372415
C -1.981690 2.328161 -0.203455
H -2.180030 2.573283 -1.251230
C -3.293284 1.958840 0.466284
H -3.164417 1.853210 1.552664
O -3.781239 0.748579 -0.094110
H -1.542355 3.212545 0.262474
H -4.060101 2.712466 0.286529
O -3.626819 -1.492107 -0.378096
C -5.063751 -1.689351 -0.131643
H -5.297345 -2.640276 -0.602682
H -5.262230 -1.743343 0.943422
H -5.641872 -0.882827 -0.578605
O 5.073650 -0.259860 0.019476
C 5.930728 0.909425 -0.042573
H 5.786773 1.452062 -0.980495
H 5.744916 1.576619 0.803150
H 6.939611 0.510956 0.008568
```

5 Full reference (35)

(35) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A. C., J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision C.01*, Gaussian, Inc.;Wallingford CT, 2009: 2009.