

# Antiaromaticity Gain Activates Tropone and Non-Benzenoid Aromatics as Normal-Electron-Demand Diels-Alder Dienes

Lucas J. Karas,<sup>a</sup> Adam T. Campbell,<sup>b</sup> Igor V. Alabugin,<sup>b</sup> Judy I. Wu<sup>a\*</sup>

<sup>a</sup>Department of Chemistry, University of Houston, Houston, TX 77204

<sup>b</sup>Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306

Correspondence: jiwu@central.uh.edu

## Table of Contents

<b>1. Computed NICS(1)<sub>zz</sub> and HOMO energies for tropone, and tropone with a q(-1) point charge at 4, 3, and 2 Å away from the carbonyl oxygen in a near linear arrangement.</b> .....	<b>2</b>
<i>Table S1. Computed NICS(1)<sub>zz</sub> and HOMO energies for tropone, and tropone with a q(-1) point charge at 4, 3, and 2 Å away from the carbonyl oxygen in a near linear arrangement.</i> .....	2
<b>2. Computed activation free energies for endo vs. exo reactions.</b> .....	<b>3</b>
<i>Table S2. Computed gas-phase activation free energies for the endo vs. exo Diels-Alder reactions of maleimide with 1, 2-prot, 2, 3-prot, 3, 4, 5-prot, and 5. Relative free energies (<math>\Delta G</math> and <math>\Delta G^\ddagger</math>) are in kcal/mol.</i> .....	3
<b>3. Computed activation free energies in implicit dichloromethane solvent for the Diels–Alder reactions of maleimide with 4, 5-prot, and 5.</b> .....	<b>4</b>
<i>Table S3. Computed activation free energies in implicit dichloromethane solvent for the Diels–Alder reactions of maleimide with 4, 5-prot, and 5. Relative free energies (<math>\Delta G</math> and <math>\Delta G^\ddagger</math>) are in kcal/mol.</i> .....	4
<b>4. Computed NICS(0)<sub>π</sub> at points along the intrinsic reaction coordinate (IRC) of the Diels–Alder reactions of maleimide with 1 and 2.</b> .....	<b>5</b>
<i>Figure S1. Computed NICS(0)<sub>π</sub> (ppm) and gas-phase <math>\Delta E</math> values (in kcal/mol) for the Diels–Alder reactions of maleimide with a) 1 and b) 2.</i> .....	5
<b>5. Computed gas-phase Diels-Alder reaction pathways of maleimide with 2, 2', and 2''.</b> .....	<b>6</b>
<i>Figure S2. Computed gas-phase reaction pathway for the Diels-Alder reaction of maleimide adding to C2 and C5 (2), C4 and C7 (2') of 2, and with an alternative conformer of 2 (N lone pair anti-periplanar to C=N, 2''). Relevant transition state (TS) and intermediate (Inter) structures are shown. Relative free energies (<math>\Delta G</math> and <math>\Delta G^\ddagger</math>) are in kcal/mol.</i> .....	6
<b>6. Computed gas-phase Diels-Alder reaction pathways of maleimide with 2-prot and 2'-prot.</b> .....	<b>7</b>
<i>Figure S3. Computed gas-phase reaction pathway for the Diels-Alder reaction of maleimide adding to C2 and C5 (2-prot), C4 and C7 (2'-prot) of 2-prot. Relevant transition state (TS) and intermediate (Inter) structures are shown. Relative free energies (<math>\Delta G</math> and <math>\Delta G^\ddagger</math>) are in kcal/mol.</i> .....	7
<b>7. Computed gas-phase Diels-Alder reaction pathways of maleimide with 4, 5, and 5-prot.</b> .....	<b>8</b>
<i>Figure S4. Computed gas-phase reaction pathway for the Diels-Alder reaction of maleimide with 4, 5, and 5-prot. Relevant transition state (TS) and intermediate (Inter) structures are shown. Relative free energies (<math>\Delta G</math> and <math>\Delta G^\ddagger</math>) are in kcal/mol.</i> .....	8
<b>8. Optimized Cartesian coordinates for all structures at ωB97X-D/6-311+G(d,p).</b> .....	<b>9</b>

**1. Computed NICS(1)<sub>zz</sub> and HOMO energies for tropone, and tropone with a q(-1) point charge at 4, 3, and 2 Å away from the carbonyl oxygen in a near linear arrangement.**

**Table S1.** Computed NICS(1)<sub>zz</sub> and HOMO energies for tropone, and tropone with a q(-1) point charge at 4, 3, and 2 Å away from the carbonyl oxygen in a near linear arrangement.

Compound	NICS(1) <sub>zz</sub> (ppm)	HOMO (eV)
Tropone	-5.0	-8.7
q(-1) at 4 Å	-1.7	-6.4
q(-1) at 3 Å	0.3	-5.9
q(-1) at 2 Å	4.7	-4.8

## 2. Computed activation free energies for *endo* vs. *exo* reactions.

**Table S2.** Computed gas-phase activation free energies for the *endo* vs. *exo* Diels-Alder reactions of maleimide with **1**, **2-prot**, **2**, **3-prot**, **3**, **4**, **5-prot**, and **5**. Relative free energies ( $\Delta G$  and  $\Delta G^\ddagger$ ) are in kcal/mol.

Compound	Product	$\Delta G^\ddagger (TS_1)$	$\Delta G_{int}$	$\Delta G^\ddagger (TS_2)$	$\Delta G_{prod}$
1	<i>endo</i>	30.2	--	--	-19.2
	<i>exo</i>	34.0	--	--	-17.1
2-prot	<i>endo</i>	30.7	--	--	-22.0
	<i>exo</i>	34.9	--	--	-19.9
2	<i>endo</i>	3.0	-9.4	-4.6	-29.0
	<i>exo</i>	4.5	-8.1	0.0	-25.4
3-prot	<i>endo</i>	31.9	--	--	-18.7
	<i>exo</i>	33.4	--	--	-20.5
3	<i>endo</i>	16.2	--	--	-26.5
	<i>exo</i>	20.0	--	--	-26.0
4	<i>endo</i>	29.3	--	--	-15.0
	<i>exo</i>	33.2	--	--	-13.6
5-prot	<i>endo</i>	28.3	--	--	-18.4
	<i>exo</i>	31.9	--	--	-17.3
5	<i>endo</i>	0.6	-18.3	-2.7	-16.5
	<i>exo</i>	5.7	-17.8	0.7	-14.6

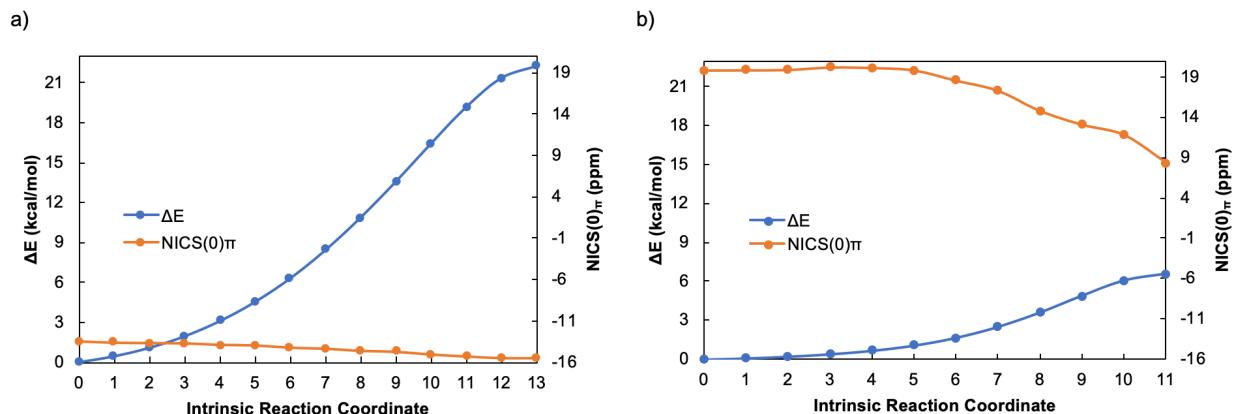
Computed gas-phase activation energies for the *endo* vs. *exo* Diels-Alder reactions of maleimide with **1**, **2-prot**, **2**, **3-prot**, **3**, **4**, **5-prot**, and **5** show that for all cases the *endo* pathway is preferred. Activation free energies ( $\Delta G$  and  $\Delta G^\ddagger$ ) were computed relative to the energies of the separate reactants.

**3. Computed activation free energies in implicit dichloromethane solvent for the Diels–Alder reactions of maleimide with **4**, **5-prot**, and **5**.**

**Table S3.** Computed activation free energies in implicit dichloromethane solvent for the Diels-Alder reactions of maleimide with **4**, **5-prot**, and **5**. Relative free energies ( $\Delta G$  and  $\Delta G^\ddagger$ ) are in kcal/mol.

Compound	$\Delta G^\ddagger (TS_1)$	$\Delta G_{int}$	$\Delta G^\ddagger (TS_2)$	$\Delta G_{prod}$
4	26.0	--	--	-18.5
5-prot	24.8	--	--	-21.9
5	11.6	-11.6	5.3	-17.9

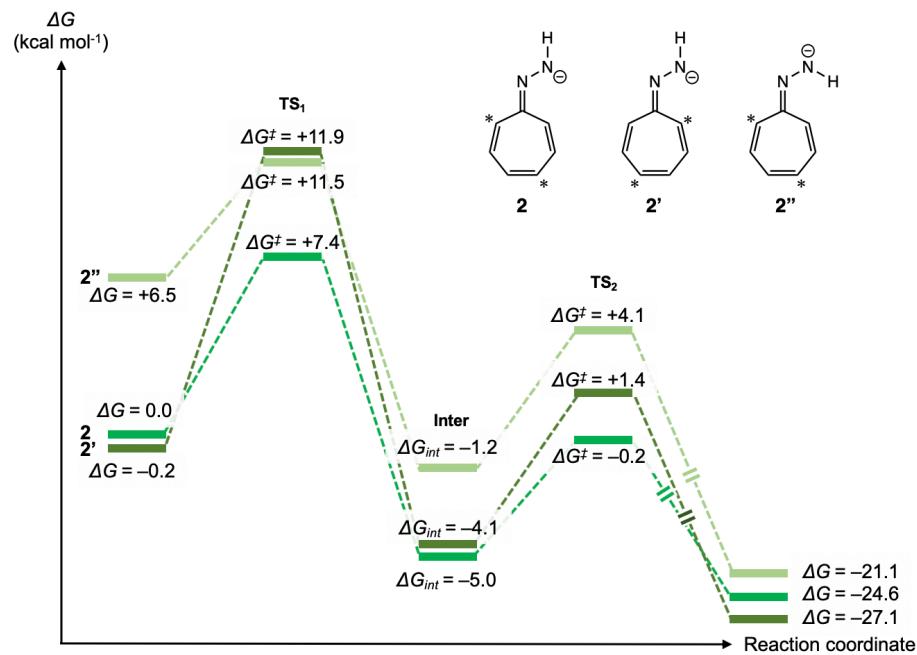
**4. Computed NICS( $0$ ) $_{\pi}$  at points along the intrinsic reaction coordinate (IRC) of the Diels–Alder reactions of maleimide with **1** and **2**.**



**Figure S1.** Computed NICS( $0$ ) $_{\pi}$  (ppm) and gas-phase  $\Delta E$  values (in kcal/mol) for the Diels–Alder reactions of maleimide with a) **1** and b) **2**.

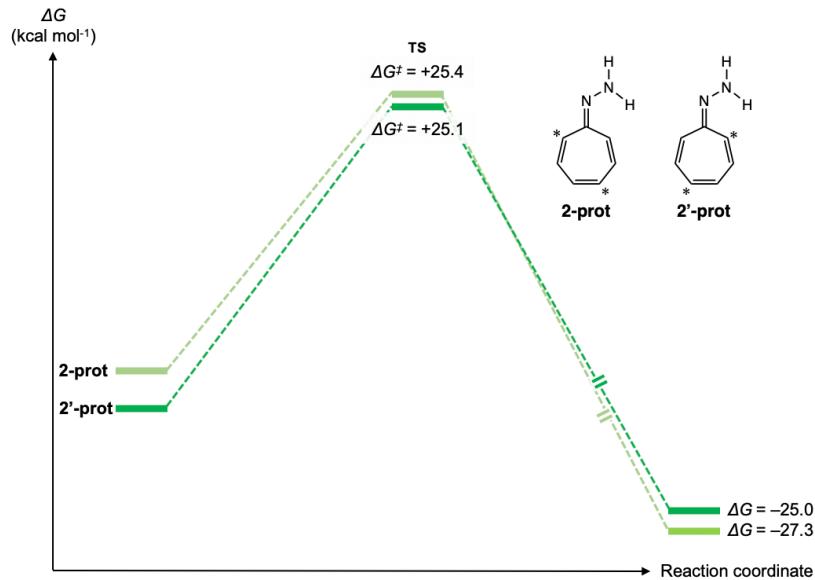
Computed NICS( $0$ ) $_{\pi}$  values along the IRC show that the aromatic character of **1** remains almost constant along the IRC. In contrast, **2** is antiaromatic and shows a relief of antiaromatic character along the IRC up to the first transition state. NICS( $0$ ) $_{\pi}$  computations were performed by placing NICS points at the ring center of **1** and **2** and including magnetic tensor contributions only from the localized  $\pi$ -molecular orbitals in the ring (three C=C and one C=O in **1**, three C=C and one C=N in **2**).

**5. Computed gas-phase Diels-Alder reaction pathways of maleimide with **2**, **2'**, and **2''**.**



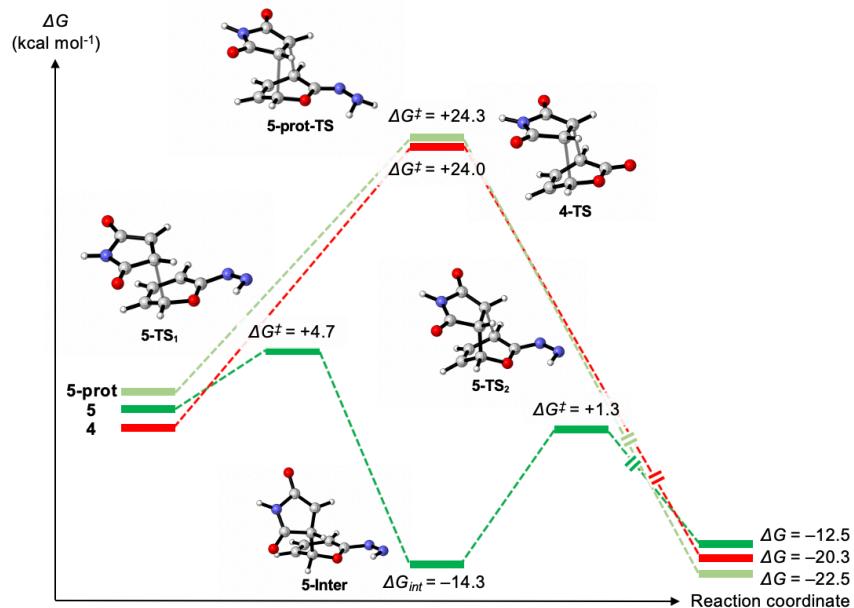
**Figure S2.** Computed gas-phase reaction pathway for the Diels-Alder reaction of maleimide adding to C2 and C5 (**2**), C4 and C7 (**2'**) of **2**, and with an alternative conformer of **2** (N lone pair anti-periplanar to C=N, **2''**). Relevant transition state (TS) and intermediate (Inter) structures are shown. Relative free energies ( $\Delta G$  and  $\Delta G^\ddagger$ ) are in kcal/mol.

## 6. Computed gas-phase Diels-Alder reaction pathways of maleimide with 2-prot and 2'-prot.



**Figure S3.** Computed gas-phase reaction pathway for the Diels-Alder reaction of maleimide adding to C2 and C5 (**2-prot**), C4 and C7 (**2'-prot**) of **2-prot**. Relevant transition state (TS) and intermediate (Inter) structures are shown. Relative free energies ( $\Delta G$  and  $\Delta G^\ddagger$ ) are in kcal/mol.

**7. Computed gas-phase Diels-Alder reaction pathways of maleimide with **4**, **5**, and **5-prot**.**



**Figure S4.** Computed gas-phase reaction pathway for the Diels-Alder reaction of maleimide with **4**, **5**, and **5-prot**. Relevant transition state (TS) and intermediate (Inter) structures are shown. Relative free energies ( $\Delta G$  and  $\Delta G^\ddagger$ ) are in kcal/mol.

































C	0.066613	-1.069676	1.587843
C	-0.355051	-1.423710	0.193169
C	-2.017391	0.220255	0.271935
H	-1.217374	1.992171	1.098703
H	0.090575	0.656864	2.848862
H	0.659840	-1.745154	2.191560
N	-3.026045	0.823183	-0.366579
O	-1.738711	-1.124552	0.006398
C	1.975990	-0.928100	-0.545120
C	0.511943	-0.588850	-0.811226
C	0.432822	0.912196	-0.611323
C	1.747497	1.392641	-0.307077
H	-0.192178	1.527672	-1.241546
N	2.582273	0.237354	-0.183019
H	3.560564	0.301631	0.049507
O	2.502302	-2.024971	-0.597147
O	2.201016	2.517913	-0.140814
N	-3.801704	0.179782	-1.159786
H	-3.491841	-0.804646	-1.214059
H	0.236026	-0.909424	-1.820917
H	-0.239886	-2.482755	-0.031552

Imaginary Frequencies

409 *i* cm<sup>-1</sup>

### 1 product

- Electronic Energy (a.u.): -704.976101883

- Number of Imaginary Frequencies: 0

xyz

O	-3.171097	1.354994	-0.346531
C	-2.283768	0.547571	-0.189106
C	-0.936060	0.977054	0.398935
C	-2.478803	-0.869936	-0.585636
C	-0.622075	0.211994	1.664421
H	-1.011138	2.048027	0.585339
C	-1.580901	-1.846594	-0.428823
H	-3.447858	-1.078745	-1.026738
C	-0.271879	-1.064398	1.561759
H	-0.688257	0.721690	2.618009
C	-0.205343	-1.675611	0.175503
H	-1.841169	-2.845245	-0.769020
H	-0.022581	-1.672078	2.423354
H	0.296927	-2.642529	0.210301
C	2.097852	-0.746400	-0.312405
C	0.632689	-0.737613	-0.733815
H	0.590012	-1.106250	-1.761207
C	1.449604	1.490282	-0.216878
C	0.192789	0.732248	-0.639225
H	-0.117390	1.134417	-1.606451
O	1.554842	2.669082	-0.015801
O	2.811354	-1.705748	-0.188970
N	2.473393	0.565603	-0.091673
H	3.402264	0.823287	0.210157

### 2 product

- Electronic Energy (a.u.): -739.845468199

- Number of Imaginary Frequencies: 0

xyz

C	-2.039715	0.166365	-0.036000
C	-0.760560	0.787288	0.490183
C	-2.078069	-1.217203	-0.387498
C	-0.305745	0.045537	1.725647
H	-0.978009	1.832835	0.714125
C	-1.052051	-2.104873	-0.323784
H	-3.049918	-1.568984	-0.723730
C	0.223401	-1.170968	1.575354
H	-0.504334	0.468800	2.705863
C	0.333352	-1.728156	0.171276
H	-1.218421	-3.144467	-0.590499
H	0.481672	-1.800333	2.422206
H	0.979637	-2.609096	0.159841

C	2.462487	-0.501249	-0.440734
C	0.985051	-0.664962	-0.749388
H	0.899125	-1.012731	-1.782196
C	1.545214	1.626739	-0.172347
C	0.374687	0.745919	-0.568471
H	-0.032789	1.136986	-1.504090
O	1.551755	2.808247	0.075919
O	3.327356	-1.346753	-0.447015
N	2.682086	0.829277	-0.137053
H	3.586769	1.185103	0.132186
N	-3.098201	0.988986	-0.113092
N	-4.222688	0.547815	-0.569851
H	-4.853308	1.350773	-0.530381

## 2 product alternative

- Electronic Energy (a.u.): -739.84974759

- Number of Imaginary Frequencies: 0

xyz			
C	-2.079238	-0.237728	-0.198674
C	-0.938600	0.574705	0.394601
C	-1.899445	-1.612171	-0.528830
C	-0.463590	-0.093832	1.660512
H	-1.323732	1.576831	0.587983
C	-0.764748	-2.349539	-0.393851
H	-2.792211	-2.098351	-0.918299
C	0.248425	-1.219008	1.558513
H	-0.777788	0.302242	2.621470
C	0.517502	-1.767512	0.172789
H	-0.765345	-3.401896	-0.659156
H	0.552166	-1.793378	2.429005
H	1.286392	-2.542883	0.212435
C	2.478621	-0.253425	-0.350796
C	1.057729	-0.628145	-0.730042
H	1.076432	-0.993929	-1.760029
C	1.256367	1.725366	-0.159804
C	0.243171	0.683157	-0.602539
H	-0.161279	1.006834	-1.564717
O	1.087852	2.897801	0.067935
O	3.453960	-0.968153	-0.304270
N	2.491418	1.095163	-0.053972
H	3.321533	1.578516	0.253918
N	-3.293927	0.286777	-0.410647
N	-3.512332	1.518701	-0.090909
H	-4.483952	1.693122	-0.354510

## 2 product alternative conformer

- Electronic Energy (a.u.): -739.838853703

- Number of Imaginary Frequencies: 0

xyz			
C	-2.046959	0.174477	-0.034782
C	-0.763230	0.789396	0.493550
C	-2.083143	-1.210965	-0.360704
C	-0.310062	0.051439	1.730645
H	-0.982702	1.834862	0.714855
C	-1.058773	-2.104734	-0.293417
H	-3.045601	-1.615791	-0.671223
C	0.224494	-1.163637	1.583976
H	-0.512500	0.476133	2.709330
C	0.331286	-1.724931	0.181367
H	-1.240500	-3.151079	-0.519158
H	0.483331	-1.790851	2.432262
H	0.976679	-2.606368	0.168795
C	2.455636	-0.508543	-0.457278
C	0.974254	-0.666610	-0.749934
H	0.875193	-1.017029	-1.780642
C	1.546934	1.620336	-0.166306
C	0.370906	0.746524	-0.563949
H	-0.033171	1.143056	-1.498928
O	1.558834	2.798745	0.093272
O	3.316777	-1.357628	-0.477396

N	2.682093	0.818915	-0.148104
H	3.590150	1.170291	0.115608
N	-3.094952	1.030241	-0.112164
N	-4.254026	0.756401	-0.577791
H	-4.295623	-0.227567	-0.910495

### 2-prot product

- Electronic Energy (a.u.): -740.423176469

- Number of Imaginary Frequencies: 0

xyz			
N	-3.012865	0.991278	-0.015329
C	-2.000231	0.205225	-0.035855
C	-0.695727	0.801631	0.458200
C	-2.029094	-1.191244	-0.497189
C	-0.239397	0.073577	1.704783
H	-0.888965	1.853945	0.664913
C	-1.007603	-2.050702	-0.412174
H	-2.935448	-1.533418	-0.985745
C	0.254696	-1.152062	1.570162
H	-0.341765	0.555984	2.669943
C	0.352187	-1.730899	0.173086
H	-1.134821	-3.045773	-0.828483
H	0.592867	-1.740935	2.414924
H	0.964955	-2.632866	0.177504
C	2.507664	-0.511795	-0.364751
C	1.042553	-0.689000	-0.743313
H	1.018197	-1.049519	-1.774613
C	1.580580	1.623317	-0.237603
C	0.417418	0.712793	-0.617765
H	0.016911	1.073403	-1.567765
O	1.545686	2.807194	-0.035129
O	3.343987	-1.370859	-0.267665
N	2.718781	0.837315	-0.149406
H	3.615978	1.211685	0.124045
N	-4.235708	0.529972	-0.432216
H	-4.948148	1.177651	-0.132137
H	-4.466888	-0.415844	-0.147052

### 2-prot product alternative

- Electronic Energy (a.u.): -740.423983367

- Number of Imaginary Frequencies: 0

xyz			
C	-2.048555	-0.322477	-0.148605
C	-0.907285	0.491579	0.444380
C	-1.806529	-1.715973	-0.542103
C	-0.353627	-0.174330	1.685811
H	-1.249581	1.492497	0.704802
C	-0.646688	-2.371976	-0.437306
H	-2.674536	-2.218380	-0.956171
C	0.390529	-1.264653	1.540776
H	-0.585567	0.246511	2.656905
C	0.626979	-1.781921	0.137407
H	-0.599358	-3.400892	-0.779062
H	0.814160	-1.793281	2.386829
H	1.411305	-2.539346	0.137657
C	2.503924	-0.147420	-0.347284
C	1.106695	-0.605268	-0.747867
H	1.161926	-0.943847	-1.785076
C	1.174438	1.758062	-0.183928
C	0.222202	0.646562	-0.608331
H	-0.219910	0.942806	-1.562461
O	0.890909	2.904571	0.046803
O	3.495588	-0.820526	-0.258443
N	2.441627	1.214434	-0.095825
H	3.244582	1.750032	0.201612
N	-3.234520	0.113308	-0.373102
N	-3.588255	1.382599	-0.026093
H	-4.427812	1.648182	-0.516430
H	-2.871636	2.097864	-0.088050



H	0.442300	1.324732	-0.594544
H	1.031682	-0.634416	-1.733812
H	2.205748	-2.527900	-0.507245
H	0.675935	1.436035	1.894214

#### 4 product

- Electronic Energy (a.u.): -702.810246669

- Number of Imaginary Frequencies: 0

xyz			
C	-1.081171	0.993009	0.277072
C	-0.722106	0.383520	1.613183
C	-0.457353	-0.917143	1.547768
C	-0.598601	-1.471945	0.153791
C	-2.223258	0.160919	-0.297548
H	-1.365736	2.040006	0.321180
H	-0.687485	0.982926	2.513433
H	-0.159386	-1.540382	2.380095
H	-0.505835	-2.552105	0.093081
O	-3.274644	0.575142	-0.682822
O	-1.911385	-1.154176	-0.360204
C	1.842061	-0.908799	-0.330179
C	0.398455	-0.749247	-0.781599
C	0.109337	0.757645	-0.700389
C	1.400360	1.382454	-0.186829
H	0.292775	-1.154003	-1.789303
H	-0.124321	1.197146	-1.671672
N	2.327193	0.359251	-0.055796
H	3.262241	0.517969	0.292110
O	2.459847	-1.932441	-0.215937
O	1.600063	2.537876	0.068967

#### 5 product

- Electronic Energy (a.u.): -737.6328059780001

- Number of Imaginary Frequencies: 0

xyz			
C	-0.725293	1.082786	0.148571
C	-0.481980	0.523687	1.532131
C	-0.273853	-0.798425	1.550582
C	-0.360391	-1.411112	0.180373
C	-1.899170	0.299755	-0.382220
H	-0.953483	2.145678	0.144689
H	-0.588338	1.135478	2.421608
H	-0.188377	-1.403489	2.445326
H	-0.260106	-2.496202	0.184371
O	-1.625005	-1.103628	-0.397843
C	2.120010	-0.994868	-0.268962
C	0.705590	-0.771805	-0.753666
C	0.501229	0.758215	-0.742374
C	1.807327	1.321960	-0.219697
H	0.593323	-1.210983	-1.746923
H	0.316522	1.160544	-1.740866
N	2.663876	0.249716	0.002517
H	3.589738	0.365386	0.386139
O	2.708916	-2.040617	-0.126454
O	2.107279	2.473628	-0.019510
N	-3.125241	0.728650	-0.233164
N	-4.184545	-0.032836	-0.284319
H	-3.878258	-1.011347	-0.407547

#### 5-prot product

- Electronic Energy (a.u.): -738.245746491

- Number of Imaginary Frequencies: 0

xyz			
C	-0.673580	1.066412	0.411707
C	-0.203326	0.476542	1.723183
C	0.001427	-0.836935	1.670595
C	-0.296035	-1.424678	0.315216
C	-1.876981	0.264946	-0.010124
H	-0.913224	2.124729	0.455371
H	-0.061616	1.091010	2.603026



C -2.402129 -0.860448 -0.444293  
C -1.127148 -0.136987 -0.743218  
H -0.372793 -0.601220 -1.364333  
O -2.677095 -2.038296 -0.582386  
O -3.350238 2.421291 0.148179  
N -3.248757 0.108596 0.050129  
H -4.220790 -0.054588 0.250983  
N 3.882116 1.974061 -0.355715  
H 4.692147 2.290746 -0.897763

Imaginary Frequencies

412*i* cm<sup>-1</sup>

#### **2-TS<sub>2</sub>-exo**

- Electronic Energy (a.u.): -739.795416414

- Number of Imaginary Frequencies: 1

xyz

N	-2.455800	1.173943	-0.106986
C	-1.708701	0.011375	-0.039632
C	-1.285500	-0.325395	1.238200
C	-1.364783	-0.755802	-1.222694
C	-0.915077	-1.675491	1.647640
H	-1.626572	0.348623	2.017394
C	-0.330592	-1.601275	-1.316178
H	-1.991686	-0.593306	-2.093346
C	-0.064904	-2.454918	0.969285
H	-1.354282	-2.034422	2.576248
C	0.676644	-1.895660	-0.211392
H	-0.185966	-2.144104	-2.245575
H	0.145640	-3.465195	1.309843
H	1.360343	-2.651730	-0.603298
C	1.131528	1.569584	0.909186
C	1.053276	0.230873	1.336577
H	1.147780	-0.010496	2.385552
C	1.812982	0.281534	-0.926628
C	1.566708	-0.675815	0.242384
H	2.545879	-1.103777	0.501119
O	2.221610	-0.012741	-2.036777
O	0.943074	2.650946	1.466292
N	1.483287	1.521880	-0.487048
H	1.508842	2.343623	-1.068734
N	-2.869422	1.527559	-1.247074
H	-3.403391	2.387409	-1.088051

Imaginary Frequencies

257*i* cm<sup>-1</sup>

#### **2-prot-TS-exo**

- Electronic Energy (a.u.): -740.326170045

- Number of Imaginary Frequencies: 1

xyz

N	-2.687176	0.176518	-0.014166
C	-1.552904	-0.417854	-0.135011
C	-0.993976	-0.908124	1.142693
C	-0.829211	-0.574926	-1.395576
C	-0.324689	-2.123280	1.330056
H	-1.594835	-0.552861	1.975282
C	0.362207	-1.167114	-1.565332
H	-1.242841	-0.057197	-2.253664
C	0.694207	-2.585111	0.520517
H	-0.442302	-2.596658	2.300474
C	1.169727	-1.895331	-0.594617
H	0.821708	-1.074471	-2.544363
H	1.303907	-3.401450	0.895632
H	2.118997	-2.237715	-0.995845
C	0.263773	1.671238	0.935105
C	0.789036	0.359542	1.433947
H	0.751994	0.168019	2.495537
C	1.946224	0.990220	-0.497128
C	1.835101	-0.021516	0.596530
H	2.711076	-0.577475	0.891020
O	2.735602	1.031325	-1.407224

O -0.543472 2.397634 1.446700  
 N 0.936092 1.912897 -0.261206  
 H 0.743622 2.700019 -0.860067  
 N -3.294671 0.666163 -1.152628  
 H -4.241295 0.923582 -0.914873  
 H -3.303756 0.019029 -1.936047

#### Imaginary Frequencies

572*i* cm<sup>-1</sup>

#### 3-TS-exo

- Electronic Energy (a.u.): -1327.69436894
- Number of Imaginary Frequencies: 1

xyz

N 1.306786 1.001120 0.070697  
 C 0.016944 1.329404 -0.189216  
 C -0.608983 1.990506 0.849135  
 C -0.619696 0.975367 -1.467357  
 C -1.951174 2.413356 0.977209  
 H 0.056797 2.231245 1.674071  
 C -1.926466 0.819012 -1.690618  
 H 0.069390 0.808208 -2.287576  
 C -3.033763 1.991176 0.234471  
 H -2.157115 3.079573 1.809700  
 C -3.049739 0.960781 -0.730516  
 H -2.227912 0.539413 -2.696156  
 H -4.004523 2.367671 0.553891  
 H -4.014863 0.800388 -1.203744  
 C -1.014702 -1.415923 1.201951  
 C -2.179393 -0.668602 1.568158  
 H -2.271271 -0.155520 2.511440  
 C -2.570207 -1.701383 -0.487898  
 C -3.097844 -0.701619 0.512845  
 H -4.172171 -0.645508 0.638018  
 O -3.113020 -2.103927 -1.497381  
 O 0.060384 -1.571546 1.759479  
 N -1.323622 -2.046827 -0.039696  
 H -0.629262 -2.500195 -0.610578  
 N 1.917530 0.329977 -0.825294  
 S 3.486716 -0.067770 -0.277720  
 O 4.341400 1.113420 -0.195404  
 O 3.920054 -1.174983 -1.118127  
 C 3.215791 -0.683486 1.381406  
 H 4.159803 -1.129824 1.693967  
 H 2.939021 0.155401 2.015092  
 H 2.404642 -1.411675 1.359492

#### Imaginary Frequencies

519*i* cm<sup>-1</sup>

#### 3-prot-TS-exo

- Electronic Energy (a.u.): -1328.21979775
- Number of Imaginary Frequencies: 1

xyz

N 1.161732 -0.758946 -0.259137  
 C -0.066196 -1.012033 0.029039  
 C -0.874324 -1.378398 -1.148057  
 C -0.652582 -0.894392 1.360247  
 C -1.977972 -2.238332 -1.176055  
 H -0.262824 -1.350047 -2.045503  
 C -1.959824 -0.958230 1.656301  
 H 0.014676 -0.608087 2.164416  
 C -3.024452 -2.193177 -0.279940  
 H -2.130553 -2.796562 -2.094638  
 C -3.081695 -1.298697 0.791917  
 H -2.243804 -0.701733 2.672204  
 H -3.936965 -2.720471 -0.539890  
 H -4.046325 -1.199730 1.280332  
 C -0.997754 1.529279 -1.033699  
 C -2.031147 0.513034 -1.411261  
 H -2.156625 0.271725 -2.455714  
 C -2.683856 1.614317 0.545297

C -3.064648 0.594217 -0.481227  
 H -4.109584 0.421135 -0.685587  
 O -3.313845 1.992014 1.498941  
 O -0.009662 1.855497 -1.636200  
 N -1.420185 2.062049 0.180109  
 H -0.892132 2.738507 0.708627  
 N 1.997729 -0.342247 0.759120  
 H 2.031902 -0.921586 1.597403  
 S 3.596775 -0.100745 0.222424  
 O 4.049334 -1.171988 -0.637046  
 O 4.313591 0.201781 1.446187  
 C 3.365865 1.362248 -0.761723  
 H 4.316977 1.553156 -1.257419  
 H 2.575866 1.162206 -1.485077  
 H 3.092221 2.179952 -0.098677

Imaginary Frequencies  
 $568i \text{ cm}^{-1}$

#### 4-TS-exo

- Electronic Energy (a.u.): -702.727064936  
 - Number of Imaginary Frequencies: 1

xyz  
 C 1.567988 1.029725 -0.394932  
 C 2.395130 0.036293 -0.922954  
 C 2.156284 -1.260061 -0.520848  
 C 1.118571 -1.441138 0.394272  
 C 1.045348 0.850145 0.959921  
 H 1.629978 2.059767 -0.721493  
 H 3.077552 0.262146 -1.733670  
 H 2.598044 -2.119418 -1.007224  
 H 0.814480 -2.413201 0.761414  
 O 0.780109 1.703313 1.754152  
 O 0.831583 -0.470090 1.297335  
 C -1.400604 1.091748 -0.578340  
 C -0.378059 0.289753 -1.327974  
 C -0.519152 -1.044697 -0.962838  
 C -1.626759 -1.122729 0.050624  
 H -0.030402 0.653506 -2.282266  
 H -0.340755 -1.892674 -1.606566  
 N -2.038083 0.185399 0.263519  
 H -2.710271 0.453958 0.965253  
 O -1.650207 2.261000 -0.681680  
 O -2.077052 -2.103735 0.579984

Imaginary Frequencies  
 $572i \text{ cm}^{-1}$

#### 5-TS<sub>1</sub>-exo

- Electronic Energy (a.u.): -737.590551235  
 - Number of Imaginary Frequencies: 1

xyz  
 C 1.159036 0.947905 1.385182  
 C 1.091987 2.182622 0.675552  
 C 1.141756 2.118212 -0.699620  
 C 1.135130 0.868237 -1.323231  
 C 1.415812 -0.205463 0.722324  
 H 0.938187 0.875445 2.442379  
 H 0.943642 3.116597 1.200981  
 H 0.944404 2.995913 -1.307074  
 H 1.293355 0.735140 -2.384487  
 N 1.414785 -1.424196 1.364395  
 O 1.722280 -0.197426 -0.625784  
 C -2.020820 0.158335 0.704553  
 C -1.758217 1.172442 -0.275221  
 C -1.071487 0.608577 -1.353077  
 C -1.031961 -0.867496 -1.124005  
 H -2.051863 2.201552 -0.140520  
 H -1.100431 0.972143 -2.372023  
 N -1.589040 -1.064791 0.119980  
 H -1.456401 -1.909706 0.651917

O	-2.525295	0.203743	1.818735
O	-0.590360	-1.738661	-1.850937
N	1.553206	-2.479053	0.689407
H	1.616034	-2.252285	-0.318500

Imaginary Frequencies

434*i* cm<sup>-1</sup>

### 5-TS<sub>2</sub>-exo

- Electronic Energy (a.u.): -737.603430076

- Number of Imaginary Frequencies: 1

xyz

C	0.989107	-0.620611	-1.275576
C	1.842377	-1.655129	-0.668356
C	1.979107	-1.599165	0.659596
C	1.143707	-0.515384	1.281307
C	1.123579	0.653587	-0.730526
H	0.718187	-0.676940	-2.321199
H	2.321778	-2.401963	-1.292897
H	2.585404	-2.279293	1.246331
N	0.837659	1.779176	-1.401356
O	1.446748	0.718021	0.625189
C	-1.865575	-0.671359	-0.737348
C	-0.751105	-1.422156	-0.259555
C	-0.364753	-0.895361	1.111026
C	-1.246578	0.344278	1.279341
H	-0.610795	-1.588595	1.924539
N	-2.014332	0.428443	0.154706
H	-2.630738	1.202975	-0.034752
O	-2.590204	-0.806811	-1.716829
O	-1.266130	1.103662	2.225906
N	0.892270	2.924637	-0.833470
H	1.126585	2.801986	0.165568
H	-0.700963	-2.476903	-0.494452
H	1.358843	-0.338243	2.334119

Imaginary Frequencies

393*i* cm<sup>-1</sup>

### 5-prot-TS-exo

- Electronic Energy (a.u.): -738.159596217

- Number of Imaginary Frequencies: 1

xyz

C	-1.442063	0.620288	1.075299
C	-2.432694	-0.350724	0.966216
C	-2.372751	-1.192445	-0.132144
C	-1.318747	-0.988719	-1.017056
C	-0.845238	1.140635	-0.144136
H	-1.350302	1.258005	1.944823
H	-3.097170	-0.555117	1.796944
H	-2.953577	-2.102992	-0.200695
H	-1.141100	-1.608769	-1.885942
N	-0.323810	2.291543	-0.241425
O	-0.828863	0.271891	-1.218036
C	1.422149	0.067373	1.263410
C	0.273985	-0.883711	1.380126
C	0.269505	-1.702952	0.253689
C	1.407226	-1.264567	-0.626546
H	-0.092551	-1.147996	2.359780
H	-0.033361	-2.739216	0.237204
N	1.991171	-0.184883	0.016565
H	2.676531	0.417695	-0.411915
O	1.808810	0.873964	2.064746
O	1.750726	-1.734340	-1.680248
N	0.340211	2.580232	-1.419277
H	0.371517	3.582050	-1.535600
H	-0.046609	2.124905	-2.240486

Imaginary Frequencies

593*i* cm<sup>-1</sup>

### 1 product - exo

- Electronic Energy (a.u.): -704.972548748

- Number of Imaginary Frequencies: 0

xyz

O	2.452969	1.496911	1.030741
C	1.670296	0.646167	0.679130
C	1.367042	0.428145	-0.808048
C	1.003288	-0.226660	1.679220
C	1.908669	-0.925319	-1.219036
H	1.867533	1.239517	-1.334335
C	0.289123	-1.318699	1.393859
H	1.172684	0.065664	2.710180
C	1.258348	-2.012116	-0.821641
H	2.822554	-0.973573	-1.798772
C	-0.004545	-1.833340	0.000112
H	-0.142644	-1.882319	2.215438
H	1.595054	-3.012630	-1.066398
H	-0.545921	-2.775153	0.084894
C	-0.913696	1.587097	-0.448514
C	-0.150293	0.461016	-1.136289
H	-0.230379	0.647824	-2.209872
C	-2.090078	-0.361480	0.076198
C	-0.905316	-0.823415	-0.762236
H	-1.300649	-1.327742	-1.646235
O	-2.936333	-1.051328	0.580168
O	-0.644446	2.756264	-0.440759
N	-2.018764	1.016377	0.169190
H	-2.681444	1.560607	0.703044

## 2-inter-exo

- Electronic Energy (a.u.): -739.806318049

- Number of Imaginary Frequencies: 0

xyz

N	-3.132397	-1.188559	0.069415
C	-2.216802	-0.102434	0.139766
C	-2.338563	0.741338	-0.909058
C	-1.333101	0.046084	1.285170
C	-1.633049	1.982163	-1.130776
H	-3.095250	0.467473	-1.638589
C	-0.243123	0.815039	1.381924
H	-1.614085	-0.548044	2.147842
C	-0.479562	2.389262	-0.577560
H	-2.103548	2.656369	-1.842988
C	0.448914	1.630651	0.323826
H	0.269267	0.813868	2.341169
H	-0.127677	3.379135	-0.865173
H	1.059692	2.370950	0.853118
C	2.509198	0.196194	0.462114
C	1.479972	0.795583	-0.510791
C	1.597691	-1.543148	-0.849263
C	0.981919	-0.384405	-1.276921
H	0.257993	-0.343566	-2.076190
O	1.562656	-2.746917	-1.150268
O	3.161892	0.816632	1.297428
N	2.520769	-1.123355	0.225140
H	3.091881	-1.781892	0.728972
N	-3.152564	-1.950114	1.052417
H	-3.848055	-2.673639	0.835775
H	2.021792	1.537857	-1.120608

## 2 product - exo

- Electronic Energy (a.u.): -739.839987051

- Number of Imaginary Frequencies: 0

xyz

C	-1.589531	0.033336	0.184978
C	-0.937208	0.207573	-1.174760
C	-1.039004	0.668874	1.338309
C	-0.892713	1.683397	-1.504924
H	-1.553273	-0.341847	-1.888410
C	0.069460	1.450971	1.388376
H	-1.599789	0.503200	2.254277

C	-0.008288	2.450565	-0.861576
H	-1.655875	2.106639	-2.151999
C	0.897343	1.789635	0.158291
H	0.381304	1.888957	2.330807
H	-0.008389	3.533550	-0.950815
H	1.706500	2.463376	0.449557
C	0.659257	-1.721320	-0.661212
C	0.512983	-0.334479	-1.258841
H	0.787693	-0.409465	-2.316077
C	2.159576	-0.386942	0.533792
C	1.535163	0.539903	-0.494483
H	2.338823	0.866137	-1.163859
O	3.042637	-0.137921	1.320522
O	0.153372	-2.752626	-1.024143
N	1.569487	-1.627194	0.385723
H	1.802822	-2.414219	0.971523
N	-2.739575	-0.663926	0.192085
N	-3.370258	-0.845552	1.301781
H	-4.187693	-1.404319	1.049139

### 2-prot product - exo

- Electronic Energy (a.u.): -740.419836784

- Number of Imaginary Frequencies: 0

xyz			
C	-1.607487	-0.006786	0.104849
C	-0.894009	0.232179	-1.213844
C	-0.998323	0.469212	1.355506
C	-0.855057	1.724163	-1.480286
H	-1.474114	-0.291481	-1.972427
C	0.081868	1.253447	1.434608
H	-1.438385	0.119708	2.283787
C	-0.017119	2.467571	-0.766707
H	-1.533952	2.151318	-2.209503
C	0.870281	1.772191	0.247356
H	0.470710	1.501822	2.416863
H	0.044180	3.544272	-0.877470
H	1.642422	2.449068	0.612904
C	0.734479	-1.689592	-0.672290
C	0.565601	-0.291175	-1.249619
H	0.851885	-0.354303	-2.302294
C	2.257118	-0.356305	0.496804
C	1.565051	0.588410	-0.476417
H	2.330848	0.997375	-1.139607
O	3.104318	-0.077574	1.304934
O	0.150585	-2.690370	-0.985244
N	1.731228	-1.618351	0.293674
H	2.020733	-2.421517	0.833103
N	-2.737860	-0.605722	0.023774
N	-3.463978	-0.828557	1.164111
H	-3.471115	-0.069033	1.836457
H	-4.402589	-1.095162	0.909992

### 3 product - exo

- Electronic Energy (a.u.): -1327.7747073

- Number of Imaginary Frequencies: 0

xyz			
N	1.334522	-0.447970	-0.263276
C	0.073769	-0.713591	-0.059144
C	-0.810314	-0.725383	-1.294890
C	-0.484351	-1.002696	1.249581
C	-1.479435	-2.074378	-1.443684
H	-0.156370	-0.510992	-2.140327
C	-1.770591	-1.289152	1.510969
H	0.234439	-0.982140	2.062292
C	-2.466830	-2.384615	-0.606407
H	-1.093815	-2.782893	-2.169445
C	-2.854380	-1.363756	0.446022
H	-2.075905	-1.485682	2.533487
H	-2.941405	-3.360919	-0.604622
H	-3.795758	-1.641880	0.923258

C	-1.433403	1.711306	-0.823185
C	-1.934199	0.343920	-1.254991
H	-2.329464	0.451122	-2.269048
C	-3.099198	1.159133	0.719580
C	-3.064657	-0.001320	-0.262098
H	-4.033485	-0.021985	-0.770695
O	-3.846064	1.312044	1.655099
O	-0.624731	2.415348	-1.368512
N	-2.125869	2.059196	0.331120
H	-1.936250	2.909449	0.840221
N	2.151484	-0.390739	0.777370
S	3.683319	-0.051976	0.265259
O	4.220925	-1.014218	-0.701715
O	4.476097	0.200174	1.467673
C	3.542338	1.509057	-0.620670
H	4.533749	1.757387	-0.999610
H	2.828517	1.373073	-1.431605
H	3.189377	2.265737	0.078602

#### 3-prot product - exo

- Electronic Energy (a.u.): -1328.31141532

- Number of Imaginary Frequencies: 0

xyz			
N	1.324922	-0.213219	-0.321900
C	0.106378	-0.520018	-0.081007
C	-0.784407	-0.619772	-1.305467
C	-0.455646	-0.766548	1.254607
C	-1.279349	-2.044806	-1.450238
H	-0.167535	-0.327980	-2.153947
C	-1.699095	-1.197706	1.490958
H	0.171006	-0.544707	2.111806
C	-2.213164	-2.472753	-0.609491
H	-0.838930	-2.683084	-2.207062
C	-2.737717	-1.501138	0.430045
H	-2.018391	-1.302435	2.522773
H	-2.599882	-3.484906	-0.634512
H	-3.625601	-1.900050	0.919830
C	-1.700005	1.718228	-0.746248
C	-2.021385	0.313366	-1.238908
H	-2.393850	0.417358	-2.260684
C	-3.408539	0.953596	0.652153
C	-3.136528	-0.195563	-0.309588
H	-4.058567	-0.389296	-0.861978
O	-4.198268	0.973300	1.558711
O	-0.869021	2.473253	-1.172452
N	-2.564880	1.993765	0.303791
H	-2.542933	2.867877	0.809495
N	2.210921	-0.100326	0.716907
H	2.134669	-0.750184	1.497179
S	3.834628	-0.020096	0.218561
O	4.127696	-0.991989	-0.810299
O	4.564049	-0.035209	1.470353
C	3.859628	1.601241	-0.511211
H	4.856298	1.735885	-0.930052
H	3.102093	1.625868	-1.293521
H	3.654142	2.332047	0.267973

#### 4 product - exo

- Electronic Energy (a.u.): -702.807831165

- Number of Imaginary Frequencies: 0

xyz			
C	1.166338	0.984452	-0.480127
C	2.265487	0.107469	-1.041554
C	2.115158	-1.180240	-0.749971
C	0.886982	-1.450513	0.083520
C	1.111811	0.694946	1.016268
H	1.301869	2.049922	-0.642806
H	3.083930	0.526253	-1.612685
H	2.779648	-1.975698	-1.059985
H	0.795877	-2.470742	0.445661

O	1.199293	1.494252	1.897609
O	0.921459	-0.621920	1.267283
C	-1.394542	1.163851	-0.490001
C	-0.174089	0.471910	-1.089343
C	-0.343063	-1.014543	-0.737752
C	-1.629183	-1.092591	0.079244
H	-0.164995	0.663481	-2.162711
H	-0.446870	-1.660110	-1.610680
N	-2.140410	0.192412	0.160697
H	-2.986259	0.409120	0.669194
O	-1.674099	2.327969	-0.560367
O	-2.122867	-2.074996	0.558905

### 5-inter-exo

- Electronic Energy (a.u.): -737.630235325

- Number of Imaginary Frequencies: 0

xyz			
C	-2.625148	0.352530	0.613383
C	-2.661282	-1.060481	0.944649
C	-1.724798	-1.874203	0.447456
C	-0.603917	-1.352712	-0.406870
C	-1.741123	0.755445	-0.309832
H	-3.247434	1.089276	1.100049
H	-3.444422	-1.440614	1.591685
H	-1.709494	-2.934426	0.677228
H	-0.445690	-2.005721	-1.270310
N	-1.655132	2.126466	-0.659630
O	-0.952941	-0.080301	-0.999696
C	1.872919	0.692230	1.088120
C	0.835613	-0.168465	1.391092
C	0.725452	-1.244784	0.357797
C	1.842636	-0.913161	-0.645941
H	0.237636	-0.105290	2.287267
H	0.930368	-2.266402	0.724319
N	2.435081	0.200005	-0.188362
H	3.220597	0.645488	-0.633898
O	2.395011	1.687902	1.608713
O	2.104937	-1.547138	-1.661908
N	-0.691496	2.491247	-1.350227
H	-0.058891	1.691562	-1.544804

### 5 product - exo

- Electronic Energy (a.u.): -737.630510875

- Number of Imaginary Frequencies: 0

xyz			
C	0.792415	0.709499	-1.048569
C	1.546331	-0.383693	-1.774710
C	1.322178	-1.612732	-1.290113
C	0.374250	-1.601743	-0.124551
C	1.229454	0.557239	0.388358
H	1.025964	1.711228	-1.402185
H	2.312681	-0.153028	-2.507625
H	1.876534	-2.500874	-1.570663
H	0.227174	-2.578069	0.337591
N	2.335303	1.139406	0.799901
O	0.886841	-0.735257	0.893670
C	-1.554328	1.335165	-0.308620
C	-0.718997	0.401095	-1.165216
C	-0.976590	-1.006876	-0.583964
C	-1.916459	-0.790332	0.589183
H	-1.049683	0.496551	-2.203029
H	-1.459316	-1.684366	-1.292663
N	-2.167422	0.566003	0.672247
H	-2.723952	0.972457	1.408640
O	-1.726028	2.519651	-0.447616
O	-2.403428	-1.625969	1.311802
N	3.048495	0.719686	1.801539
H	2.627357	-0.152700	2.160498

### 5-prot product - exo

- Electronic Energy (a.u.): -738.243960475

- Number of Imaginary Frequencies: 0

xyz

C	-0.904611	-0.101158	1.301274
C	-1.573542	-1.458737	1.360803
C	-1.309376	-2.226943	0.307331
C	-0.410122	-1.553983	-0.699288
C	-1.295158	0.502251	-0.021930
H	-1.164485	0.572589	2.113085
H	-2.217847	-1.738552	2.184824
H	-1.694737	-3.225908	0.149588
H	-0.260505	-2.110068	-1.620901
N	-1.829066	1.639416	-0.152007
O	-0.999561	-0.295724	-1.093370
C	1.423637	0.918976	1.027768
C	0.629533	-0.364498	1.238572
C	0.925966	-1.226172	-0.002958
C	1.821987	-0.363810	-0.886195
H	0.955829	-0.825382	2.171485
H	1.454209	-2.152340	0.228285
N	2.038610	0.825473	-0.212872
H	2.588667	1.577882	-0.602423
O	1.518980	1.846389	1.782624
O	2.271841	-0.652501	-1.961491
N	-2.043639	2.086531	-1.441880
H	-2.797995	2.756101	-1.434229
H	-2.204432	1.344874	-2.116770

### 1...maleimide (implicit solvent, DCM)

- Electronic Energy (a.u.): -704.944357365

- Number of Imaginary Frequencies: 1

xyz

O	3.065442	-0.054532	-1.694739
C	2.443238	-0.024705	-0.629676
C	2.088808	-1.286029	0.020128
C	2.112746	1.271060	-0.037729
C	1.268952	-1.533329	1.069098
H	2.542263	-2.143920	-0.467909
C	1.297810	1.580930	0.998326
H	2.582081	2.097201	-0.563966
C	0.521410	-0.627836	1.887577
H	1.141350	-2.581052	1.325401
C	0.533910	0.727558	1.856733
H	1.189730	2.641399	1.206763
H	-0.117471	-1.095032	2.630035
H	-0.096105	1.239816	2.576607
C	-1.974411	1.138400	-0.385293
C	-1.015671	0.642983	-1.426877
H	-0.442961	1.315363	-2.048066
C	-1.977923	-1.149791	-0.354625
C	-1.017692	-0.685316	-1.409135
H	-0.447424	-1.375855	-2.012440
O	-2.235456	-2.280266	-0.025586
O	-2.228651	2.278082	-0.086831
N	-2.523691	0.002640	0.189645
H	-3.183362	0.013787	0.952153

### 2...maleimide (implicit solvent, DCM)

- Electronic Energy (a.u.): -739.8676979169999

- Number of Imaginary Frequencies: 0

xyz

N	3.059617	-1.189856	-0.256647
C	2.227362	-0.255775	0.211340
C	1.345975	-0.693341	1.256502
C	2.283560	1.126212	-0.274197
C	0.294181	-0.076246	1.859623
H	1.565279	-1.705863	1.593328
C	1.438053	2.150815	-0.067351
H	3.159616	1.326510	-0.884855
C	-0.271019	1.228227	1.552578

H	-0.222551	-0.637206	2.632394
C	0.187733	2.166279	0.702443
H	1.700852	3.102488	-0.523709
H	-1.205464	1.453556	2.062432
H	-0.409238	3.068462	0.596875
C	-2.416982	0.571487	-0.801492
C	-1.135099	0.116513	-1.418223
H	-0.569780	0.734046	-2.099228
C	-1.926650	-1.526099	-0.018584
C	-0.850589	-1.102312	-0.963609
H	0.005745	-1.722374	-1.180064
O	-2.059653	-2.580783	0.556759
O	-3.034357	1.591824	-0.999691
N	-2.803743	-0.451911	0.052986
H	-3.664235	-0.457217	0.577631
N	3.875791	-0.892516	-1.234559
H	4.411053	-1.745302	-1.397993

### 2-prot...maleimide (implicit solvent, DCM)

- Electronic Energy (a.u.): -740.3849964359999  
- Number of Imaginary Frequencies: 0

xyz			
N	3.620008	-0.415348	-0.667744
C	2.439138	-0.299226	-0.158996
C	1.650539	-1.530454	-0.113961
C	1.855835	0.990572	0.229664
C	0.613908	-1.836422	0.688925
H	1.999422	-2.297259	-0.800044
C	0.871507	1.238071	1.113925
H	2.277648	1.850807	-0.283848
C	-0.017175	-1.026547	1.707853
H	0.204547	-2.836622	0.582970
C	0.100594	0.303345	1.903359
H	0.606535	2.282152	1.256749
H	-0.702586	-1.559815	2.360032
H	-0.497077	0.744013	2.695287
C	-2.272866	1.348583	-0.315969
C	-1.336855	0.860295	-1.380448
H	-0.663790	1.523677	-1.902166
C	-2.541801	-0.911223	-0.546401
C	-1.492514	-0.451959	-1.513792
H	-0.979514	-1.136186	-2.172429
O	-2.942801	-2.032045	-0.355761
O	-2.405712	2.470851	0.104369
N	-2.975110	0.231363	0.108307
H	-3.651686	0.235631	0.855765
N	4.393347	0.725266	-0.777330
H	5.350025	0.446693	-0.942898
H	4.355011	1.337295	0.034115

### 3...maleimide (implicit solvent, DCM)

- Electronic Energy (a.u.): -1327.8088825500001  
- Number of Imaginary Frequencies: 0

xyz			
N	-1.303755	-0.731916	0.591817
C	-0.164466	-1.345661	0.501014
C	0.667364	-1.314316	1.702060
C	0.226018	-2.107914	-0.690795
C	2.002294	-1.459629	1.806672
H	0.115305	-1.083900	2.609771
C	1.458772	-2.440346	-1.112016
H	-0.616540	-2.420012	-1.300630
C	2.971526	-1.707130	0.754553
H	2.424678	-1.340738	2.800415
C	2.740621	-2.123630	-0.505940
H	1.518819	-3.003703	-2.039817
H	4.009671	-1.562594	1.041168
H	3.608006	-2.284020	-1.140082
C	3.082570	1.409288	-0.736373
C	1.857476	0.996376	-1.490853

H	1.911300	0.499290	-2.447620
C	1.235437	1.973755	0.493176
C	0.783337	1.317682	-0.777449
H	-0.259336	1.134094	-1.000398
O	0.565255	2.437305	1.381482
O	4.238771	1.301622	-1.065631
N	2.623209	1.968219	0.445541
H	3.217515	2.360626	1.158827
N	-2.056121	-0.668433	-0.542514
S	-3.467575	0.066207	-0.223485
O	-4.256408	-0.561358	0.854285
O	-4.163409	0.202953	-1.512881
C	-3.083296	1.721332	0.353884
H	-4.018906	2.208841	0.626075
H	-2.421134	1.636475	1.214371
H	-2.591106	2.258243	-0.455877

### 3-prot...maleimide (implicit solvent, DCM)

- Electronic Energy (a.u.): -1328.28325651
- Number of Imaginary Frequencies: 0

xyz			
N	-1.563508	0.735210	-1.544953
C	-0.603322	1.363467	-0.933873
C	0.622857	1.473120	-1.715772
C	-0.744145	2.027861	0.353374
C	1.879227	1.735338	-1.298128
H	0.478183	1.264296	-2.771285
C	0.215720	2.381743	1.233775
H	-1.772840	2.235468	0.627529
C	2.368543	1.979051	0.031456
H	2.643317	1.716417	-2.069374
C	1.643843	2.240325	1.142582
H	-0.136855	2.834046	2.156557
H	3.448792	1.980815	0.135711
H	2.192074	2.432486	2.058934
C	2.659611	-1.146602	1.254154
C	1.209918	-1.305818	0.914114
H	0.431276	-1.248890	1.659380
C	2.467593	-1.518028	-0.997822
C	1.096102	-1.519615	-0.392699
H	0.193811	-1.663620	-0.968675
O	2.778610	-1.688441	-2.149916
O	3.160023	-0.948586	2.333439
N	3.341333	-1.275721	0.052768
H	4.344767	-1.237610	-0.038527
N	-2.786353	0.657633	-0.825045
H	-3.535152	0.625656	-1.511291
S	-3.036266	-0.727828	0.135412
O	-2.002372	-1.720661	-0.107783
O	-4.435469	-1.071439	-0.068914
C	-2.849080	-0.138169	1.802162
H	-3.085813	-0.981572	2.450518
H	-1.820789	0.183931	1.952183
H	-3.548361	0.680935	1.957827

### 4...maleimide (implicit solvent, DCM)

- Electronic Energy (a.u.): -702.785024924
- Number of Imaginary Frequencies: 0

xyz			
C	1.633927	-0.831159	0.963248
C	0.943736	0.069099	1.701008
C	0.823138	1.421114	1.257452
C	1.422961	1.760021	0.103116
C	2.277206	-0.442743	-0.271355
H	1.739561	-1.866506	1.257015
H	0.467964	-0.236790	2.625585
H	0.266770	2.160668	1.814456
H	1.407629	2.744753	-0.343449
O	2.919802	-1.147154	-1.012205
O	2.130631	0.885449	-0.632775

C	-2.026564	0.865753	-0.368108
C	-1.123155	0.336407	-1.441772
C	-0.888465	-0.950832	-1.205622
C	-1.624299	-1.352978	0.038349
H	-0.763017	0.957267	-2.248650
H	-0.288669	-1.649410	-1.770298
N	-2.256137	-0.202237	0.486570
H	-2.861538	-0.164730	1.292275
O	-2.475792	1.977657	-0.250243

**5...maleimide (implicit solvent, DCM)**

- Electronic Energy (a.u.): -737.684597341
- Number of Imaginary Frequencies: 0

xyz			
C	1.325310	-1.146189	1.008584
C	0.329136	-0.656851	1.788740
C	0.099905	0.774097	1.765582
C	0.887440	1.551015	1.007330
C	2.139095	-0.306256	0.195016
H	1.535945	-2.208290	0.953751
H	-0.284156	-1.307399	2.398763
H	-0.708090	1.232277	2.321103
H	0.775338	2.625197	0.923013
N	3.029030	-0.768010	-0.627473
O	1.937625	1.099910	0.278063
C	-2.058395	1.048904	-0.602916
C	-0.896694	0.467287	-1.338398
C	-0.900435	-0.854768	-1.165733
C	-2.061326	-1.224424	-0.304034
H	-0.199576	1.075535	-1.894595
H	-0.205044	-1.588027	-1.544181
N	-2.682611	-0.025571	0.017119
H	-3.530786	0.046734	0.556650
O	-2.431635	2.198265	-0.558117
O	-2.433535	-2.323144	0.038823
N	3.726346	0.071067	-1.387115
H	4.343156	-0.535574	-1.927410

**5-prot...maleimide (implicit solvent, DCM)**

- Electronic Energy (a.u.): -738.214410138
- Number of Imaginary Frequencies: 0

xyz			
C	-1.821989	1.565149	-0.600420
C	-1.051429	2.388417	0.129823
C	-0.414414	1.891696	1.330992
C	-0.643415	0.629338	1.703721
C	-1.992105	0.183157	-0.204903
H	-2.315551	1.875767	-1.511653
H	-0.900116	3.417374	-0.171666
H	0.226576	2.518507	1.934318
H	-0.243210	0.149492	2.585881
N	-2.615405	-0.673317	-0.914521
O	-1.431509	-0.219373	0.991973
C	1.706593	-1.433186	0.304598
C	0.800009	-1.235370	-0.873843
C	1.105976	-0.079295	-1.453332
C	2.229160	0.559244	-0.693038
H	0.018370	-1.940162	-1.123193
H	0.652238	0.391859	-2.312411
N	2.538579	-0.324140	0.330242
H	3.246090	-0.159732	1.029504
O	1.725164	-2.350024	1.087120
O	2.765764	1.618422	-0.901204
N	-2.593170	-1.989297	-0.471677
H	-3.388641	-2.472586	-0.864160
H	-2.591467	-2.080332	0.540380

**1 product (implicit solvent, DCM)**

- Electronic Energy (a.u.): -704.9916346120001
- Number of Imaginary Frequencies: 0

xyz

O	-3.174259	1.359093	-0.320274
C	-2.280805	0.545765	-0.183685
C	-0.934509	0.969706	0.402741
C	-2.476648	-0.860003	-0.599609
C	-0.625401	0.197315	1.666391
H	-1.006879	2.039094	0.598302
C	-1.578261	-1.839132	-0.450413
H	-3.440895	-1.068474	-1.051173
C	-0.278391	-1.079196	1.556104
H	-0.692428	0.704163	2.621241
C	-0.207819	-1.680899	0.166072
H	-1.835585	-2.831434	-0.808846
H	-0.032129	-1.693798	2.413474
H	0.282673	-2.653059	0.196367
C	2.098066	-0.738508	-0.302960
C	0.638124	-0.739198	-0.733392
H	0.606482	-1.101855	-1.762721
C	1.446948	1.487240	-0.219252
C	0.193619	0.728375	-0.639267
H	-0.116304	1.126363	-1.607648
O	1.551069	2.673864	-0.035284
O	2.822231	-1.695032	-0.181611
N	2.467751	0.570513	-0.071543
H	3.398942	0.833223	0.222771

### 2-inter (implicit solvent, DCM)

- Electronic Energy (a.u.): -739.887628411
- Number of Imaginary Frequencies: 0

xyz

N	-3.418021	0.936674	0.104982
C	-2.345398	0.022342	0.295711
C	-1.659719	0.243687	1.441021
C	-2.119468	-1.056409	-0.654753
C	-0.554636	-0.523597	1.965237
H	-2.024883	1.059727	2.057661
C	-0.996635	-1.762905	-0.834220
H	-2.977379	-1.308772	-1.268993
C	0.272677	-1.341453	1.295338
H	-0.388489	-0.417068	3.033859
C	0.351832	-1.566161	-0.188981
H	-1.042165	-2.574416	-1.557372
H	1.020829	-1.869612	1.881496
H	0.906744	-2.498831	-0.331082
C	2.607943	-0.452996	-0.316898
C	1.202798	-0.482347	-0.928750
H	1.309755	-0.853231	-1.958903
C	1.715901	1.711575	-0.227742
C	0.761826	0.946737	-0.847506
H	-0.196843	1.315351	-1.178316
O	1.827882	2.923323	0.090454
O	3.376163	-1.406099	-0.203446
N	2.824519	0.810647	0.085939
H	3.678046	1.124123	0.522041
N	-4.057498	0.812306	-0.954306
H	-4.783697	1.536709	-0.943505

### 2 product (implicit solvent, DCM)

- Electronic Energy (a.u.): -739.920867345
- Number of Imaginary Frequencies: 0

xyz

C	-2.042374	0.169256	-0.024738
C	-0.753052	0.778290	0.495872
C	-2.074538	-1.221539	-0.402494
C	-0.280395	0.035859	1.726544
H	-0.960261	1.824098	0.728635
C	-1.047110	-2.097094	-0.343746
H	-3.036991	-1.580870	-0.754826
C	0.242837	-1.180254	1.568188
H	-0.431492	0.473927	2.708351

C	0.338842	-1.731720	0.159931
H	-1.204415	-3.127868	-0.647344
H	0.545629	-1.797514	2.408207
H	0.974428	-2.618858	0.141352
C	2.461562	-0.486198	-0.431069
C	0.989080	-0.665098	-0.755641
H	0.923520	-1.004789	-1.792167
C	1.535109	1.626448	-0.186290
C	0.368740	0.737524	-0.576447
H	-0.037690	1.124439	-1.513744
O	1.514496	2.810844	0.057947
O	3.322764	-1.336223	-0.414970
N	2.675324	0.845778	-0.142260
H	3.581980	1.213808	0.111282
N	-3.092707	0.978135	-0.090884
N	-4.242672	0.541236	-0.541485
H	-4.864608	1.347766	-0.491805

### 2-prot product (implicit solvent, DCM)

- Electronic Energy (a.u.): -740.439028508
- Number of Imaginary Frequencies: 0

xyz

N	-3.009586	0.993630	-0.010838
C	-2.000406	0.201127	-0.025067
C	-0.694714	0.789543	0.477130
C	-2.031432	-1.193879	-0.490107
C	-0.233161	0.050919	1.715823
H	-0.886150	1.839365	0.697894
C	-1.007026	-2.051434	-0.415223
H	-2.942515	-1.543926	-0.962961
C	0.263617	-1.172344	1.567403
H	-0.333277	0.525089	2.685351
C	0.356283	-1.736370	0.163950
H	-1.137639	-3.046646	-0.828823
H	0.605046	-1.769670	2.404887
H	0.963209	-2.641449	0.156922
C	2.504687	-0.498788	-0.372727
C	1.042022	-0.685010	-0.745726
H	1.017013	-1.034345	-1.780333
C	1.573642	1.622157	-0.231955
C	0.412445	0.712753	-0.607752
H	0.007593	1.075083	-1.554849
O	1.535737	2.811871	-0.034882
O	3.353271	-1.353295	-0.292005
N	2.711317	0.845092	-0.138659
H	3.612029	1.224256	0.121016
N	-4.232988	0.547083	-0.453286
H	-4.948462	1.177875	-0.122782
H	-4.465849	-0.406922	-0.196245

### 3 product (implicit solvent, DCM)

- Electronic Energy (a.u.): -1327.85749061
- Number of Imaginary Frequencies: 0

xyz

C	-0.458160	-0.401853	0.199208
C	0.707166	0.457779	0.656367
C	-0.217589	-1.769424	-0.262788
C	1.448956	-0.191959	1.804100
H	0.293123	1.420880	0.955050
C	0.977378	-2.373536	-0.315752
H	-1.098324	-2.315980	-0.580648
C	2.210529	-1.250582	1.542311
H	1.326198	0.199229	2.808082
C	2.285817	-1.732219	0.106972
H	1.033235	-3.393388	-0.684629
H	2.754638	-1.783223	2.314555
H	3.092035	-2.457350	-0.008929
C	4.017869	-0.027260	-0.602394
C	2.596084	-0.521884	-0.810760
H	2.511935	-0.836445	-1.853394

C	2.673764	1.813907	-0.169411
C	1.701138	0.696549	-0.511050
H	1.137511	1.014280	-1.390956
O	2.409960	2.950273	0.141775
O	5.039213	-0.665928	-0.701814
N	3.956787	1.309205	-0.268464
H	4.779101	1.864691	-0.075275
N	-1.626207	0.151495	0.233564
N	-2.689921	-0.577817	-0.179848
S	-4.043595	0.319226	-0.083429
C	-5.227628	-0.896492	-0.630012
H	-5.212043	-1.740499	0.056627
H	-6.201211	-0.406992	-0.614231
H	-4.973386	-1.210116	-1.640423
O	-4.095568	1.444611	-1.043240
O	-4.418837	0.713413	1.292220

### 3-prot product (implicit solvent, DCM)

- Electronic Energy (a.u.): -1328.33131443
- Number of Imaginary Frequencies: 0

xyz			
N	1.564979	-0.586068	1.419045
C	0.581004	0.175251	1.095107
C	-0.783014	-0.464943	1.266569
C	0.694626	1.531599	0.553825
C	-1.784687	0.395742	2.000329
C	-0.328612	2.242196	0.068763
H	1.677649	1.982919	0.598807
C	-2.275197	1.463347	1.381029
H	-2.091917	0.109419	2.999018
C	-1.760793	1.766432	-0.013299
H	-0.131593	3.251243	-0.279588
H	-3.008981	2.118695	1.834966
C	-3.309089	0.158279	-1.197702
C	-1.856485	0.481424	-0.879296
C	-2.509015	-1.716667	-0.089069
C	-1.321678	-0.766351	-0.159317
O	-2.543704	-2.803828	0.430982
O	-4.110331	0.872307	-1.748917
N	-3.570308	-1.114867	-0.735133
H	-4.477548	-1.553264	-0.820624
N	2.851420	-0.069932	1.108910
H	3.511222	-0.566812	1.700487
S	3.371807	-0.356590	-0.502381
O	2.189575	-0.500888	-1.333073
O	4.375493	-1.410018	-0.483534
C	4.186378	1.170862	-0.900525
H	4.613263	1.043211	-1.895068
H	3.449518	1.970890	-0.896660
H	4.969692	1.346213	-0.165191
H	-0.537223	-1.262567	-0.734996
H	-1.343226	0.652350	-1.827332
H	-2.365480	2.539209	-0.486705
H	-0.625817	-1.413596	1.779095

### 4 product (implicit solvent, DCM)

- Electronic Energy (a.u.): -702.8273837
- Number of Imaginary Frequencies: 0

xyz			
C	-1.10478	-0.69715	-0.71778
C	0.08010	-0.74176	-1.65867
C	0.81043	0.36835	-1.64406
C	0.26902	1.41271	-0.70378
C	-1.88713	0.55929	-1.06662
H	-1.74951	-1.56923	-0.76605
H	0.28237	-1.61642	-2.26217
H	1.70982	0.53752	-2.22018
H	0.76687	2.37470	-0.76709
O	-3.05509	0.61988	-1.33896
O	-1.12483	1.66663	-1.02691

C	1.63760	0.43305	1.21257
C	0.25617	0.84824	0.73545
C	-0.57253	-0.44481	0.72586
C	0.39140	-1.53258	1.17557
H	-0.14047	1.60513	1.41295
H	-1.40729	-0.41391	1.42729
N	1.60047	-0.92567	1.45797
H	2.40999	-1.44454	1.77149
O	2.60314	1.14012	1.35167
O	0.16598	-2.71143	1.27413

**5-inter (implicit solvent, DCM)**

- Electronic Energy (a.u.): -737.7077298
- Number of Imaginary Frequencies: 0

xyz

C	-1.04924	-0.62670	-1.01573
C	0.37372	-0.79314	-1.24563
C	1.22873	0.04711	-0.65618
C	0.75309	1.12299	0.27730
C	-1.46269	0.47953	-0.38101
H	-1.78029	-1.35523	-1.33627
H	0.72201	-1.59009	-1.89126
H	2.30036	-0.03589	-0.79804
H	1.28960	2.05125	0.07078
N	-2.83974	0.69900	-0.17113
O	-0.63465	1.45804	0.03018
C	2.43533	0.59704	2.05094
C	0.94048	0.78682	1.77288
C	0.32541	-0.48153	2.28488
C	1.29448	-1.31806	2.77992
H	0.62250	1.68887	2.31499
H	-0.73086	-0.70484	2.27731
N	2.56862	-0.61838	2.60667
H	3.45074	-1.00618	2.90427
O	3.32949	1.39840	1.79113
O	1.30947	-2.45489	3.31149
N	-3.19418	1.71692	0.44971
H	-2.37072	2.27423	0.74199

**5 product (implicit solvent, DCM)**

- Electronic Energy (a.u.): -737.7235411
- Number of Imaginary Frequencies: 0

xyz

C	-1.13459	-0.67155	-0.70259
C	0.04151	-0.73638	-1.65398
C	0.78997	0.36603	-1.64533
C	0.26879	1.41990	-0.69972
C	-1.89962	0.57704	-1.05162
H	-1.78421	-1.54204	-0.74759
H	0.21824	-1.59585	-2.28998
H	1.66400	0.53396	-2.26204
H	0.82040	2.35628	-0.74520
O	-1.09055	1.72571	-1.02909
C	1.62895	0.44396	1.22283
C	0.25114	0.84822	0.74152
C	-0.57277	-0.45311	0.73357
C	0.39829	-1.52988	1.17572
H	-0.15294	1.60613	1.41461
H	-1.40319	-0.42427	1.44079
N	1.60821	-0.91758	1.45448
H	2.42309	-1.43148	1.76097
O	2.59404	1.15484	1.37748
O	0.19324	-2.71605	1.27578
N	-3.13194	0.62832	-1.38569
N	-3.76765	1.77472	-1.72650
H	-3.09015	2.54516	-1.66547

**5-prot product (implicit solvent, DCM)**

- Electronic Energy (a.u.): -738.2620962
- Number of Imaginary Frequencies: 0

xyz

C	-1.15162	-0.67044	-0.67369
C	0.00448	-0.70667	-1.65041
C	0.73890	0.40269	-1.64402
C	0.23732	1.43552	-0.66935
C	-1.92016	0.58841	-0.97907
H	-1.80056	-1.54008	-0.71719
H	0.18391	-1.56667	-2.28251
H	1.61093	0.58051	-2.25913
H	0.75174	2.38975	-0.72639
O	-1.15686	1.71539	-0.94932
C	1.65066	0.42577	1.19559
C	0.25827	0.84543	0.75964
C	-0.57023	-0.45105	0.75392
C	0.40726	-1.54116	1.16002
H	-0.12217	1.59145	1.45849
H	-1.38474	-0.42905	1.47937
N	1.62321	-0.93662	1.41991
H	2.44158	-1.45848	1.70362
O	2.62004	1.13177	1.32268
O	0.19000	-2.72366	1.24670
N	-3.15821	0.61612	-1.24109
N	-3.72640	1.87240	-1.43898
H	-3.08149	2.53946	-1.85486
H	-4.53754	1.76114	-2.03116

### 1-TS (implicit solvent, DCM)

- Electronic Energy (a.u.): -704.908235405
- Number of Imaginary Frequencies: 1

xyz

O	-3.097522	1.373095	-0.521416
C	-2.303269	0.519472	-0.137695
C	-1.146331	0.948615	0.686837
C	-2.481006	-0.878503	-0.511434
C	-0.524677	0.213386	1.707494
H	-1.158561	2.027335	0.819148
C	-1.597567	-1.874971	-0.319578
H	-3.374471	-1.075647	-1.093958
C	-0.128517	-1.099034	1.584181
H	-0.129277	0.780589	2.543592
C	-0.362360	-1.869250	0.438943
H	-1.822265	-2.826431	-0.793713
H	0.563723	-1.493853	2.319790
H	0.205899	-2.790905	0.364514
C	2.088564	-0.696219	-0.431398
C	0.753394	-0.566101	-1.077031
H	0.465739	-1.236796	-1.871400
C	1.407779	1.493175	-0.207629
C	0.325319	0.747911	-0.928753
H	-0.310769	1.278136	-1.622644
O	1.488441	2.675073	0.021150
O	2.831807	-1.648206	-0.405501
N	2.342558	0.536585	0.157034
H	3.192278	0.750899	0.657937

Imaginary Frequencies  
537*i* cm<sup>-1</sup>

### 2-TS<sub>1</sub> (implicit solvent, DCM)

- Electronic Energy (a.u.): -739.854848769
- Number of Imaginary Frequencies: 1

xyz

N	-3.452774	0.862778	-0.137776
C	-2.347726	0.119541	0.241867
C	-1.530602	0.772025	1.128522
C	-2.130705	-1.235373	-0.290279
C	-0.328065	0.355448	1.759569
H	-1.888149	1.761532	1.404724
C	-1.035597	-2.000282	-0.178329
H	-2.974226	-1.642396	-0.836004
C	0.388974	-0.805787	1.541884

H	0.049936	1.024476	2.525483
C	0.247266	-1.719898	0.489560
H	-1.085199	-2.980439	-0.648549
H	1.267616	-0.941450	2.168504
H	0.925870	-2.566956	0.512456
C	2.588515	-0.573182	-0.425613
C	1.270507	-0.563135	-1.118129
H	1.009478	-1.352102	-1.808624
C	1.713415	1.565568	-0.382346
C	0.826179	0.749224	-1.158902
H	-0.059280	1.129523	-1.642538
O	1.735030	2.774751	-0.154213
O	3.396050	-1.483780	-0.307343
N	2.731182	0.693748	0.086738
H	3.552994	1.013768	0.573936
N	-4.253774	0.331976	-0.961189
H	-4.993084	1.021863	-1.118188

Imaginary Frequencies  
 $450i \text{ cm}^{-1}$

### 2-TS<sub>2</sub> (implicit solvent, DCM)

- Electronic Energy (a.u.): -739.874172315
- Number of Imaginary Frequencies: 1

xyz			
N	-3.099446	1.028568	0.027075
C	-2.138014	0.078495	0.278706
C	-1.068000	0.535216	1.054004
C	-2.153259	-1.222969	-0.361900
C	-0.198676	-0.329452	1.840610
H	-1.179254	1.553863	1.413990
C	-1.083911	-2.011520	-0.557723
H	-3.115817	-1.559479	-0.733637
C	0.393066	-1.424903	1.351828
H	-0.026763	-0.031515	2.871704
C	0.338589	-1.709459	-0.121128
H	-1.241205	-2.980981	-1.023820
H	1.009087	-2.049496	1.990833
H	0.949454	-2.588307	-0.336638
C	2.452961	-0.412757	-0.423766
C	1.001377	-0.523455	-0.897293
H	1.008095	-0.798489	-1.959793
C	1.495616	1.701895	-0.222360
C	0.456464	0.865647	-0.671317
H	-0.345770	1.276308	-1.264042
O	1.564597	2.920022	-0.004391
O	3.289940	-1.303135	-0.401670
N	2.631706	0.861126	0.007385
H	3.508263	1.211055	0.364295
N	-4.062808	0.712330	-0.736147
H	-4.665830	1.537358	-0.780555

Imaginary Frequencies  
 $422i \text{ cm}^{-1}$

### 2-prot-TS (implicit solvent, DCM)

- Electronic Energy (a.u.): -740.349320297
- Number of Imaginary Frequencies: 1

xyz			
N	-3.023698	0.975972	-0.034536
C	-2.055834	0.145599	0.153039
C	-0.896044	0.731568	0.854704
C	-2.043765	-1.237880	-0.315429
C	-0.059618	0.093840	1.775567
H	-1.034703	1.798594	1.005058
C	-1.016871	-2.095798	-0.225809
H	-2.903147	-1.572105	-0.884472
C	0.495745	-1.158542	1.589773
H	0.373985	0.719620	2.548921
C	0.266440	-1.937616	0.455874
H	-1.129815	-3.048957	-0.734388
H	1.318808	-1.446353	2.235357

H	0.936996	-2.780281	0.319106
C	2.465895	-0.446383	-0.566781
C	1.076367	-0.487057	-1.093844
H	0.812727	-1.178437	-1.878905
C	1.518575	1.627853	-0.233069
C	0.494735	0.759522	-0.879753
H	-0.279738	1.201965	-1.488323
O	1.469048	2.809395	0.019761
O	3.333195	-1.288130	-0.628585
N	2.600063	0.797947	0.035794
H	3.454363	1.119613	0.465981
N	-4.157023	0.541433	-0.694936
H	-4.891813	1.216084	-0.535657
H	-4.484746	-0.377954	-0.411964

Imaginary Frequencies

555*i* cm<sup>-1</sup>

### 3-TS (implicit solvent, DCM)

- Electronic Energy (a.u.): -1327.7731456
- Number of Imaginary Frequencies: 1

xyz			
N	-1.729820	-0.159198	0.520794
C	-0.540647	-0.721284	0.566480
C	0.370879	-0.071950	1.452530
C	-0.194912	-1.904786	-0.225477
C	1.630725	-0.452955	1.903465
H	-0.081265	0.774000	1.964355
C	1.034121	-2.354181	-0.493662
H	-1.040141	-2.435070	-0.648972
C	2.520323	-1.302993	1.264110
H	1.999614	0.073029	2.777952
C	2.339424	-1.809793	-0.037240
H	1.118310	-3.238229	-1.120005
H	3.508560	-1.403684	1.702787
H	3.180814	-2.391135	-0.405048
C	3.924952	0.246533	-0.719242
C	2.554439	-0.192179	-1.164499
H	2.477791	-0.763272	-2.081870
C	2.390408	1.853921	-0.086507
C	1.676559	0.850837	-0.837137
H	0.670513	0.993428	-1.194583
O	2.040108	2.937826	0.356834
O	4.996021	-0.280547	-0.943276
N	3.717913	1.374487	0.034227
H	4.461498	1.911020	0.454119
N	-2.626814	-0.694978	-0.295724
S	-4.057184	0.118212	-0.166644
O	-4.596242	0.132386	1.201396
O	-4.930748	-0.444696	-1.201016
C	-3.711904	1.819954	-0.600392
H	-4.646424	2.374323	-0.520820
H	-2.969950	2.203183	0.097999
H	-3.332624	1.842342	-1.620767

Imaginary Frequencies

553*i* cm<sup>-1</sup>

### 3-prot-TS (implicit solvent, DCM)

- Electronic Energy (a.u.): -1328.24593368
- Number of Imaginary Frequencies: 1

xyz			
N	1.583388	-0.144792	1.557872
C	0.554753	0.555435	1.181979
C	-0.719805	-0.003399	1.652561
C	0.610695	1.759256	0.373282
C	-1.923726	0.671586	1.886583
H	-0.554092	-0.894883	2.251394
C	-0.432958	2.340950	-0.238382
H	1.598753	2.161496	0.194116
C	-2.478997	1.596278	1.028788
H	-2.566655	0.252540	2.653441

C	-1.849615	2.019700	-0.146755
H	-0.209990	3.172252	-0.901339
H	-3.524877	1.851171	1.160927
H	-2.471562	2.568954	-0.846470
C	-3.186384	-0.204624	-1.268186
C	-1.718459	0.041176	-1.201461
H	-1.206690	0.507983	-2.028804
C	-2.269490	-1.773321	0.149313
C	-1.161496	-0.900862	-0.343174
H	-0.151599	-1.279029	-0.414553
O	-2.208871	-2.769354	0.829680
O	-4.018262	0.331789	-1.962035
N	-3.439049	-1.212007	-0.346531
H	-4.355861	-1.601554	-0.184068
N	2.823595	0.326121	1.039152
H	3.535772	0.061756	1.715373
S	3.256013	-0.436844	-0.432046
O	2.044378	-0.502054	-1.234600
O	4.003873	-1.662997	-0.190642
C	4.364487	0.772533	-1.113016
H	4.727801	0.361313	-2.054611
H	3.813451	1.695937	-1.275968
H	5.190819	0.919002	-0.418576

Imaginary Frequencies  
 $555i \text{ cm}^{-1}$

#### 4-TS (implicit solvent, DCM)

- Electronic Energy (a.u.): -702.75060726
- Number of Imaginary Frequencies: 1

xyz			
C	-1.297451	0.910400	0.678661
C	-0.668689	0.188363	1.695939
C	-0.400519	-1.140042	1.446103
C	-0.806309	-1.630451	0.205311
C	-2.216938	0.205553	-0.209376
H	-1.462672	1.976436	0.763368
H	-0.270801	0.695533	2.565610
H	0.242011	-1.740833	2.074589
H	-0.637598	-2.653674	-0.100936
O	-3.170562	0.670748	-0.780222
O	-1.914244	-1.112199	-0.401543
C	1.886832	-0.816452	-0.377815
C	0.585359	-0.601349	-1.074351
C	0.258723	0.746330	-0.958247
C	1.342230	1.416251	-0.177288
H	0.302847	-1.236492	-1.901350
H	-0.335335	1.319010	-1.655435
N	2.197893	0.398300	0.219995
H	3.035861	0.555368	0.760611
O	2.556047	-1.819073	-0.316352
O	1.483886	2.588641	0.070612

Imaginary Frequencies  
 $562i \text{ cm}^{-1}$

#### 5-TS<sub>1</sub> (implicit solvent, DCM)

- Electronic Energy (a.u.): -737.6679539679999
- Number of Imaginary Frequencies: 1

xyz			
C	1.493924	-1.303707	0.838101
C	0.384750	-1.015990	1.666454
C	-0.039582	0.301263	1.721727
C	0.492495	1.220411	0.827965
C	2.158572	-0.310723	0.180246
H	1.847630	-2.316387	0.688888
H	-0.097522	-1.796979	2.237696
H	-0.913094	0.591204	2.292748
H	0.263485	2.276329	0.867038
N	3.216710	-0.573390	-0.625420
O	1.773516	1.016160	0.314792

C	-1.992364	1.141807	-0.326434
C	-0.713626	0.706363	-0.944583
C	-0.797978	-0.665540	-1.160290
C	-2.004451	-1.158516	-0.562480
H	-0.106369	1.404939	-1.504456
H	-0.087507	-1.298782	-1.666384
N	-2.655621	-0.024009	-0.016604
H	-3.581053	-0.054261	0.380921
O	-2.402327	2.272484	-0.104391
O	-2.496592	-2.285526	-0.506605
N	3.790980	0.370121	-1.259519
H	3.322726	1.267738	-1.060244

Imaginary Frequencies  
 $548i \text{ cm}^{-1}$

#### 5-TS<sub>2</sub> (implicit solvent, DCM)

- Electronic Energy (a.u.): -737.683252713

- Number of Imaginary Frequencies: 1

xyz			
C	-1.071206	0.905966	1.016446
C	-0.251466	0.129339	1.941911
C	0.057483	-1.112532	1.554378
C	-0.346696	-1.427184	0.148803
C	-2.014031	0.213403	0.264512
H	-1.255199	1.956778	1.195810
H	0.067092	0.563862	2.882266
H	0.653741	-1.802922	2.137178
N	-3.038886	0.823612	-0.334992
O	-1.731845	-1.107723	-0.050326
C	1.993502	-0.906512	-0.534746
C	0.533613	-0.578052	-0.833339
C	0.450453	0.916635	-0.633990
C	1.745524	1.398780	-0.300390
H	-0.199930	1.541896	-1.226381
N	2.587003	0.257502	-0.155170
H	3.562258	0.326519	0.095675
O	2.524554	-2.003143	-0.581094
O	2.185398	2.537468	-0.129895
N	-3.805366	0.192804	-1.155963
H	-3.472797	-0.777401	-1.263148
H	0.285627	-0.896235	-1.850734
H	-0.247957	-2.481800	-0.098791

Imaginary Frequencies  
 $479i \text{ cm}^{-1}$

#### 5-prot-TS (implicit solvent, DCM)

- Electronic Energy (a.u.): -738.181421312

- Number of Imaginary Frequencies: 1

xyz			
C	-0.856763	1.011711	0.874690
C	-0.082756	0.344107	1.820499
C	0.112060	-1.012733	1.624146
C	-0.484524	-1.574116	0.500950
C	-1.905913	0.264474	0.195322
H	-0.986431	2.085580	0.906154
H	0.485412	0.895445	2.558650
H	0.851288	-1.581784	2.171264
H	-0.364246	-2.614121	0.230945
N	-2.970821	0.793234	-0.249785
O	-1.668237	-1.077599	0.025265
C	2.100026	-0.897674	-0.551585
C	0.721769	-0.629274	-1.042725
C	0.482179	0.737418	-0.918597
C	1.701069	1.364387	-0.336214
H	0.271995	-1.274843	-1.782787
H	-0.191107	1.322125	-1.527435
N	2.557691	0.310968	-0.041111
H	3.476967	0.435614	0.356388
O	2.726454	-1.931900	-0.565719
O	1.942269	2.533814	-0.147340

N -3.826863 -0.029434 -0.972497  
H -4.758634 0.357191 -0.917033  
H -3.832058 -0.992901 -0.648966

Imaginary Frequencies  
 $577i \text{ cm}^{-1}$