Supporting Information

Effects of Solvents on the DACBO-catalyzed vinylogous Henry reaction of isatin with 3,5-dimethyl-4-nitroisoxazole "on water" and in solution from QM/MM MC simulations

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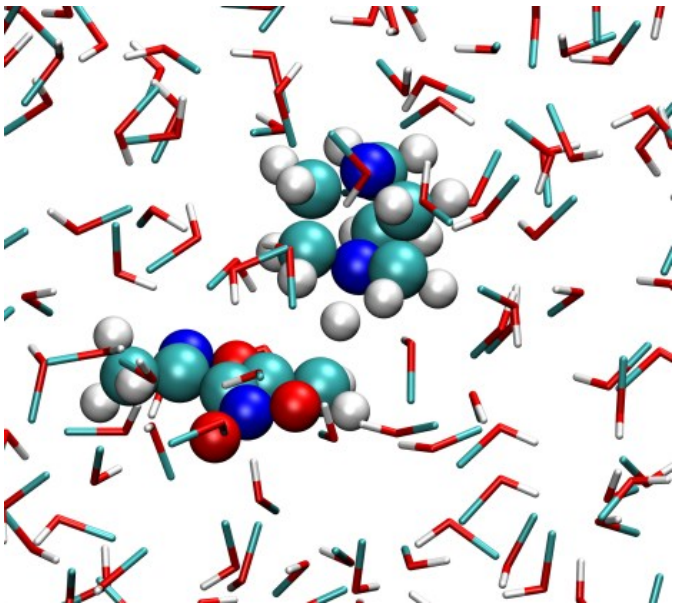


Fig. S1 Illustration of the transition structure of the proton migration process for DACBO-catalyzed vinylogous Henry reactions of isatin with 3,5-dimethyl-4-nitroisoxazole in methanol from QM/MM calculations.

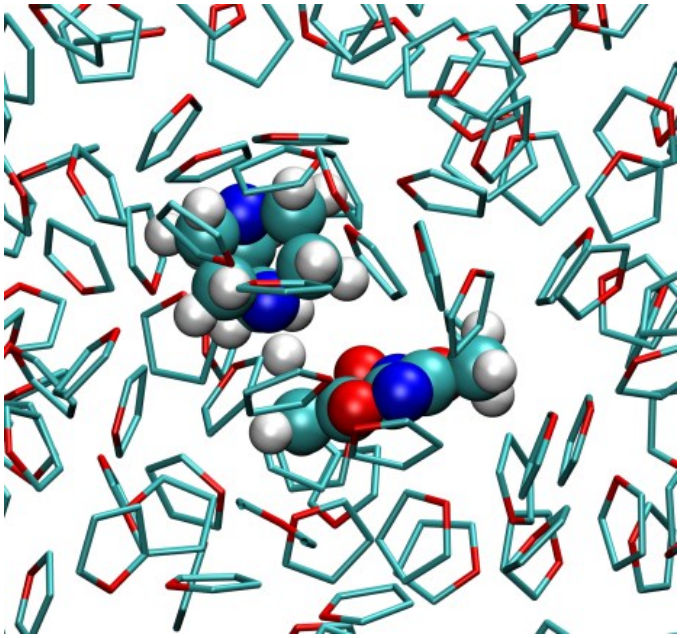
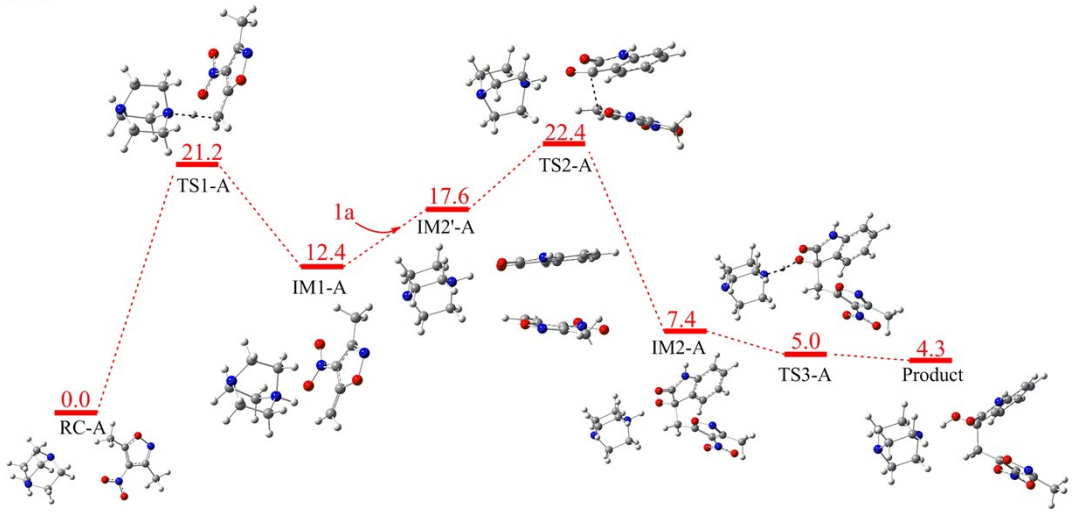
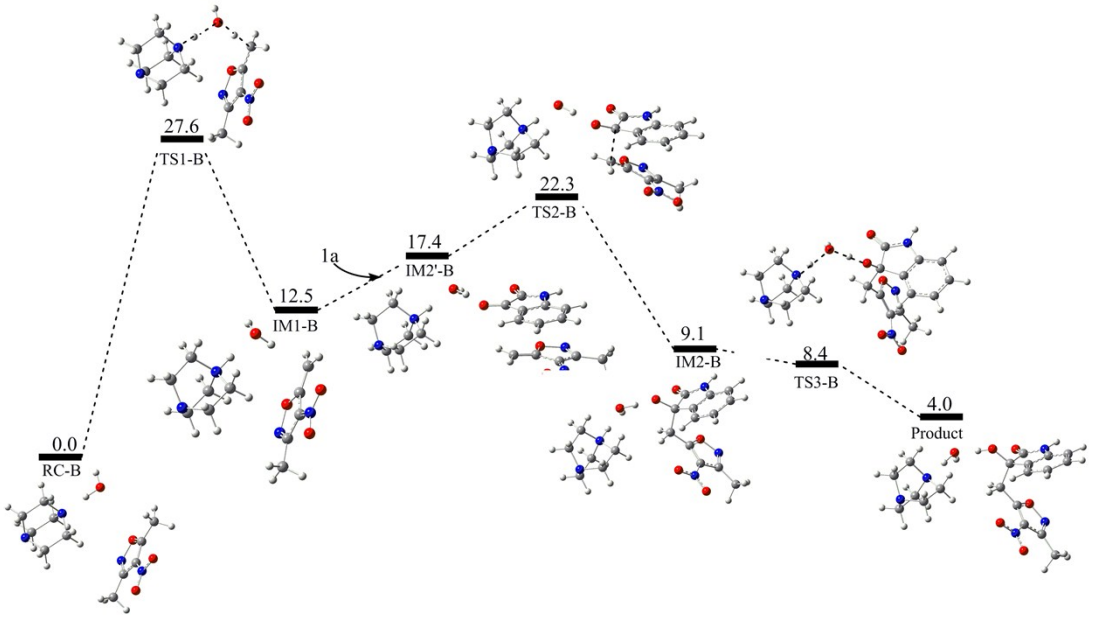


Fig. S2 Illustration of the transition structure of the proton migration process for DACBO-catalyzed vinylogous Henry reactions of isatin with 3,5-dimethyl-4-nitroisoxazole in THF from QM/MM calculations.

Path A


21.2
TS1-A
22.4
TS2-A
1a
17.6
IM2'-A
12.4
IM1-A
7.4
IM2-A
5.0
TS3-A
4.3
Product
0.0
RC-A

Path B


27.6
TS1-B'
22.3
TS2-B
1a
17.4
IM2'-B
12.5
IM1-B
9.1
IM2-B
8.4
TS3-B
4.0
Product
0.0
RC-B

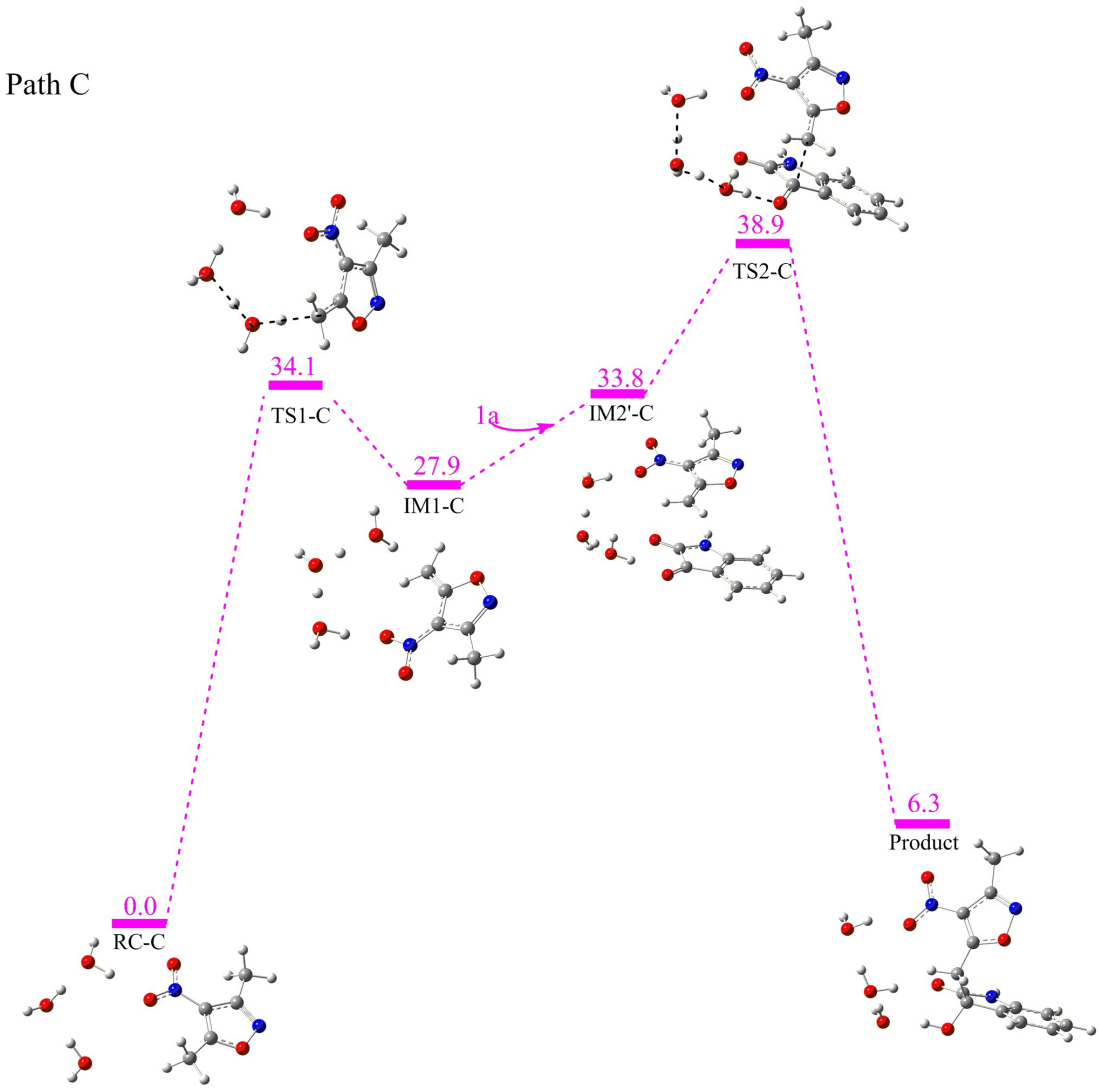


Fig. S3 DFT calculated free energy profiles of three pathways for the vinylogous Henry reaction of isatin with 3,5-dimethyl-4-nitroisoxazole in water and the corresponding optimized structures. Gibbs free energies are given in kcal mol^{-1}.

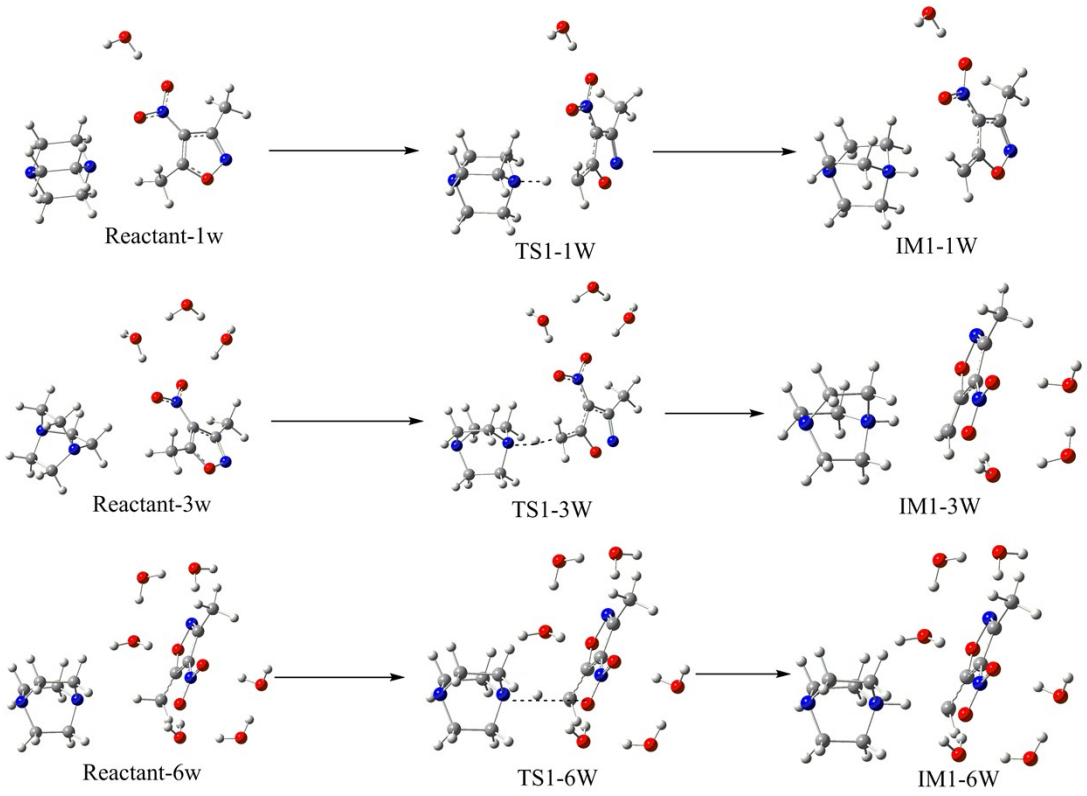


Fig. S4 The geometry structures of reactant, transition, intermidate for the proton migration process (rate-limiting step) in DACBO-catalyzed vinylogous Henry reactions of isatin with 3,5-dimethyl-4-nitroisoxazole by employing microsolvent models with the introducing one-, three- and six-water clusters.

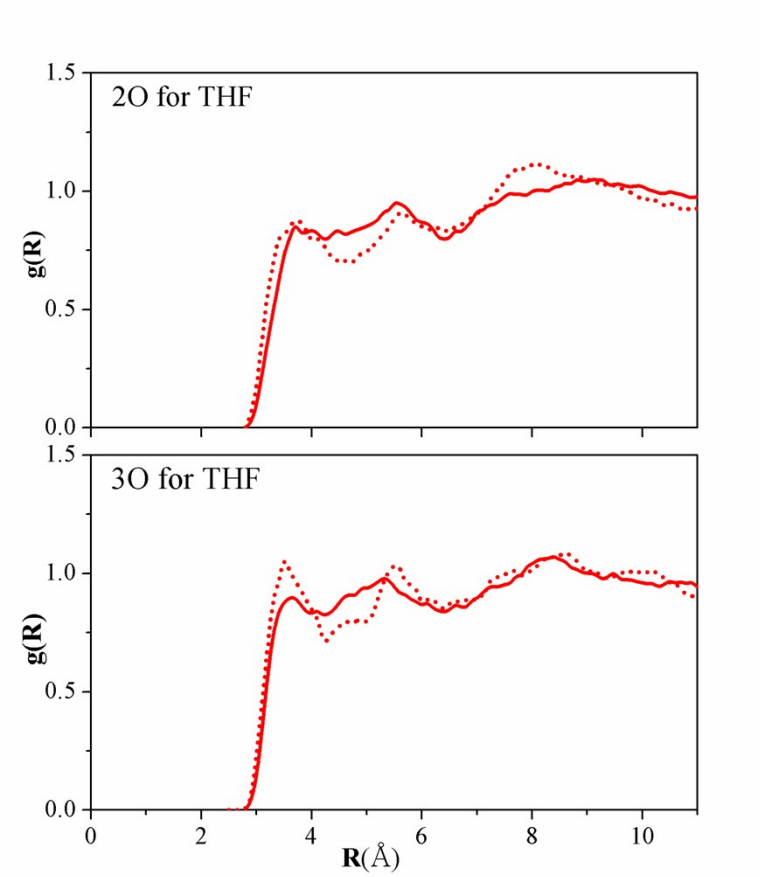


Fig. S5 Computed O(solute)-CH2(THF) radial distribution functions for the rate-limiting step of DACBO-catalyzed vinylogous Henry reaction in THF: transition structure (dash red), reactants (solid red) at 25 ℃ and 1 atm.

Coordinates of all stationary points:

DABCO catalyzes directly the vinylogous Henry reaction of **1a** and **2** in water (Path A).

DABCO

Sum of electronic and zero-point Energies=	-345.177467
Sum of electronic and thermal Energies=	-345.171095
Sum of electronic and thermal Enthalpies=	-345.170150
Sum of electronic and thermal Free Energies=	-345.207942

N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.62398859
C	1.38183719	0.00000000	0.53481518
C	1.38013416	-0.10564268	2.08863911
H	1.92212469	-0.84086029	0.08680746
H	1.87127720	0.92327368	0.21155942
H	1.80302223	-1.05888849	2.41963610
H	1.98344632	0.68882219	2.54085485
C	-0.70078441	-1.18937450	0.53828103
H	-1.70815970	-1.20820714	0.10882544
H	-0.17687755	-2.08428390	0.18980601
C	-0.77595093	-1.14709417	2.09383580
H	-1.81006484	-1.05279622	2.43797609
H	-0.36373653	-2.06426672	2.52774054
C	-0.67207450	1.20809022	0.53078384
C	-0.60282377	1.24685134	2.09012744
H	-1.60467075	1.34779239	2.52073561
H	-0.00431654	2.09378134	2.43828175
H	-1.70828157	1.20989390	0.17961811
H	-0.17373395	2.08368059	0.10163429

2

Sum of electronic and zero-point Energies=	-529.102237
Sum of electronic and thermal Energies=	-529.093011
Sum of electronic and thermal Enthalpies=	-529.092067
Sum of electronic and thermal Free Energies=	-529.136857

C	-1.1401	-0.74977	-0.00001
C	-0.00421	0.12669	-0.00002
C	1.10736	-0.68684	-0.00001
N	-0.73668	-1.99708	0.
O	0.6827	-1.95143	-0.00001
N	0.00333	1.55427	-0.00001

C	-2.60007	-0.43309	0.00001
C	2.57333	-0.45079	0.00003
H	-2.86421	0.16093	-0.87895
H	-3.17095	-1.36358	-0.00001
H	-2.86418	0.16087	0.87901
H	2.86434	0.13265	0.87821
H	3.09862	-1.40764	-0.00025
H	2.8643	0.1332	-0.8778
O	-1.08712	2.13461	0.00003
O	1.10288	2.12258	-0.00003

1a

Sum of electronic and zero-point Energies= -512.999847
Sum of electronic and thermal Energies= -512.991865
Sum of electronic and thermal Enthalpies= -512.990921
Sum of electronic and thermal Free Energies= -513.032854

C	0.37222	0.6128	0.00001
C	0.53358	-0.78891	0.
C	1.80399	-1.36632	0.00001
C	2.91661	-0.51984	0.00002
C	2.74089	0.87107	0.00003
C	1.46614	1.46382	0.00002
C	-1.7784	-0.1508	0.
C	-0.80129	-1.36911	-0.00001
H	1.91658	-2.44603	0.
H	3.91824	-0.93644	0.00002
H	3.61436	1.51628	0.00004
H	1.35321	2.5419	0.00004
N	-1.00073	0.96565	-0.00001
O	-1.18285	-2.53131	-0.00002
O	-3.00603	-0.22104	0.00001
H	-1.33736	1.90728	-0.00003

TS1-A

Sum of electronic and zero-point Energies= -874.275212
Sum of electronic and thermal Energies= -874.258843
Sum of electronic and thermal Enthalpies= -874.257899
Sum of electronic and thermal Free Energies= -874.320613

C	3.18492	-0.7269	0.56278
C	2.36789	0.13046	-0.25099
C	1.54269	-0.71313	-1.02733
N	2.90286	-1.98037	0.32932

O	1.87142	-1.98363	-0.67757
N	2.35203	1.51121	-0.26345
C	4.2328	-0.3768	1.56435
C	0.48012	-0.51468	-1.93414
H	3.81006	0.24125	2.3613
H	4.6469	-1.2893	1.99859
H	5.03686	0.19511	1.09277
H	0.255	-1.39398	-2.53978
H	-0.64623	-0.337	-1.19483
H	0.53038	0.41665	-2.49369
O	3.1428	2.14904	0.48138
O	1.53642	2.1085	-1.01474
C	-1.47598	-0.60467	0.93127
C	-2.76625	-0.451	1.78735
H	-1.13566	-1.64269	0.88673
H	-0.6564	0.01199	1.30946
H	-3.11413	-1.42664	2.13638
H	-2.57129	0.1701	2.66547
C	-2.89303	-0.95502	-1.01521
H	-3.03767	-0.65014	-2.05498
H	-2.59472	-2.00655	-1.00231
C	-4.1615	-0.70127	-0.15017
H	-4.94213	-0.22077	-0.74556
H	-4.56079	-1.64602	0.22751
C	-3.36656	1.47498	0.48713
H	-4.18242	1.96158	-0.05349
H	-3.10768	2.10415	1.34268
C	-2.13468	1.28158	-0.44651
H	-2.35389	1.57585	-1.47626
H	-1.2633	1.84685	-0.10416
N	-1.76968	-0.15797	-0.45662
N	-3.85385	0.17526	1.00225

IM1-A

Sum of electronic and zero-point Energies= -874.284935
Sum of electronic and thermal Energies= -874.267814
Sum of electronic and thermal Enthalpies= -874.266869
Sum of electronic and thermal Free Energies= -874.332592

C	3.12738	-0.73114	0.55627
C	2.29776	0.13282	-0.24201
C	1.47112	-0.7273	-1.04766
N	2.8615	-1.98482	0.31809
O	1.82324	-2.01932	-0.67981

N	2.2711	1.48646	-0.24322
C	4.17757	-0.3789	1.55666
C	0.51466	-0.54086	-1.99322
H	3.75299	0.22552	2.36307
H	4.60466	-1.2914	1.97887
H	4.97345	0.20759	1.0892
H	0.09037	-1.40336	-2.49792
H	-1.00551	-0.31055	-0.97578
H	0.30813	0.4523	-2.36644
O	3.06545	2.15621	0.50187
O	1.43687	2.09597	-0.99384
C	-1.57958	-0.62232	0.99084
C	-2.88308	-0.45305	1.80954
H	-1.24624	-1.65953	0.93134
H	-0.75998	-0.00495	1.36235
H	-3.24147	-1.42461	2.15623
H	-2.69756	0.17149	2.68585
C	-2.98696	-0.97215	-1.00639
H	-3.0988	-0.65322	-2.04387
H	-2.67517	-2.01761	-0.98554
C	-4.2525	-0.70478	-0.15238
H	-5.02314	-0.22383	-0.75843
H	-4.65696	-1.64617	0.22511
C	-3.45994	1.47511	0.48865
H	-4.26595	1.9544	-0.07079
H	-3.21707	2.10928	1.34386
C	-2.21531	1.29426	-0.41881
H	-2.4029	1.57508	-1.45648
H	-1.33921	1.8341	-0.05563
N	-1.87168	-0.16596	-0.40894
N	-3.94992	0.17508	0.99839

IM1'-A

Sum of electronic and zero-point Energies= -1387.286028
Sum of electronic and thermal Energies= -1387.258944
Sum of electronic and thermal Enthalpies= -1387.258000
Sum of electronic and thermal Free Energies= -1387.347797

C	3.11105	-2.72463	0.25731
C	2.7388	-1.66678	-0.64525
C	1.29847	-1.59754	-0.61819
N	2.05901	-3.26175	0.80885
O	0.9041	-2.58056	0.28954
N	3.55826	-0.89122	-1.39087

C	4.46756	-3.23781	0.6105
C	0.36053	-0.83923	-1.23062
H	5.083	-2.44019	1.03592
H	4.37741	-4.04727	1.33863
H	4.9822	-3.61177	-0.27886
H	-0.69015	-1.02273	-1.03679
H	0.64866	-0.08852	-1.95044
C	-0.18561	1.64708	0.47381
O	-1.29403	1.84501	-0.01807
O	4.82839	-1.06222	-1.36524
O	3.05707	0.02666	-2.12606
H	-2.82604	0.72534	0.02825
N	-3.75597	0.28588	-0.08407
C	-4.80021	1.37321	-0.06454
C	-6.18789	0.69317	-0.20053
H	-4.68421	1.91265	0.87666
H	-4.57441	2.04549	-0.89349
H	-6.79136	0.88933	0.68816
H	-6.71837	1.0941	-1.0667
C	-3.99167	-0.67749	1.0495
H	-3.18099	-1.40615	1.026
H	-3.93148	-0.10278	1.97452
C	-5.385	-1.32228	0.83207
H	-5.28284	-2.40179	0.70259
H	-6.02081	-1.14304	1.70153
C	-3.80184	-0.44855	-1.39952
C	-5.22633	-1.04211	-1.55383
H	-5.16603	-2.12287	-1.6984
H	-5.72427	-0.61105	-2.42485
H	-3.0276	-1.21608	-1.36326
H	-3.55655	0.27124	-2.18158
N	-6.05998	-0.77114	-0.36298
C	1.09911	2.28004	0.21798
C	2.02365	1.73512	1.13451
C	1.49662	3.24528	-0.71085
C	2.83345	3.64735	-0.71649
C	3.74216	3.08924	0.19668
C	3.35266	2.12683	1.14183
C	0.07596	0.64785	1.64671
H	0.78009	3.66138	-1.4122
H	3.17531	4.3908	-1.42873
H	4.77861	3.41196	0.17711
H	4.06361	1.7069	1.84525
N	1.38811	0.79821	1.97324

O	-0.75751	-0.07789	2.18132
H	1.8567	0.26562	2.69798

TS2-A

Sum of electronic and zero-point Energies= -1387.278498
Sum of electronic and thermal Energies= -1387.252987
Sum of electronic and thermal Enthalpies= -1387.252043
Sum of electronic and thermal Free Energies= -1387.335703

C	3.12037	-2.55853	0.07657
C	2.63374	-1.51181	-0.77805
C	1.25061	-1.38972	-0.52069
N	2.14436	-3.04737	0.79574
O	0.96263	-2.32764	0.42573
N	3.36007	-0.80512	-1.7242
C	4.49735	-3.11233	0.22204
C	0.2192	-0.53063	-0.93456
H	5.20147	-2.32409	0.502
H	4.50098	-3.88903	0.98979
H	4.83924	-3.54109	-0.72414
H	-0.7836	-0.89334	-0.73379
H	-2.74546	0.70188	-0.05335
H	0.3704	-0.00507	-1.86807
O	4.58533	-1.05049	-1.86673
O	2.78122	0.06302	-2.42208
C	-4.72988	1.37099	-0.10006
C	-6.13021	0.70931	-0.19805
H	-4.58671	1.91658	0.83404
H	-4.51797	2.03729	-0.93775
H	-6.70807	0.91558	0.7054
H	-6.67834	1.11514	-1.05098
C	-3.92453	-0.68087	1.00199
H	-3.12115	-1.41761	0.96757
H	-3.83997	-0.10411	1.92406
C	-5.32797	-1.31518	0.81846
H	-5.23833	-2.39547	0.68525
H	-5.94115	-1.13227	1.70343
C	-5.2228	-1.03831	-1.57025
H	-5.18103	-2.11942	-1.71937
H	-5.73544	-0.59833	-2.4284
C	-3.78757	-0.4655	-1.44605
H	-3.02427	-1.24481	-1.42238
H	-3.5468	0.24513	-2.23815
N	-3.70021	0.27383	-0.13831

N	-6.02723	-0.75789	-0.36045
C	2.0522	1.6477	0.97993
C	1.14338	1.99004	-0.03684
C	1.49145	2.91394	-1.0151
C	2.77845	3.46862	-0.984
C	3.68616	3.09711	0.01725
C	3.33522	2.18269	1.02351
C	0.14995	0.50332	1.53887
C	-0.11028	1.23476	0.21029
H	0.78443	3.18576	-1.79352
H	3.07663	4.18755	-1.74078
H	4.68176	3.53089	0.02535
H	4.03819	1.91592	1.80539
N	1.44739	0.75676	1.89378
O	-1.27469	1.61169	-0.14325
O	-0.66387	-0.17462	2.17795
H	1.919	0.34175	2.67182

IM2-A

Sum of electronic and zero-point Energies= -1387.294377

Sum of electronic and thermal Energies= -1387.268943

Sum of electronic and thermal Enthalpies= -1387.267999

Sum of electronic and thermal Free Energies= -1387.352063

C	-3.44455	-2.00433	-1.3093
C	-2.48034	-1.94061	-0.24646
C	-1.42316	-1.18062	-0.71746
N	-3.0042	-1.33441	-2.34475
O	-1.72653	-0.81954	-1.96915
N	-2.58869	-2.54894	1.02769
C	-4.76827	-2.68564	-1.36874
C	-0.12843	-0.70622	-0.17486
H	-5.4337	-2.29635	-0.59318
H	-5.22211	-2.52276	-2.34832
H	-4.65236	-3.75955	-1.1988
H	0.65015	-0.91153	-0.9172
H	2.44459	0.423	0.39609
H	0.09539	-1.25302	0.73939
O	-3.61192	-3.20833	1.27596
O	-1.66828	-2.40317	1.84771
C	4.43441	0.81008	1.05459
C	5.86079	0.27514	0.76031
H	4.31299	1.85605	0.76671
H	4.15646	0.69989	2.10453

H	6.44441	1.01762	0.21082
H	6.38284	0.06404	1.69647
C	3.83442	0.05615	-1.1989
H	3.04556	-0.44291	-1.76443
H	3.85929	1.10934	-1.48492
C	5.21209	-0.63681	-1.36401
H	5.10801	-1.56678	-1.92801
H	5.8965	0.01457	-1.91252
C	4.93759	-1.93906	0.63428
H	4.97053	-2.88187	0.08321
H	5.34379	-2.11652	1.63294
C	3.47761	-1.42208	0.72393
H	2.79668	-1.98418	0.08213
H	3.09065	-1.43456	1.74464
N	3.45722	0.00143	0.25141
N	5.81136	-0.96088	-0.04999
C	-1.85786	2.37061	0.23633
C	-1.23576	1.34599	0.96342
C	-1.7122	1.00554	2.22171
C	-2.82405	1.6936	2.7389
C	-3.43542	2.70914	1.99671
C	-2.95732	3.06804	0.72578
C	-0.1611	1.68311	-1.13465
C	-0.03928	0.83005	0.17046
H	-1.23449	0.22039	2.80066
H	-3.20997	1.43515	3.72047
H	-4.29332	3.23453	2.40614
H	-3.42995	3.85962	0.1541
N	-1.19636	2.56097	-0.9997
O	1.17499	1.09758	0.78704
O	0.5999	1.61497	-2.10988
H	-1.45021	3.25963	-1.6686

TS3-A

Sum of electronic and zero-point Energies= -1387.296979
Sum of electronic and thermal Energies= -1387.271874
Sum of electronic and thermal Enthalpies= -1387.270930
Sum of electronic and thermal Free Energies= -1387.353724

C	3.59635	-1.99874	1.01199
C	2.67255	-1.71567	-0.05096
C	1.54454	-1.1727	0.54035
N	3.06865	-1.65115	2.15891
O	1.77321	-1.13206	1.85801

N	2.87191	-1.96834	-1.43024
C	4.96124	-2.59434	0.96826
C	0.23834	-0.65627	0.06706
H	5.62777	-1.97823	0.35868
H	5.36184	-2.66738	1.9813
H	4.92633	-3.59163	0.52102
H	-0.54903	-1.08482	0.69597
H	0.08373	-0.96956	-0.96393
C	0.05636	0.90937	0.10464
O	-1.15577	1.25046	-0.47398
H	-2.19662	0.60173	-0.29131
O	3.96251	-2.44585	-1.78505
O	1.96043	-1.70756	-2.23149
N	-3.4167	0.03079	-0.21976
C	-4.36427	1.002	-0.85913
C	-5.79114	0.3953	-0.80959
H	-4.28931	1.93923	-0.30443
H	-4.0157	1.16708	-1.88037
H	-6.46215	1.04869	-0.24716
H	-6.19423	0.28657	-1.81928
C	-3.81913	-0.2086	1.20379
H	-3.08735	-0.89215	1.63815
H	-3.7582	0.74927	1.72357
C	-5.25633	-0.79608	1.20823
H	-5.26288	-1.78117	1.68061
H	-5.92832	-0.14672	1.77412
C	-3.43719	-1.26358	-0.97417
C	-4.8845	-1.82621	-0.92923
H	-4.89493	-2.81185	-0.45833
H	-5.28076	-1.93221	-1.94178
H	-2.71514	-1.92934	-0.49769
H	-3.10265	-1.05066	-1.99144
N	-5.78703	-0.9363	-0.16549
C	1.2401	1.66996	-0.49225
C	1.79537	2.50274	0.48911
C	1.75476	1.69007	-1.78207
C	2.8349	2.54138	-2.0715
C	3.38071	3.35823	-1.07471
C	2.86425	3.3524	0.23044
C	0.09603	1.41719	1.58652
H	1.32874	1.06068	-2.55817
H	3.24738	2.56664	-3.07567
H	4.21536	4.01186	-1.31079
H	3.28	3.98952	1.00495

N	1.09502	2.33236	1.70195
O	-0.68187	1.08505	2.48939
H	1.28267	2.85194	2.55258

Product

Sum of electronic and zero-point Energies= -1387.296498
Sum of electronic and thermal Energies= -1387.271048
Sum of electronic and thermal Enthalpies= -1387.270104
Sum of electronic and thermal Free Energies= -1387.354648

C	3.37887	-2.11267	1.30757
C	2.51452	-1.94996	0.17195
C	1.43509	-1.20397	0.6045
N	2.8615	-1.50325	2.34505
O	1.63318	-0.93247	1.8978
N	2.71995	-2.47875	-1.12888
C	4.67722	-2.83178	1.43225
C	0.17151	-0.71089	-0.00358
H	5.40969	-2.42082	0.73215
H	5.05537	-2.73363	2.45178
H	4.5488	-3.89179	1.19598
H	-0.65079	-1.00357	0.65811
C	0.07867	0.82851	-0.22315
O	-1.11103	1.13041	-0.9278
H	-1.94226	0.67025	-0.54065
H	0.03494	-1.19212	-0.9709
O	3.74892	-3.14212	-1.33062
O	1.87369	-2.26201	-2.00922
N	-3.45739	0.01519	-0.253
C	-4.41595	0.70522	-1.15419
C	-5.82614	0.05768	-1.02467
H	-4.43433	1.76353	-0.87594
H	-4.03359	0.63154	-2.17713
H	-6.57434	0.80736	-0.75079
H	-6.13766	-0.39531	-1.97057
C	-3.9264	0.16263	1.14807
H	-3.22309	-0.37155	1.79343
H	-3.88795	1.22362	1.41272
C	-5.3686	-0.40483	1.28624
H	-5.40937	-1.17571	2.06155
H	-6.07506	0.38377	1.5619
C	-3.43735	-1.4292	-0.59769
C	-4.85183	-2.04207	-0.39346
H	-4.83431	-2.81024	0.38529

H	-5.21034	-2.51064	-1.3147
H	-2.69667	-1.91998	0.04016
H	-3.10456	-1.52233	-1.63621
N	-5.82654	-1.00179	0.01057
C	1.26812	1.44272	-0.9312
C	1.82775	2.42476	-0.10258
C	1.80757	1.19716	-2.18559
C	2.92336	1.94469	-2.59928
C	3.47436	2.91669	-1.7583
C	2.93199	3.17585	-0.48908
C	0.08975	1.60021	1.13386
H	1.3768	0.44211	-2.8361
H	3.35956	1.76488	-3.57702
H	4.3383	3.48559	-2.08913
H	3.36087	3.93387	0.1576
N	1.10701	2.50538	1.11204
O	-0.72126	1.43567	2.05121
H	1.32131	3.14486	1.85037

The vinylogous Henry reaction of **1a** and **2** by one water auxiliary to activating the catalyst (Path B).

H_2O

Sum of electronic and zero-point Energies=	-76.427052
Sum of electronic and thermal Energies=	-76.424215
Sum of electronic and thermal Enthalpies=	-76.423271
Sum of electronic and thermal Free Energies=	-76.444714

O	-1.67183	1.37647	-0.07598
H	-0.71183	1.37647	-0.07598
H	-1.99228	2.2814	-0.07598

TS1-B

Sum of electronic and zero-point Energies=	-950.698214
Sum of electronic and thermal Energies=	-950.679253
Sum of electronic and thermal Enthalpies=	-950.678308
Sum of electronic and thermal Free Energies=	-950.747442

C	-2.75924	-1.3264	-1.20351
C	-1.88705	-0.04463	-1.25077
H	-2.13756	-2.21144	-1.35337
H	-3.51096	-1.3046	-1.99506
H	-0.81977	-0.26307	-1.31936
H	-2.16393	0.62024	-2.07033

C	-2.45024	-1.45118	1.17595
H	-2.96762	-1.58562	2.13035
H	-1.7856	-2.30738	1.0274
C	-1.63955	-0.1272	1.18818
H	-1.80832	0.45968	2.09299
H	-0.56694	-0.28733	1.06494
C	-3.5509	1.04736	0.1914
H	-3.64522	1.64646	1.09876
H	-3.83691	1.65775	-0.66667
C	-4.34586	-0.28351	0.26791
H	-4.84651	-0.37334	1.23442
H	-5.10974	-0.30982	-0.51232
N	-3.45774	-1.45275	0.09344
N	-2.09875	0.70788	0.02972
C	2.51708	-1.20443	-0.79577
C	2.44422	-0.07199	0.08533
C	2.17786	1.05307	-0.72108
O	2.08457	0.59124	-1.99064
N	2.29932	-0.8334	-2.02977
N	2.61436	-0.06403	1.46164
O	2.89489	-1.13519	2.05491
O	2.47707	1.0151	2.0887
C	1.93791	2.43076	-0.48144
H	2.43058	2.80542	0.41335
H	2.11145	3.04483	-1.36705
H	0.66208	2.60489	-0.22369
C	2.79396	-2.63773	-0.49068
H	3.78026	-2.74539	-0.03059
H	2.05597	-3.03295	0.2123
H	2.76253	-3.22318	-1.41197
O	-0.59981	2.88936	0.05224
H	-0.87832	3.49436	-0.65172
H	-1.50865	1.61785	0.00773

IM1-B

Sum of electronic and zero-point Energies=	-950.714115
Sum of electronic and thermal Energies=	-950.693803
Sum of electronic and thermal Enthalpies=	-950.692859
Sum of electronic and thermal Free Energies=	-950.766992

C	-2.80277	-1.33026	-1.25305
C	-1.95545	-0.03127	-1.28158
H	-2.16112	-2.20044	-1.40616
H	-3.54813	-1.31384	-2.05118

H	-0.8835	-0.22492	-1.35014
H	-2.24741	0.64456	-2.08702
C	-2.50657	-1.48616	1.12666
H	-3.02412	-1.6401	2.07586
H	-1.83104	-2.32941	0.96848
C	-1.70946	-0.15538	1.16435
H	-1.88353	0.41659	2.07729
H	-0.63578	-0.29914	1.03198
C	-3.64679	1.01042	0.18194
H	-3.74746	1.58539	1.104
H	-3.93457	1.63785	-0.6634
C	-4.4179	-0.33396	0.22442
H	-4.92612	-0.44932	1.18412
H	-5.17312	-0.35786	-0.56397
N	-3.50783	-1.48475	0.03787
N	-2.18705	0.69109	0.01675
C	2.42261	-1.1718	-0.83236
C	2.36117	-0.0847	0.10946
C	2.20198	1.12017	-0.66817
O	2.10789	0.68769	-1.98925
N	2.26936	-0.74264	-2.05346
N	2.45102	-0.15323	1.45651
O	2.65331	-1.27177	2.04695
O	2.32309	0.91561	2.14724
C	2.16586	2.44607	-0.39021
H	2.29414	2.79277	0.62529
H	2.12599	3.16385	-1.20297
H	0.15191	2.85294	-0.09143
C	2.63825	-2.62823	-0.5855
H	3.60609	-2.79386	-0.10347
H	1.86757	-3.02953	0.07799
H	2.61407	-3.17026	-1.53371
O	-0.78263	3.09857	0.08478
H	-1.03806	3.66731	-0.65741
H	-1.65138	1.58914	0.01149

IM1’-B

Sum of electronic and zero-point Energies= -1463.716177
Sum of electronic and thermal Energies= -1463.685954
Sum of electronic and thermal Enthalpies= -1463.685010
Sum of electronic and thermal Free Energies= -1463.782790

C	6.22879	-1.68677	-1.09488
C	5.12564	-1.72594	-0.00358

H	5.88934	-2.2107	-1.99092
H	7.13377	-2.18088	-0.73496
H	4.2017	-2.18838	-0.35426
H	5.45181	-2.22683	0.90941
N	6.5716	-0.29827	-1.46645
C	5.34795	0.38095	-1.94266
H	5.61076	1.39358	-2.2557
H	4.97571	-0.15811	-2.8165
C	4.26117	0.42885	-0.83699
H	4.03163	1.44577	-0.51458
H	3.33576	-0.06963	-1.12948
C	7.07551	0.40552	-0.268
C	6.0332	0.38629	0.88021
H	5.73538	1.38656	1.19839
H	6.37362	-0.17779	1.75028
H	7.31135	1.43488	-0.54634
H	8.00003	-0.07808	0.0544
N	4.79932	-0.30402	0.36366
H	4.06951	-0.29537	1.11094
O	2.81547	-0.10604	2.34447
H	2.46932	-0.94355	2.68605
H	2.05618	0.31817	1.89043
O	0.89633	1.32026	0.84083
C	-0.32213	1.33719	0.99384
C	-1.0692	0.47455	2.06286
N	-2.37461	0.84898	1.98963
C	-0.90811	-1.28129	-0.78654
H	-0.01227	-1.66722	-0.31317
H	-0.82197	-0.5534	-1.57875
C	-2.11964	-1.75196	-0.41348
O	-2.20378	-2.71363	0.59533
N	-3.57936	-3.05507	0.83644
C	-3.48648	-1.49552	-0.8009
N	-3.89365	-0.62876	-1.75453
O	-5.13911	-0.48596	-2.02706
O	-3.02409	0.06325	-2.38793
C	-4.30822	-2.34428	0.0224
C	-5.79388	-2.48714	0.05307
H	-6.26799	-1.52756	0.27737
H	-6.17047	-2.8211	-0.91779
H	-6.07771	-3.21452	0.81708
C	-2.57983	1.8053	0.97504
C	-3.77108	2.39595	0.58544
C	-1.35625	2.13278	0.35249

C	-1.30667	3.07598	-0.67778
C	-2.50011	3.67605	-1.08293
C	-3.71023	3.33277	-0.45851
H	-4.71133	2.14355	1.064
H	-0.36128	3.32359	-1.15042
H	-2.49708	4.40765	-1.88396
H	-4.62965	3.80782	-0.78717
O	-0.55569	-0.33877	2.82536
H	-3.11477	0.44293	2.55175

TS2-B

Sum of electronic and zero-point Energies= -1463.708099
Sum of electronic and thermal Energies= -1463.679427
Sum of electronic and thermal Enthalpies= -1463.678482
Sum of electronic and thermal Free Energies= -1463.771580

C	6.05974	-1.69884	-1.03759
C	4.98964	-1.66108	0.08547
H	5.65181	-2.16936	-1.9353
H	6.92363	-2.28368	-0.71157
H	4.05936	-2.15475	-0.20156
H	5.34748	-2.09109	1.02278
C	5.36676	0.43026	-1.92008
H	5.70384	1.44971	-2.12468
H	5.04833	-0.01787	-2.86401
C	4.18827	0.44279	-0.91222
H	3.86425	1.45197	-0.65345
H	3.32691	-0.12902	-1.26194
C	5.88613	0.4944	0.87759
H	5.60625	1.53808	1.03404
H	6.1329	0.04347	1.84081
C	7.01565	0.3289	-0.1718
H	7.42029	1.30706	-0.44619
H	7.83109	-0.27417	0.23781
N	6.51712	-0.33838	-1.39376
N	4.6659	-0.21599	0.35438
C	-4.07964	-2.3518	0.05176
C	-3.21904	-1.49032	-0.71035
C	-1.96687	-1.48976	-0.05748
O	-2.10442	-2.31758	1.01728
N	-3.43614	-2.84493	1.07701
N	-3.52487	-0.84121	-1.89608
O	-4.67889	-0.95764	-2.38254
O	-2.64187	-0.15276	-2.46487

C	-0.74762	-0.81344	-0.22358
H	-0.55336	-0.4013	-1.20516
H	0.09496	-1.24896	0.30449
H	1.87771	0.52941	1.73416
C	-5.50747	-2.71858	-0.17128
H	-6.13495	-1.82264	-0.19322
H	-5.62544	-3.23063	-1.13034
H	-5.84777	-3.37727	0.63113
O	2.66227	0.19339	2.24529
H	2.33987	-0.57934	2.73445
H	3.90683	-0.15149	1.07332
C	-3.89034	2.46658	0.60635
C	-2.71799	1.79508	0.93219
C	-1.55881	1.89479	0.14307
C	-1.5444	2.71212	-0.98267
C	-2.71548	3.40022	-1.32618
C	-3.87259	3.26957	-0.5437
H	-4.78025	2.37988	1.22233
H	-0.64709	2.8019	-1.58844
H	-2.73028	4.03829	-2.2044
H	-4.77341	3.80697	-0.82525
C	-0.5059	1.05715	0.77713
O	0.7463	1.26949	0.69938
N	-2.46397	0.96832	2.04357
C	-1.17154	0.52954	2.06413
O	-0.64117	-0.14162	2.95526
H	-3.13785	0.75832	2.77155

IM2-B

Sum of electronic and zero-point Energies= -1463.722027
Sum of electronic and thermal Energies= -1463.693519
Sum of electronic and thermal Enthalpies= -1463.692575
Sum of electronic and thermal Free Energies= -1463.785730

C	6.271	-1.64675	-1.06447
C	5.18007	-1.66542	0.04012
H	5.90361	-2.13983	-1.96708
H	7.16	-2.18169	-0.72343
H	4.26287	-2.16168	-0.2811
H	5.5278	-2.1238	0.96731
C	5.47463	0.45229	-1.92456
H	5.76752	1.47791	-2.15931
H	5.15069	-0.02751	-2.85058
C	4.32164	0.44687	-0.88767

H	4.00764	1.45109	-0.59953
H	3.44999	-0.11391	-1.22854
C	6.03366	0.48519	0.88813
H	5.72436	1.50886	1.10561
H	6.31749	-0.00637	1.8202
C	7.14356	0.41386	-0.19317
H	7.4732	1.41989	-0.46126
H	8.00771	-0.13603	0.18611
N	6.66226	-0.2657	-1.41451
N	4.82602	-0.23772	0.35467
C	-4.02241	-2.14294	0.06395
C	-3.18858	-1.21248	-0.64513
C	-1.93679	-1.23514	-0.03572
O	-2.012	-2.16458	0.93634
N	-3.32609	-2.72244	1.00941
N	-3.55918	-0.4591	-1.77938
O	-4.73102	-0.54197	-2.19057
O	-2.70152	0.24798	-2.33417
C	-0.66825	-0.47212	-0.14623
H	-0.5043	-0.16097	-1.17677
H	0.1446	-1.11505	0.19709
H	1.97184	0.35613	1.67161
C	-5.46415	-2.48232	-0.11866
H	-6.0801	-1.58374	-0.02504
H	-5.63789	-2.9034	-1.11273
H	-5.76784	-3.20846	0.63809
O	2.76233	0.02456	2.20923
H	2.4608	-0.78851	2.63905
H	4.06548	-0.21166	1.07744
C	-3.7145	2.5034	0.76819
C	-2.57485	1.74647	1.01273
C	-1.4367	1.8145	0.19634
C	-1.38767	2.73777	-0.84105
C	-2.51721	3.53667	-1.09214
C	-3.67191	3.39901	-0.31205
H	-4.59648	2.41504	1.39517
H	-0.50001	2.82689	-1.46137
H	-2.49931	4.2569	-1.90472
H	-4.54595	4.0053	-0.53144
C	-0.44726	0.75347	0.66484
O	0.86181	1.07608	0.68163
N	-2.33841	0.8377	2.06772
C	-1.07372	0.33008	2.02153
O	-0.54865	-0.39186	2.87676

H	-2.98293	0.66939	2.83276

TS3-B

Sum of electronic and zero-point Energies= -1463.724188
Sum of electronic and thermal Energies= -1463.696399
Sum of electronic and thermal Enthalpies= -1463.695455
Sum of electronic and thermal Free Energies= -1463.786097

C	5.52844	1.80972	-0.41557
C	4.37171	0.94559	-0.98357
H	5.1376	2.73706	0.00915
H	6.22689	2.07428	-1.21276
H	3.40031	1.43612	-0.89739
H	4.53354	0.66323	-2.02575
N	6.27538	1.08623	0.63771
C	5.35508	0.78241	1.75533
H	5.90504	0.1975	2.49616
H	5.04834	1.72012	2.22423
C	4.10807	0.00042	1.26405
H	3.96741	-0.94277	1.79526
H	3.19045	0.58686	1.33739
C	6.75852	-0.19335	0.06842
C	5.57715	-1.10063	-0.36523
H	5.49296	-1.99998	0.24796
H	5.63712	-1.39465	-1.41476
H	7.36601	-0.70445	0.81864
H	7.39972	0.03357	-0.78649
N	4.30607	-0.32408	-0.18711
H	3.4691	-0.92217	-0.53922
O	2.3086	-1.81954	-1.02969
H	2.06623	-1.56696	-1.93209
H	1.24551	-1.85019	-0.37954
O	0.30281	-1.94915	0.32419
C	-0.85157	-1.31567	-0.15452
C	-1.33959	-2.02361	-1.46423
N	-2.5626	-2.56536	-1.22301
C	-3.0086	-2.2982	0.08789
C	-2.0398	-1.54775	0.76796
C	-0.54104	0.1983	-0.42691
C	-1.70689	1.03163	-0.81328
C	-2.47502	2.00897	-0.20695
C	-3.48147	2.38741	-1.15994

O	-2.20858	0.83893	-2.03752
N	-3.33106	1.69168	-2.25933
N	-2.29752	2.54714	1.09249
O	-3.09698	3.4149	1.47849
O	-1.35897	2.13734	1.79306
H	-0.09872	0.60537	0.48071
H	0.19578	0.24192	-1.23623
C	-4.5781	3.38997	-1.05303
H	-5.245	3.13614	-0.22429
H	-4.16803	4.38466	-0.85801
H	-5.14926	3.41096	-1.98339
C	-4.19902	-2.69421	0.68479
C	-2.25301	-1.18111	2.09027
C	-3.44859	-1.57012	2.7177
C	-4.40634	-2.31448	2.01975
H	-4.93665	-3.27593	0.14088
H	-1.50882	-0.60588	2.63291
H	-3.63033	-1.29083	3.75104
H	-5.32635	-2.60831	2.51655
O	-0.70871	-2.10917	-2.52335
H	-3.07562	-3.11325	-1.9053

Product

Sum of electronic and zero-point Energies= -1463.722027
Sum of electronic and thermal Energies= -1463.693519
Sum of electronic and thermal Enthalpies= -1463.692575
Sum of electronic and thermal Free Energies= -1463.785730

C	6.271	-1.64675	-1.06447
C	5.18007	-1.66542	0.04012
H	5.90361	-2.13983	-1.96708
H	7.16	-2.18169	-0.72343
H	4.26287	-2.16168	-0.2811
H	5.5278	-2.1238	0.96731
C	5.47463	0.45229	-1.92456
H	5.76752	1.47791	-2.15931
H	5.15069	-0.02751	-2.85058
C	4.32164	0.44687	-0.88767
H	4.00764	1.45109	-0.59953
H	3.44999	-0.11391	-1.22854
C	6.03366	0.48519	0.88813
H	5.72436	1.50886	1.10561
H	6.31749	-0.00637	1.8202
C	7.14356	0.41386	-0.19317

H	7.4732	1.41989	-0.46126
H	8.00771	-0.13603	0.18611
N	6.66226	-0.2657	-1.41451
N	4.82602	-0.23772	0.35467
C	-4.02241	-2.14294	0.06395
C	-3.18858	-1.21248	-0.64513
C	-1.93679	-1.23514	-0.03572
O	-2.012	-2.16458	0.93634
N	-3.32609	-2.72244	1.00941
N	-3.55918	-0.4591	-1.77938
O	-4.73102	-0.54197	-2.19057
O	-2.70152	0.24798	-2.33417
C	-0.66825	-0.47212	-0.14623
H	-0.5043	-0.16097	-1.17677
H	0.1446	-1.11505	0.19709
H	1.97184	0.35613	1.67161
C	-5.46415	-2.48232	-0.11866
H	-6.0801	-1.58374	-0.02504
H	-5.63789	-2.9034	-1.11273
H	-5.76784	-3.20846	0.63809
O	2.76233	0.02456	2.20923
H	2.4608	-0.78851	2.63905
H	4.06548	-0.21166	1.07744
C	-3.7145	2.5034	0.76819
C	-2.57485	1.74647	1.01273
C	-1.4367	1.8145	0.19634
C	-1.38767	2.73777	-0.84105
C	-2.51721	3.53667	-1.09214
C	-3.67191	3.39901	-0.31205
H	-4.59648	2.41504	1.39517
H	-0.50001	2.82689	-1.46137
H	-2.49931	4.2569	-1.90472
H	-4.54595	4.0053	-0.53144
C	-0.44726	0.75347	0.66484
O	0.86181	1.07608	0.68163
N	-2.33841	0.8377	2.06772
C	-1.07372	0.33008	2.02153
O	-0.54865	-0.39186	2.87676
H	-2.98293	0.66939	2.83276

The three water molecules auxiliary without catalyst (Path C).

$3H_2O$

Sum of electronic and zero-point Energies= -229.284549

Sum of electronic and thermal Energies= -229.275965
Sum of electronic and thermal Enthalpies= -229.275021
Sum of electronic and thermal Free Energies= -229.317771

H	-2.3152	-0.87219	-1.29211
O	-3.1995	-1.27694	-1.3874
H	-3.08013	-2.19768	-1.11062
H	-4.32711	-0.46811	-0.27219
O	-4.942	-0.03278	0.36531
H	-5.54475	0.49427	-0.17898
O	-3.37539	1.59311	1.99615
H	-3.96563	1.04382	1.43051
H	-3.96599	2.05088	2.61112

TS1-C

Sum of electronic and zero-point Energies= -758.354420
Sum of electronic and thermal Energies= -758.338151
Sum of electronic and thermal Enthalpies= -758.337206
Sum of electronic and thermal Free Energies= -758.398878

H	-1.23878	-1.94754	0.08984
C	-0.28795	-1.74517	1.25591
C	0.81241	-1.14784	0.65332
C	1.15386	0.181	0.27058
C	2.40967	0.10029	-0.42585
N	2.82445	-1.13481	-0.48107
O	1.83273	-1.93448	0.20087
N	0.40373	1.30077	0.50573
C	3.22681	1.18627	-1.03987
H	3.49491	1.93329	-0.28764
H	4.13762	0.76477	-1.47047
H	2.66073	1.69576	-1.82478
H	-0.15284	-2.77527	1.58144
H	-0.91595	-1.11173	1.87283
O	0.79157	2.42961	0.09778
O	-0.69225	1.18166	1.13747
H	-2.21899	1.88879	0.38375
O	-3.12332	2.01485	0.02552
H	-3.03252	2.66571	-0.68576
H	-3.57358	0.47737	-0.57982
O	-3.82563	-0.42316	-0.91868
H	-4.59956	-0.69477	-0.40247
O	-1.9742	-2.15019	-0.76173
H	-2.72973	-1.43505	-0.78078

H	-2.38851	-3.01672	-0.60318

IM1-C

Sum of electronic and zero-point Energies= -758.358355
Sum of electronic and thermal Energies= -758.341554
Sum of electronic and thermal Enthalpies= -758.340609
Sum of electronic and thermal Free Energies= -758.405685

H	1.36275	1.99944	-0.24039
C	0.05316	1.75885	1.49442
C	-0.90139	1.14954	0.7531
C	-1.13834	-0.20048	0.29532
C	-2.34515	-0.15669	-0.49286
N	-2.82608	1.05211	-0.54011
O	-1.95313	1.89866	0.22757
N	-0.36418	-1.27059	0.54638
C	-3.04748	-1.2613	-1.2092
H	-3.32493	-2.05723	-0.5127
H	-3.94804	-0.87416	-1.69118
H	-2.39535	-1.70058	-1.96959
H	-0.02454	2.82121	1.7008
H	0.84212	1.18052	1.95225
O	-0.63063	-2.42457	0.06631
O	0.68283	-1.11968	1.29058
H	2.13286	-1.59623	0.55237
O	3.03415	-1.74008	0.15326
H	2.93874	-2.46017	-0.48948
H	3.4644	-0.56924	-0.47341
O	3.8073	0.32851	-0.9575
H	4.59267	0.66014	-0.489
O	1.99946	2.0987	-0.9813
H	3.07301	1.06465	-0.93186
H	2.37336	2.98918	-0.88774

IM1’-C

Sum of electronic and zero-point Energies= -1271.360944
Sum of electronic and thermal Energies= -1271.334626
Sum of electronic and thermal Enthalpies= -1271.333682
Sum of electronic and thermal Free Energies= -1271.419817

C	-0.67018	3.17076	0.02844
C	-1.24165	1.94755	0.53588
C	-0.23046	1.34475	1.37641
N	0.54075	3.33976	0.47633

O	0.85544	2.22256	1.32064
N	-2.46578	1.45385	0.28894
C	-1.26997	4.18778	-0.88426
C	-0.14142	0.21518	2.10942
H	-2.18097	4.60778	-0.44888
H	-0.5535	4.99354	-1.05975
H	-1.54087	3.73411	-1.84169
H	-0.97114	-0.47425	2.15828
H	0.76729	0.00106	2.66105
O	-3.29321	2.04539	-0.48989
O	-2.81458	0.34446	0.85736
C	2.62306	-0.1819	-0.99466
C	2.66481	-1.21244	-0.03088
C	3.8226	-1.44814	0.71641
C	4.93462	-0.63606	0.48654
C	4.87672	0.3829	-0.47767
C	3.72095	0.62749	-1.23676
C	0.52478	-1.08826	-1.11082
C	1.36375	-1.85806	-0.03615
H	3.84656	-2.24224	1.45609
H	5.84773	-0.79121	1.05119
H	5.75123	1.00445	-0.64475
H	3.68998	1.41886	-1.97807
N	1.35841	-0.14068	-1.61604
O	0.93829	-2.82091	0.59492
O	-0.63381	-1.32933	-1.43116
H	1.09421	0.52271	-2.3366
H	-0.80226	-3.29921	0.80307
H	-3.95978	-0.5254	0.00267
O	-4.58061	-1.17548	-0.43604
H	-4.86695	-0.75997	-1.26431
H	-3.8742	-2.36526	-0.68326
O	-3.35927	-3.29644	-0.81704
H	-2.8874	-3.27009	-1.66733
O	-1.69237	-3.64836	1.03753
H	-2.64927	-3.41926	-0.05722
H	-1.9691	-3.15056	1.82293

TS2-C

Sum of electronic and zero-point Energies=	-1271.352166
Sum of electronic and thermal Energies=	-1271.327205
Sum of electronic and thermal Enthalpies=	-1271.326261
Sum of electronic and thermal Free Energies=	-1271.407641

C	3.94929	-1.50809	-0.93612
C	2.63592	-1.71114	-0.39355
C	1.77424	-0.82115	-1.07327
N	3.92076	-0.58125	-1.85789
O	2.55994	-0.144	-1.95723
N	2.26446	-2.63406	0.56951
C	5.23913	-2.17114	-0.59002
C	0.42206	-0.46414	-0.99158
H	5.17851	-3.24759	-0.77264
H	6.04436	-1.74869	-1.19481
H	5.47084	-2.02738	0.46908
H	-0.24659	-1.16855	-0.5141
H	0.03914	0.07246	-1.85285
O	3.1319	-3.4084	1.05024
O	1.06565	-2.67967	0.94297
C	2.06306	1.68871	1.16151
C	1.22047	2.0356	0.0892
C	1.6324	2.97352	-0.85168
C	2.90123	3.55431	-0.70956
C	3.73289	3.19033	0.35736
C	3.32407	2.24842	1.31568
C	0.14794	0.48447	1.55736
C	-0.03504	1.25502	0.23337
H	0.98465	3.24542	-1.68002
H	3.24253	4.28892	-1.43228
H	4.71299	3.64814	0.45297
H	3.96447	1.97763	2.14928
N	1.41137	0.75731	1.99389
O	-1.18455	1.61241	-0.1743
O	-0.703	-0.19638	2.13925
H	1.80085	0.38445	2.85258
H	-2.31614	-0.01905	-0.50727
H	0.11229	-2.62427	2.34093
O	-0.52375	-2.47036	3.09264
H	-0.08919	-1.84957	3.69802
H	-1.70631	-1.92891	2.59186
O	-2.63913	-1.49199	2.11478
H	-2.5772	-0.55159	2.35571
O	-2.85547	-0.81714	-0.31669
H	-2.73323	-1.25213	1.10791
H	-2.52606	-1.505	-0.91658

Product

Sum of electronic and zero-point Energies= -1271.394266

Sum of electronic and thermal Energies= -1271.368293
Sum of electronic and thermal Enthalpies= -1271.367349
Sum of electronic and thermal Free Energies= -1271.451289

C	0.60156	3.21037	-0.1896
C	1.13876	1.88934	-0.35668
C	0.11027	1.10626	-0.84761
N	-0.65682	3.22007	-0.55197
O	-0.96259	1.89123	-0.96534
N	2.47095	1.48228	-0.08902
C	1.25166	4.4606	0.29152
C	-0.03274	-0.3167	-1.25935
H	2.10498	4.71442	-0.34331
H	0.5301	5.2797	0.27019
H	1.62236	4.33132	1.31173
H	0.96003	-0.7621	-1.31086
H	-0.48383	-0.33788	-2.25686
O	3.25056	2.311	0.39948
O	2.80528	0.31616	-0.35842
C	-0.92604	-1.21166	-0.34515
C	-2.36698	-0.75609	-0.22745
C	-2.65158	-0.47894	1.11415
C	-3.34939	-0.60349	-1.19527
C	-4.62365	-0.16891	-0.79639
C	-4.88994	0.10714	0.54969
C	-3.90178	-0.04431	1.53401
C	-0.45925	-1.1591	1.14937
H	-3.13739	-0.8139	-2.23929
H	-5.40647	-0.04378	-1.53757
H	-5.87953	0.44475	0.84312
H	-4.10688	0.167	2.57833
N	-1.50106	-0.72024	1.89578
O	-0.8925	-2.54277	-0.82917
O	0.65339	-1.47517	1.58521
H	-1.45678	-0.61979	2.90505
H	0.03299	-2.8409	-1.03085
H	4.4909	-0.53918	0.23191
O	5.04587	-1.32269	0.40137
H	5.49342	-1.14482	1.24202
H	3.63707	-2.46782	0.63178
O	2.84573	-3.04301	0.73148
H	2.12276	-2.45352	1.03131
O	1.49367	-3.67428	-1.53351
H	2.10036	-3.45644	-0.78041

H	1.86372	-3.22268	-2.30614

Microsovlent models
One-water
TS1-1W

Sum of electronic and zero-point Energies= -950.704509
Sum of electronic and thermal Energies= -950.684573
Sum of electronic and thermal Enthalpies= -950.683629
Sum of electronic and thermal Free Energies= -950.755442

C	1.52077	0.2467	0.89623
C	2.73244	0.80366	1.69823
H	0.78928	1.02714	0.67075
H	1.01454	-0.5627	1.42879
H	2.59235	1.86603	1.91409
H	2.83642	0.27726	2.65055
N	3.99134	0.64332	0.93749
C	3.85311	1.35143	-0.3553
C	2.66053	0.78399	-1.18057
H	2.98877	0.35726	-2.13202
H	1.90266	1.54523	-1.38555
H	4.78997	1.24036	-0.90738
H	3.70513	2.41507	-0.15153
C	4.19063	-0.79746	0.66076
H	5.12105	-0.91076	0.09839
H	4.30683	-1.3191	1.61416
C	2.99149	-1.38648	-0.14023
H	3.30611	-1.79031	-1.10618
H	2.47725	-2.17614	0.41383
N	2.01232	-0.299	-0.3968
H	0.92802	-0.76861	-1.08207
C	-0.12501	-1.16985	-1.82288
C	-1.20035	-1.39844	-0.93845
C	-2.13818	-0.5763	-0.27268
C	-2.89587	-1.43462	0.59698
N	-2.48051	-2.66789	0.49201
O	-1.41624	-2.65792	-0.48146
N	-2.25664	0.78849	-0.41624
C	-4.00601	-1.10035	1.53462
H	-4.84741	-0.66266	0.99023
H	-4.33976	-2.00412	2.04869
H	-3.67241	-0.36717	2.27422
H	0.22918	-2.07185	-2.32355
H	-0.25099	-0.30907	-2.47629

O	-3.14889	1.40445	0.23676
O	-1.4715	1.40244	-1.18197
H	-3.0446	3.27574	0.09975
O	-3.07011	4.25436	0.10902
H	-2.34542	4.52371	-0.47313

IM1-1W

Sum of electronic and zero-point Energies= -950.715004
Sum of electronic and thermal Energies= -950.694594
Sum of electronic and thermal Enthalpies= -950.693650
Sum of electronic and thermal Free Energies= -950.766935

C	-1.53933	0.30176	-0.87272
C	-2.75154	0.8341	-1.68026
H	-0.83434	1.08754	-0.59785
H	-1.00538	-0.49831	-1.38715
H	-2.62585	1.89916	-1.88553
H	-2.82526	0.31067	-2.63572
N	-4.01926	0.64319	-0.94304
C	-3.92633	1.34483	0.35579
C	-2.76084	0.79207	1.21833
H	-3.10322	0.32539	2.14307
H	-2.01079	1.54824	1.4537
H	-4.8746	1.22213	0.88324
H	-3.77852	2.40949	0.16362
C	-4.21239	-0.80109	-0.69029
H	-5.14781	-0.93073	-0.14216
H	-4.30705	-1.31287	-1.65009
C	-3.03044	-1.40165	0.11716
H	-3.34137	-1.8191	1.07607
H	-2.47484	-2.15716	-0.44037
N	-2.07206	-0.2784	0.41275
H	-1.27161	-0.64563	0.95844
C	0.50002	-1.17016	2.1349
C	1.3265	-1.38924	1.08485
C	2.16103	-0.56	0.24802
C	2.7897	-1.4424	-0.70201
N	2.41184	-2.67482	-0.51437
O	1.49523	-2.68319	0.59517
N	2.30674	0.77525	0.3575
C	3.75178	-1.12543	-1.79814
H	4.65457	-0.65806	-1.39555
H	4.02817	-2.0428	-2.32285
H	3.30761	-0.42405	-2.51013

H	0.00463	-2.00866	2.61339
H	0.39809	-0.17861	2.55182
O	3.09525	1.41689	-0.43498
O	1.65397	1.41371	1.25074
H	3.09271	3.20931	-0.1202
O	3.16216	4.1886	-0.05501
H	2.62224	4.42277	0.71309

Three-water

TS1-3W

Sum of electronic and zero-point Energies= -1103.563745

Sum of electronic and thermal Energies= -1103.538196

Sum of electronic and thermal Enthalpies= -1103.537252

Sum of electronic and thermal Free Energies= -1103.622694

C	-1.85324	-1.16506	-4.02026
C	-3.34782	-0.92444	-3.66207
H	-1.55665	-2.2053	-3.86304
H	-1.18473	-0.52336	-3.44044
H	-3.82796	-1.86147	-3.36866
H	-3.43126	-0.22755	-2.82417
N	-4.08914	-0.3652	-4.81572
C	-4.02504	-1.34169	-5.9271
C	-2.55019	-1.67788	-6.29363
H	-2.33046	-1.46418	-7.34289
H	-2.31019	-2.726	-6.09695
H	-4.54683	-0.91372	-6.78691
H	-4.55919	-2.24646	-5.62593
C	-3.41143	0.87821	-5.24832
H	-3.97983	1.31151	-6.07527
H	-3.43492	1.58653	-4.41617
C	-1.94409	0.59548	-5.68774
H	-1.78861	0.80138	-6.75005
H	-1.22187	1.18132	-5.11251
N	-1.64939	-0.84233	-5.45736
H	-0.35123	-1.09243	-5.75753
C	0.92165	-1.33709	-6.1349
C	1.71037	-1.56437	-4.90665
C	2.11635	-2.68238	-4.19939
C	2.87413	-2.20753	-3.07687
N	2.92163	-0.89907	-3.10252
O	2.18317	-0.49768	-4.2629
N	1.82356	-4.01758	-4.53927
C	3.5517	-2.96432	-1.98788

H	4.30059	-3.64288	-2.40585
H	4.03867	-2.26803	-1.3025
H	2.82632	-3.56761	-1.43478
H	1.21008	-0.37741	-6.56688
H	0.93965	-2.24788	-6.74122
O	2.25599	-4.92229	-3.80441
O	1.14612	-4.2331	-5.55954
H	2.04561	-6.87984	-3.92175
O	2.07307	-7.85136	-3.84816
H	1.44214	-8.06729	-3.14572
H	0.23625	-5.73891	-6.51189
O	-0.18575	-6.3728	-7.11796
H	-1.11705	-6.39201	-6.85254
H	0.62043	-7.97982	-6.65118
O	1.09421	-8.77568	-6.32997
H	1.44415	-8.50505	-5.45439

IM1-3W

Sum of electronic and zero-point Energies=	-1103.575774
Sum of electronic and thermal Energies=	-1103.549838
Sum of electronic and thermal Enthalpies=	-1103.548893
Sum of electronic and thermal Free Energies=	-1103.635297

C	-2.25049	-0.13616	1.03292
C	-3.41821	-0.78686	1.83282
H	-1.33032	-0.71607	1.10302
H	-2.05141	0.88714	1.35581
H	-3.0736	-1.69394	2.33162
H	-3.78124	-0.0947	2.59875
N	-4.54524	-1.1385	0.94716
C	-4.0562	-2.08374	-0.0763
C	-2.89335	-1.4677	-0.90509
H	-3.13473	-1.39654	-1.96532
H	-1.96353	-2.02883	-0.79156
H	-4.88881	-2.34701	-0.73278
H	-3.71919	-2.99362	0.42584
C	-5.00972	0.08866	0.26746
H	-5.85038	-0.17289	-0.38288
H	-5.37658	0.78338	1.02354
C	-3.87186	0.74268	-0.56727
H	-4.10379	0.77943	-1.62913
H	-3.63309	1.75114	-0.22148
N	-2.63094	-0.07799	-0.41186
H	-1.88913	0.30692	-0.91138

C	-0.57577	0.88977	-1.89986
C	0.26976	1.62534	-1.10571
C	1.32614	1.32216	-0.18598
C	1.75317	2.57837	0.38102
N	1.05358	3.56525	-0.10822
O	0.12103	2.98705	-1.04579
N	1.77946	0.07927	0.11074
C	2.82624	2.84892	1.37979
H	3.79087	2.49263	1.00785
H	2.88849	3.92204	1.57216
H	2.61758	2.32615	2.31743
H	-1.14512	1.45234	-2.64441
H	-0.23062	-0.09846	-2.2049
O	2.71781	-0.07254	0.95643
O	1.24934	-0.93207	-0.44641
H	4.55972	-0.26369	0.46843
O	5.4993	-0.44308	0.25495
H	5.96928	-0.341	1.09593
H	2.05438	-2.60715	-0.2077
O	2.43279	-3.51325	-0.25779
H	2.23802	-3.9202	0.59882
H	4.26094	-3.31151	-0.40029
O	5.23106	-3.18388	-0.47607
H	5.37735	-2.25025	-0.21746

Six-water
TS1-6W

Sum of electronic and zero-point Energies=	-1332.850827
Sum of electronic and thermal Energies=	-1332.816160
Sum of electronic and thermal Enthalpies=	-1332.815216
Sum of electronic and thermal Free Energies=	-1332.922091

C	-1.14852	-1.99676	1.02962
C	-1.90909	-3.06671	1.86769
H	-0.08736	-2.23815	0.92225
H	-1.23405	-0.9997	1.47031
H	-1.20515	-3.77932	2.30518
H	-2.46116	-2.5943	2.68431
N	-2.87552	-3.80902	1.02703
C	-2.14196	-4.3809	-0.12575
C	-1.52891	-3.25687	-1.00881
H	-2.00626	-3.2014	-1.99071
H	-0.45383	-3.39265	-1.15496
H	-2.83275	-4.99255	-0.71195

H	-1.35905	-5.03713	0.26319
C	-3.88	-2.85059	0.51314
H	-4.55291	-3.39087	-0.15777
H	-4.47007	-2.47756	1.35409
C	-3.19441	-1.66831	-0.23444
H	-3.5867	-1.54423	-1.24725
H	-3.31308	-0.72404	0.30372
N	-1.73936	-1.95145	-0.33217
H	-1.07999	-0.96597	-1.05512
C	-0.42458	-0.11154	-1.83121
C	0.02694	0.9542	-1.02451
C	1.1267	1.16293	-0.16204
C	0.93996	2.45078	0.44694
N	-0.16786	2.99053	0.01598
O	-0.74667	2.06394	-0.91592
N	2.15841	0.27858	0.06171
C	1.78991	3.17673	1.43264
H	2.79154	3.33683	1.02462
H	1.33692	4.14138	1.66988
H	1.89381	2.59041	2.34981
H	-1.16956	0.18824	-2.56934
H	0.36992	-0.74353	-2.22277
O	3.0915	0.59544	0.84818
O	2.14031	-0.84137	-0.51576
H	4.86938	1.01873	0.21074
O	5.77057	1.19992	-0.11704
H	6.23478	1.59903	0.63357
H	3.49071	-2.08297	-0.09734
O	4.15875	-2.79551	-0.02299
H	4.15254	-3.05273	0.91061
H	5.76861	-1.96315	-0.37169
O	6.60146	-1.47941	-0.56093
H	6.37559	-0.53819	-0.40597
O	-3.73551	1.99724	-1.2917
H	-2.76962	1.96271	-1.17973
H	-4.0633	1.20911	-0.83272
O	-1.71255	5.36504	0.68409
H	-1.16695	4.59501	0.4135
H	-1.5173	6.05727	0.03581
O	-4.31338	4.35645	0.20975
H	-4.12941	3.55587	-0.32375
H	-3.42711	4.73159	0.40067

IM1-6W

Sum of electronic and zero-point Energies= -1332.863740
Sum of electronic and thermal Energies= -1332.829017
Sum of electronic and thermal Enthalpies= -1332.828072
Sum of electronic and thermal Free Energies= -1332.934357

C	-1.41353	-1.77325	1.09206
C	-2.14538	-2.90674	1.85714
H	-0.35815	-1.98916	0.92026
H	-1.50994	-0.80146	1.57836
H	-1.4692	-3.74619	2.03251
H	-2.48891	-2.53959	2.82636
N	-3.31139	-3.40206	1.09636
C	-2.84202	-3.98955	-0.17505
C	-1.996	-2.97447	-0.98567
H	-2.37852	-2.81162	-1.99428
H	-0.94144	-3.24769	-1.04077
H	-3.71658	-4.30215	-0.74959
H	-2.24607	-4.87746	0.04574
C	-4.20539	-2.26505	0.79675
H	-5.10222	-2.64216	0.30124
H	-4.50524	-1.80775	1.74196
C	-3.50278	-1.21931	-0.1103
H	-3.92647	-1.17489	-1.11476
H	-3.49499	-0.21893	0.32544
N	-2.06684	-1.65364	-0.26082
H	-1.55371	-0.95129	-0.81442
C	-0.07194	0.14782	-2.24698
C	0.28574	0.93637	-1.21848
C	1.23935	0.84903	-0.13985
C	1.10497	2.05724	0.62983
N	0.18456	2.82112	0.12016
O	-0.34636	2.16627	-1.03808
N	2.06997	-0.16478	0.08095
C	1.84362	2.49912	1.84818
H	2.91697	2.54804	1.64597
H	1.48885	3.48431	2.15789
H	1.69274	1.78853	2.66575
H	-0.83182	0.48436	-2.94372
H	0.42557	-0.7967	-2.41204
O	2.88646	-0.15094	1.0617
O	2.03307	-1.1717	-0.69596
H	4.57512	0.50647	0.79065
O	5.49854	0.80144	0.63083
H	5.88128	0.92593	1.51164

H	3.41387	-2.34051	-0.69669
O	4.12368	-3.00286	-0.85737
H	4.04021	-3.64694	-0.13947
H	5.71408	-2.08509	-0.67223
O	6.53274	-1.55531	-0.56579
H	6.22757	-0.72369	-0.14614
O	-3.21802	2.38471	-1.52338
H	-2.2728	2.22957	-1.34364
H	-3.67143	1.60093	-1.17699
O	-0.93125	5.44277	0.48445
H	-0.50039	4.56487	0.37086
H	-0.64737	5.9643	-0.2809
O	-3.63096	4.63657	0.17876
H	-3.54571	3.85873	-0.41099
H	-2.71242	4.96771	0.27843

The first sep for DABCO catalyzes directly the vinylogous Henry reaction of **1a** and **2** in CH_3OH.

2

Sum of electronic and zero-point Energies= -529.103355
Sum of electronic and thermal Energies= -529.094135
Sum of electronic and thermal Enthalpies= -529.093191
Sum of electronic and thermal Free Energies= -529.138030

C	-1.1401	-0.74977	-0.00001
C	-0.00421	0.12669	-0.00002
C	1.10736	-0.68684	-0.00001
N	-0.73668	-1.99708	0.
O	0.6827	-1.95143	-0.00001
N	0.00333	1.55427	-0.00001
C	-2.60007	-0.43309	0.00001
C	2.57333	-0.45079	0.00003
H	-2.86421	0.16093	-0.87895
H	-3.17095	-1.36358	-0.00001
H	-2.86418	0.16087	0.87901
H	2.86434	0.13265	0.87821
H	3.09862	-1.40764	-0.00025
H	2.8643	0.1332	-0.8778
O	-1.08712	2.13461	0.00003
O	1.10288	2.12258	-0.00003

DABCO

Sum of electronic and zero-point Energies= -345.187531
Sum of electronic and thermal Energies= -345.181234

Sum of electronic and thermal Enthalpies= -345.180290
Sum of electronic and thermal Free Energies= -345.217838

C	-0.78284	1.37853	-0.14177
C	0.78288	1.37848	-0.14202
H	-1.18609	1.79416	-1.07252
H	-1.18566	1.97537	0.68478
H	1.1859	1.79481	-1.07257
H	1.18598	1.97464	0.68488
N	-1.28869	0.00021	0.00059
C	-0.78354	-0.81231	-1.12223
H	-1.18623	-1.82633	-1.01609
H	-1.18743	-0.39548	-2.0522
C	0.78224	-0.812	-1.12333
H	1.18552	-1.82592	-1.01849
H	1.18463	-0.39438	-2.0536
N	1.28869	0.00003	-0.00075
C	0.78356	-0.5667	1.26422
H	1.18624	-1.5811	1.36678
H	1.18731	0.03104	2.08964
C	-0.78231	-0.56613	1.26524
H	-1.18563	-1.58015	1.36902
H	-1.18451	0.03248	2.09078

TS1

Sum of electronic and zero-point Energies= -874.277897
Sum of electronic and thermal Energies= -874.261532
Sum of electronic and thermal Enthalpies= -874.260588
Sum of electronic and thermal Free Energies= -874.323469

C	3.20921	-0.70673	0.56683
C	2.37674	0.12944	-0.25309
C	1.55706	-0.73469	-1.01337
N	2.94338	-1.96692	0.34941
O	1.90705	-1.99641	-0.65229
N	2.3418	1.50939	-0.2826
C	4.25435	-0.3302	1.56171
C	0.48078	-0.55818	-1.90817
H	3.82394	0.29008	2.35284
H	4.68305	-1.2316	2.00486
H	5.04874	0.24863	1.08235
H	0.24806	-1.4482	-2.49452
H	-0.63426	-0.36932	-1.15387
H	0.51359	0.36644	-2.48005

O	3.12991	2.16812	0.44726
O	1.51285	2.08563	-1.03502
N	-1.76891	-0.17469	-0.43795
C	-1.49918	-0.59384	0.96295
C	-2.80121	-0.41775	1.79583
H	-1.16197	-1.63342	0.94475
H	-0.68363	0.02776	1.3416
H	-3.15657	-1.38443	2.16174
H	-2.61538	0.22176	2.66254
C	-2.88564	-0.97971	-0.99811
H	-3.01531	-0.6936	-2.04512
H	-2.58933	-2.03123	-0.96148
C	-4.16685	-0.70828	-0.15705
H	-4.93927	-0.2409	-0.77318
H	-4.57106	-1.64475	0.2357
C	-2.13003	1.26624	-0.46198
C	-3.38045	1.4799	0.44186
H	-4.1865	1.94921	-0.12795
H	-3.13974	2.13283	1.28478
H	-2.32469	1.54361	-1.50132
H	-1.26477	1.83387	-0.1087
N	-3.87655	0.19327	0.98127

IM1

Sum of electronic and zero-point Energies=	-874.286889
Sum of electronic and thermal Energies=	-874.269691
Sum of electronic and thermal Enthalpies=	-874.268747
Sum of electronic and thermal Free Energies=	-874.335144

C	3.04923	-0.59339	0.76684
C	2.33987	0.13084	-0.25534
C	1.71199	-0.85921	-1.09691
N	2.90499	-1.87982	0.61569
O	2.07476	-2.08646	-0.54373
N	2.26354	1.47041	-0.41441
C	3.86659	-0.07136	1.90177
C	0.91581	-0.82563	-2.1926
H	3.26323	0.57675	2.54355
H	4.25141	-0.90513	2.49346
H	4.70624	0.5224	1.52989
H	0.59717	-1.75401	-2.65491
H	-0.94103	-0.56091	-0.99661
H	0.66116	0.11734	-2.65407
O	2.87076	2.26458	0.38745

O	1.57069	1.94943	-1.37728
C	-1.44622	-0.50074	1.02231
C	-2.73485	-0.19782	1.82885
H	-1.10205	-1.52897	1.14176
H	-0.62923	0.18149	1.26039
H	-3.11355	-1.10794	2.29859
H	-2.51545	0.52469	2.61749
C	-2.9337	-1.18084	-0.82469
H	-3.05833	-1.09687	-1.90516
H	-2.65464	-2.20533	-0.5731
C	-4.17187	-0.68171	-0.03469
H	-4.90752	-0.2471	-0.71483
H	-4.64348	-1.51726	0.48686
C	-3.26974	1.52925	0.24307
H	-4.07818	1.98242	-0.33439
H	-2.93412	2.25626	0.9857
C	-2.10213	1.14269	-0.70075
H	-2.36691	1.21852	-1.75643
H	-1.19431	1.71971	-0.51841
N	-1.77255	-0.30355	-0.43571
N	-3.79883	0.34883	0.95894

The first step for DABCO catalyzes directly the vinylogous Henry reaction of **1a** and **2** in THF.

2

Sum of electronic and zero-point Energies=	-529.105086
Sum of electronic and thermal Energies=	-529.095727
Sum of electronic and thermal Enthalpies=	-529.094783
Sum of electronic and thermal Free Energies=	-529.140265

C	-1.1401	-0.74977	-0.00001
C	-0.00421	0.12669	-0.00002
C	1.10736	-0.68684	-0.00001
N	-0.73668	-1.99708	0.
O	0.6827	-1.95143	-0.00001
N	0.00333	1.55427	-0.00001
C	-2.60007	-0.43309	0.00001
C	2.57333	-0.45079	0.00003
H	-2.86421	0.16093	-0.87895
H	-3.17095	-1.36358	-0.00001
H	-2.86418	0.16087	0.87901
H	2.86434	0.13265	0.87821
H	3.09862	-1.40764	-0.00025
H	2.8643	0.1332	-0.8778

O	-1.08712	2.13461	0.00003
O	1.10288	2.12258	-0.00003

DABCO

Sum of electronic and zero-point Energies= -345.183109
Sum of electronic and thermal Energies= -345.176748
Sum of electronic and thermal Enthalpies= -345.175804
Sum of electronic and thermal Free Energies= -345.213514

C	-0.78284	1.37853	-0.14177
C	0.78288	1.37848	-0.14202
H	-1.18609	1.79416	-1.07252
H	-1.18566	1.97537	0.68478
H	1.1859	1.79481	-1.07257
H	1.18598	1.97464	0.68488
N	-1.28869	0.00021	0.00059
C	-0.78354	-0.81231	-1.12223
H	-1.18623	-1.82633	-1.01609
H	-1.18743	-0.39548	-2.0522
C	0.78224	-0.812	-1.12333
H	1.18552	-1.82592	-1.01849
H	1.18463	-0.39438	-2.0536
N	1.28869	0.00003	-0.00075
C	0.78356	-0.5667	1.26422
H	1.18624	-1.5811	1.36678
H	1.18731	0.03104	2.08964
C	-0.78231	-0.56613	1.26524
H	-1.18563	-1.58015	1.36902
H	-1.18451	0.03248	2.09078

TS1

Sum of electronic and zero-point Energies= -874.272544
Sum of electronic and thermal Energies= -874.256004
Sum of electronic and thermal Enthalpies= -874.255060
Sum of electronic and thermal Free Energies= -874.319247

C	3.20921	-0.70673	0.56683
C	2.37674	0.12944	-0.25309
C	1.55706	-0.73469	-1.01337
N	2.94338	-1.96692	0.34941
O	1.90705	-1.99641	-0.65229
N	2.3418	1.50939	-0.2826
C	4.25435	-0.3302	1.56171
C	0.48078	-0.55818	-1.90817

H	3.82394	0.29008	2.35284
H	4.68305	-1.2316	2.00486
H	5.04874	0.24863	1.08235
H	0.24806	-1.4482	-2.49452
H	-0.63426	-0.36932	-1.15387
H	0.51359	0.36644	-2.48005
O	3.12991	2.16812	0.44726
O	1.51285	2.08563	-1.03502
N	-1.76891	-0.17469	-0.43795
C	-1.49918	-0.59384	0.96295
C	-2.80121	-0.41775	1.79583
H	-1.16197	-1.63342	0.94475
H	-0.68363	0.02776	1.3416
H	-3.15657	-1.38443	2.16174
H	-2.61538	0.22176	2.66254
C	-2.88564	-0.97971	-0.99811
H	-3.01531	-0.6936	-2.04512
H	-2.58933	-2.03123	-0.96148
C	-4.16685	-0.70828	-0.15705
H	-4.93927	-0.2409	-0.77318
H	-4.57106	-1.64475	0.2357
C	-2.13003	1.26624	-0.46198
C	-3.38045	1.4799	0.44186
H	-4.1865	1.94921	-0.12795
H	-3.13974	2.13283	1.28478
H	-2.32469	1.54361	-1.50132
H	-1.26477	1.83387	-0.1087
N	-3.87655	0.19327	0.98127

IM1

Sum of electronic and zero-point Energies=	-874.273827
Sum of electronic and thermal Energies=	-874.256631
Sum of electronic and thermal Enthalpies=	-874.255687
Sum of electronic and thermal Free Energies=	-874.321865

C	3.04923	-0.59339	0.76684
C	2.33987	0.13084	-0.25534
C	1.71199	-0.85921	-1.09691
N	2.90499	-1.87982	0.61569
O	2.07476	-2.08646	-0.54373
N	2.26354	1.47041	-0.41441
C	3.86659	-0.07136	1.90177
C	0.91581	-0.82563	-2.1926

H	3.26323	0.57675	2.54355
H	4.25141	-0.90513	2.49346
H	4.70624	0.5224	1.52989
H	0.59717	-1.75401	-2.65491
H	-0.94103	-0.56091	-0.99661
H	0.66116	0.11734	-2.65407
O	2.87076	2.26458	0.38745
O	1.57069	1.94943	-1.37728
C	-1.44622	-0.50074	1.02231
C	-2.73485	-0.19782	1.82885
H	-1.10205	-1.52897	1.14176
H	-0.62923	0.18149	1.26039
H	-3.11355	-1.10794	2.29859
H	-2.51545	0.52469	2.61749
C	-2.9337	-1.18084	-0.82469
H	-3.05833	-1.09687	-1.90516
H	-2.65464	-2.20533	-0.5731
C	-4.17187	-0.68171	-0.03469
H	-4.90752	-0.2471	-0.71483
H	-4.64348	-1.51726	0.48686
C	-3.26974	1.52925	0.24307
H	-4.07818	1.98242	-0.33439
H	-2.93412	2.25626	0.9857
C	-2.10213	1.14269	-0.70075
H	-2.36691	1.21852	-1.75643
H	-1.19431	1.71971	-0.51841
N	-1.77255	-0.30355	-0.43571
N	-3.79883	0.34883	0.95894