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Table 1: Cartesian coordinates and energies for the structure 'EP01'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.180464	-1.142789	0.000000
2	6	0	1.000614	-1.755348	0.000000
3	6	0	0.901732	-3.238964	0.000000
4	6	0	-0.199467	-0.924611	0.000000
5	8	0	-1.328529	-1.479485	0.000000
6	6	0	0.000000	0.512578	0.000000
7	6	0	-1.157520	1.353502	0.000000
8	6	0	1.312594	1.075358	0.000000
9	6	0	1.563276	2.563608	0.000000
10	6	0	2.387171	0.216738	0.000000
11	1	0	1.133957	3.042611	0.886412
12	1	0	3.419141	0.538859	0.000000
13	1	0	3.009842	-1.732469	0.000000
14	1	0	-4.184704	1.448892	0.888998
15	1	0	-4.184704	1.448892	-0.888998
16	6	0	-3.594117	1.686044	0.000000
17	7	0	-2.375496	0.882447	0.000000
18	1	0	-2.415379	-0.158981	0.000000
19	1	0	-3.342819	2.748118	0.000000
20	1	0	1.883307	-3.719409	0.000000
21	1	0	0.334008	-3.572976	0.875245
22	1	0	0.334008	-3.572976	-0.875245
23	1	0	-1.046757	2.435345	0.000000
24	1	0	2.633906	2.776320	0.000000
25	1	0	1.133957	3.042611	-0.886412

Sum of electronic and zero-point Energies= -535.128658
Sum of electronic and thermal Energies= -535.116575
Sum of electronic and thermal Enthalpies= -535.115631
Sum of electronic and thermal Free Energies= -535.166317

Table 2: Cartesian coordinates and energies for the structure 'V01'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.407386	-1.637988	-0.318885
2	6	0	1.595013	-0.408113	-0.365185
3	6	0	0.133459	-0.787747	-0.068382
4	6	0	-0.852640	0.351403	-0.330058
5	6	0	-2.272428	0.012750	0.060274

6	8	0	-3.152936	0.937559	-0.406497
7	6	0	2.106789	0.668061	0.566846
8	6	0	2.602395	1.849524	0.184142
9	8	0	-2.629787	-0.941164	0.719357
10	1	0	2.982786	2.570982	0.901604
11	1	0	2.646206	2.134333	-0.865357
12	1	0	2.081969	0.415319	1.629652
13	1	0	1.656273	-0.029142	-1.394849
14	1	0	-0.123330	-1.654324	-0.686435
15	1	0	0.043017	-1.113331	0.975833
16	1	0	3.392413	-1.420150	-0.447418
17	1	0	2.316747	-2.097459	0.585582
18	1	0	-0.851986	0.648982	-1.385456
19	1	0	-0.573638	1.254100	0.229617
20	1	0	-4.035904	0.670179	-0.099275

Sum of electronic and zero-point Energies=	-440.322595
Sum of electronic and thermal Energies=	-440.312193
Sum of electronic and thermal Enthalpies=	-440.311249
Sum of electronic and thermal Free Energies=	-440.359805

Table 3: Cartesian coordinates and energies of for the structure 'pre-reaction complex'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.103065	-0.342550	0.297261
2	6	0	2.108778	-0.882747	1.170791
3	6	0	0.877122	-0.274491	1.200596
4	7	0	0.617872	0.820508	0.413598
5	6	0	1.479206	1.386226	-0.421650
6	6	0	2.815583	0.810271	-0.534287
7	6	0	2.360541	-2.085151	2.046874
8	6	0	1.098830	2.579038	-1.227676
9	8	0	3.645266	1.327397	-1.329602
10	6	0	4.404200	-0.923205	0.217007
11	7	0	5.339390	-0.462481	-0.572786
12	6	0	6.685055	-1.010789	-0.698112
13	7	0	-2.890086	-2.861828	-0.381950
14	6	0	-3.853730	-1.761164	-0.186526
15	6	0	-3.043639	-0.466553	0.014955
16	6	0	-3.896572	0.739878	0.405739
17	6	0	-3.100660	1.991267	0.668306
18	8	0	-3.879290	3.042293	0.942418
19	6	0	-4.865388	-1.641782	-1.304620
20	6	0	-6.184780	-1.804457	-1.167840
21	8	0	-1.876217	2.091468	0.650743
22	1	0	1.472007	-2.328682	2.632405

23	1	0	0.058488	-0.609922	1.821582
24	1	0	-0.330849	1.231860	0.484286
25	1	0	0.087655	2.918146	-0.997583
26	1	0	1.811853	3.389278	-1.042695
27	1	0	1.177309	2.346680	-2.295578
28	1	0	4.657344	-1.788329	0.825861
29	1	0	2.612450	-2.969584	1.451748
30	1	0	3.180335	-1.906653	2.751277
31	1	0	-4.449526	-1.434829	-2.293769
32	1	0	-2.299913	-0.669398	0.792198
33	1	0	-2.490922	-0.242812	-0.908213
34	1	0	-2.405561	-2.756084	-1.272370
35	1	0	-4.477526	0.536940	1.315506
36	1	0	-4.643353	0.976288	-0.361112
37	1	0	-3.317111	3.817462	1.117883
38	1	0	7.418233	-0.241804	-0.440038
39	1	0	6.804377	-1.866240	-0.030559
40	1	0	6.855872	-1.327213	-1.730691
41	1	0	5.032925	0.364356	-1.130352
42	1	0	-6.635837	-2.020576	-0.201496
43	1	0	-6.860027	-1.735467	-2.015271
44	1	0	-4.390954	-1.977253	0.746394
45	1	0	-3.381254	-3.751565	-0.424829

Sum of electronic and zero-point Energies=	-975.475433
Sum of electronic and thermal Energies=	-975.451819
Sum of electronic and thermal Enthalpies=	-975.450875
Sum of electronic and thermal Free Energies=	-975.531316

Table 4: Cartesian coordinates and energies for the structure '00TS01'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.586704	-0.398163	0.458857
2	6	0	-1.275865	-1.167205	1.596935
3	6	0	-0.976362	-2.509341	1.412539
4	7	0	-0.991684	-3.033024	0.155951
5	6	0	-1.282493	-2.365698	-0.968516
6	6	0	-1.611696	-0.962287	-0.865509
7	6	0	-1.267255	-0.603857	2.999822
8	6	0	-1.259121	-3.056982	-2.287795
9	8	0	-1.871173	-0.275453	-1.899701
10	6	0	-1.917045	1.045287	0.567859
11	7	0	-3.055441	1.471976	-0.005597
12	6	0	-3.624211	2.797870	0.214722
13	7	0	-0.467133	1.870962	-0.480932
14	6	0	0.979602	1.927997	-0.078849

15	6	0	1.627466	0.559877	-0.337364
16	6	0	3.072501	0.457037	0.155032
17	6	0	3.560161	-0.979143	0.148787
18	8	0	4.898719	-1.048650	0.279874
19	6	0	1.660561	3.059006	-0.811867
20	6	0	2.113465	4.170726	-0.225405
21	8	0	2.849511	-1.961947	0.060254
22	1	0	-1.007498	-1.375529	3.727452
23	1	0	-0.722024	-3.187335	2.215084
24	1	0	-0.746063	-4.014877	0.060987
25	1	0	-0.987428	-4.112180	-2.196908
26	1	0	-2.239031	-2.977428	-2.770252
27	1	0	-0.548170	-2.560559	-2.956732
28	1	0	-1.673458	1.539821	1.504266
29	1	0	-0.536031	0.204748	3.108983
30	1	0	-2.249200	-0.206544	3.277179
31	1	0	1.768993	2.927912	-1.889475
32	1	0	1.039549	-0.216346	0.154690
33	1	0	1.591994	0.344171	-1.413079
34	1	0	-0.620757	1.353850	-1.356608
35	1	0	3.165638	0.816431	1.189429
36	1	0	3.762129	1.068339	-0.434408
37	1	0	5.156125	-1.987112	0.295625
38	1	0	-4.710855	2.742450	0.123049
39	1	0	-3.381352	3.138035	1.224567
40	1	0	-3.256019	3.535481	-0.509896
41	1	0	-3.308662	0.983782	-0.862576
42	1	0	2.030894	4.328285	0.847953
43	1	0	2.594347	4.957944	-0.797518
44	1	0	0.995979	2.145882	0.997511
45	1	0	-0.813761	2.819048	-0.624192

Sum of electronic and zero-point Energies=	-975.442160
Sum of electronic and thermal Energies=	-975.418965
Sum of electronic and thermal Enthalpies=	-975.418020
Sum of electronic and thermal Free Energies=	-975.497125

Table 5: Cartesian coordinates and energies for the structure '01'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.579938	0.128090	-0.270839
2	6	0	2.189531	-0.558177	-1.339501
3	6	0	2.834321	-1.756526	-1.068277
4	7	0	2.862956	-2.230123	0.203753
5	6	0	2.303175	-1.631487	1.267984
6	6	0	1.627156	-0.387005	1.061777

7	6	0	2.170470	-0.040986	-2.757193
8	6	0	2.395709	-2.252268	2.620450
9	8	0	1.081802	0.208153	2.072950
10	6	0	0.905904	1.472615	-0.525749
11	7	0	1.878013	2.513506	-0.588893
12	6	0	1.456401	3.842476	-1.029876
13	7	0	-0.174529	1.721810	0.562308
14	6	0	-1.611969	1.366853	0.233844
15	6	0	-1.747025	-0.153906	0.063103
16	6	0	-3.151891	-0.583733	-0.365783
17	6	0	-3.199252	-2.061854	-0.700479
18	8	0	-4.462817	-2.479273	-0.913135
19	6	0	-2.480576	1.927077	1.332022
20	6	0	-3.352537	2.923811	1.158955
21	8	0	-2.232430	-2.792103	-0.783887
22	1	0	2.763749	-0.679100	-3.415313
23	1	0	3.331354	-2.355242	-1.819349
24	1	0	3.342393	-3.111504	0.365268
25	1	0	2.927579	-3.207366	2.598998
26	1	0	2.905139	-1.574728	3.313657
27	1	0	1.391739	-2.411418	3.027345
28	1	0	0.358889	1.456797	-1.475538
29	1	0	1.150231	-0.017982	-3.157844
30	1	0	2.574297	0.974124	-2.805885
31	1	0	-2.366696	1.463223	2.312131
32	1	0	-1.034662	-0.512853	-0.685098
33	1	0	-1.481819	-0.647795	1.004371
34	1	0	0.248521	1.130111	1.439572
35	1	0	-3.484547	-0.037661	-1.258800
36	1	0	-3.901147	-0.376359	0.404853
37	1	0	-4.436877	-3.425672	-1.138519
38	1	0	2.340276	4.475329	-1.130905
39	1	0	0.985082	3.765683	-2.015072
40	1	0	0.755296	4.355986	-0.351702
41	1	0	2.517596	2.520280	0.198542
42	1	0	-3.499521	3.399329	0.191554
43	1	0	-3.961217	3.290647	1.979384
44	1	0	-1.852389	1.871217	-0.711617
45	1	0	-0.146909	2.714499	0.799741

Sum of electronic and zero-point Energies=	-975.452573
Sum of electronic and thermal Energies=	-975.429599
Sum of electronic and thermal Enthalpies=	-975.428654
Sum of electronic and thermal Free Energies=	-975.506924

Table 6: Cartesian coordinates and energies for the structure '01TS02'

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.469064	-1.341317	1.125832
2	6	0	-2.258156	-2.381491	0.647863
3	7	0	-3.020548	-2.193466	-0.463129
4	6	0	-3.101307	-1.060017	-1.177345
5	6	0	-2.315490	0.068206	-0.745084
6	6	0	-1.498343	-0.121794	0.423995
7	6	0	-3.980797	-0.979105	-2.377795
8	8	0	-2.346575	1.174496	-1.370188
9	6	0	-0.697322	1.083868	0.831950
10	7	0	0.188835	1.717183	-0.216341
11	6	0	1.661193	1.460825	-0.214703
12	6	0	2.295504	2.362619	-1.244314
13	6	0	3.158074	3.340024	-0.959356
14	6	0	-0.617408	-1.590080	2.350703
15	6	0	1.958099	-0.031064	-0.449615
16	6	0	3.437219	-0.396437	-0.283632
17	6	0	3.617709	-1.876443	-0.001302
18	8	0	2.763366	-2.607089	0.461963
19	8	0	4.863903	-2.292583	-0.292939
20	7	0	-1.488825	2.352363	1.054795
21	6	0	-1.892888	2.716149	2.425178
22	1	0	-0.751621	-0.813564	3.110153
23	1	0	-2.307023	-3.359010	1.107202
24	1	0	-3.580508	-2.980725	-0.779291
25	1	0	-3.388006	-0.718067	-3.260954
26	1	0	-4.510121	-1.917173	-2.567031
27	1	0	-4.712423	-0.173650	-2.253512
28	1	0	-0.091564	0.907749	1.721590
29	1	0	-0.878888	-2.543959	2.813642
30	1	0	0.446292	-1.641335	2.092529
31	1	0	2.025382	2.162053	-2.282174
32	1	0	1.381710	-0.632508	0.257939
33	1	0	1.613586	-0.317235	-1.451637
34	1	0	-0.246179	1.572847	-1.135668
35	1	0	3.875934	0.133012	0.574118
36	1	0	4.041001	-0.114286	-1.149753
37	1	0	4.935593	-3.233256	-0.052834
38	1	0	-2.574626	1.973604	2.852088
39	1	0	-1.006410	2.804507	3.057506
40	1	0	-2.397882	3.683066	2.392374
41	1	0	-2.273609	2.345903	0.391665
42	1	0	3.457769	3.563539	0.062083
43	1	0	3.601471	3.948348	-1.741239
44	1	0	2.020557	1.749546	0.781527
45	1	0	-0.464354	2.745793	0.327460

Sum of electronic and zero-point Energies= -975.413880
Sum of electronic and thermal Energies= -975.391086
Sum of electronic and thermal Enthalpies= -975.390142
Sum of electronic and thermal Free Energies= -975.468506

Table 7: Cartesian coordinates and energies for the structure '01TS02_H_2O'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.142357	-1.416445	1.331391
2	6	0	-1.456080	-2.718651	0.959668
3	7	0	-1.939071	-2.962778	-0.287395
4	6	0	-2.165901	-2.039368	-1.236024
5	6	0	-1.872931	-0.664716	-0.924288
6	6	0	-1.335438	-0.397795	0.382334
7	6	0	-2.707940	-2.436829	-2.566416
8	8	0	-2.079514	0.265197	-1.770498
9	6	0	-1.032101	1.064404	0.644757
10	7	0	-0.101216	1.689461	-0.356469
11	6	0	1.383802	1.522178	-0.158887
12	6	0	2.069994	2.413344	-1.168230
13	6	0	2.786724	3.495334	-0.857344
14	6	0	-0.596074	-1.172939	2.720352
15	6	0	1.836971	0.057121	-0.274269
16	6	0	3.331663	-0.138170	-0.001659
17	6	0	3.675332	-1.601677	0.198002
18	8	0	2.872744	-2.485851	0.424749
19	8	0	5.003344	-1.814654	0.119218
20	7	0	-2.296598	1.885988	0.587136
21	6	0	-3.184690	1.731923	1.761739
22	1	0	-1.216018	-0.468435	3.284252
23	1	0	-1.327382	-3.576693	1.604719
24	1	0	-2.145251	-3.929700	-0.523361
25	1	0	-2.029022	-2.109908	-3.360985
26	1	0	-2.857875	-3.517159	-2.646132
27	1	0	-3.660509	-1.928900	-2.751743
28	1	0	-0.594424	1.221975	1.632756
29	1	0	-0.557304	-2.103347	3.290380
30	1	0	0.422853	-0.772190	2.688359
31	1	0	1.967939	2.111659	-2.211941
32	1	0	1.280472	-0.566079	0.427073
33	1	0	1.593446	-0.317817	-1.276662
34	1	0	-0.402504	1.349553	-1.280483
35	1	0	3.636823	0.384378	0.915939
36	1	0	3.961073	0.270204	-0.797239
37	1	0	5.170590	-2.758990	0.285104
38	1	0	-3.461724	0.686661	1.926411
39	1	0	-2.681162	2.124603	2.648361
40	1	0	-4.090403	2.315706	1.588898
41	1	0	-2.772220	1.593817	-0.276819
42	1	0	2.917411	3.823063	0.171374
43	1	0	3.273600	4.089608	-1.624310
44	1	0	1.596505	1.899445	0.849426

45	1	0	-0.397840	2.964859	-0.266614
46	1	0	-1.224564	4.605811	-0.498410
47	1	0	-1.862983	3.099885	0.395822
48	8	0	-1.012470	3.914434	0.143552

Sum of electronic and zero-point Energies= -1051.857920
Sum of electronic and thermal Energies= -1051.833453
Sum of electronic and thermal Enthalpies= -1051.832509
Sum of electronic and thermal Free Energies= -1051.914276

Table 8: Cartesian coordinates and energies for the structure '02a'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.462282	-0.052393	0.420845
2	6	0	-1.140483	-1.197028	1.174506
3	6	0	-1.742514	-2.398602	0.818322
4	7	0	-2.618975	-2.432876	-0.218086
5	6	0	-3.005383	-1.373312	-0.950703
6	6	0	-2.435272	-0.098004	-0.633773
7	6	0	-0.172470	-1.196528	2.336078
8	6	0	-3.995146	-1.534994	-2.054215
9	8	0	-2.796521	0.954277	-1.279309
10	6	0	-0.776491	1.294580	0.621460
11	7	0	-1.874830	2.371214	0.625144
12	6	0	-2.741736	2.450424	1.830363
13	7	0	0.139602	1.706764	-0.411453
14	6	0	1.597570	1.503130	-0.232406
15	6	0	2.034710	0.072391	-0.613744
16	6	0	3.493356	-0.255470	-0.265611
17	6	0	3.702260	-1.740860	-0.040706
18	8	0	4.974558	-2.113280	-0.276894
19	6	0	2.333489	2.555971	-1.027664
20	6	0	3.173815	3.452706	-0.507717
21	8	0	2.846547	-2.515814	0.343549
22	1	0	-0.390674	-0.393892	3.047436
23	1	0	-1.548206	-3.337339	1.318895
24	1	0	-3.024635	-3.333902	-0.455876
25	1	0	-3.558721	-1.208838	-3.004186
26	1	0	-4.334527	-2.569600	-2.155125
27	1	0	-4.861765	-0.889237	-1.877933
28	1	0	-0.267326	1.348926	1.585828
29	1	0	-0.227344	-2.140503	2.882085
30	1	0	0.862079	-1.085402	1.996692
31	1	0	2.156415	2.542731	-2.104234
32	1	0	1.390371	-0.646689	-0.102557
33	1	0	1.869594	-0.075690	-1.689294

34	1	0	-0.179900	1.429065	-1.336713
35	1	0	3.785034	0.232370	0.675870
36	1	0	4.199006	0.104171	-1.017792
37	1	0	5.056753	-3.061075	-0.070733
38	1	0	-3.242242	1.492285	1.972493
39	1	0	-2.138887	2.690054	2.708839
40	1	0	-3.491425	3.227181	1.674005
41	1	0	-2.431875	2.070891	-0.260356
42	1	0	3.381206	3.495029	0.559493
43	1	0	3.688823	4.176251	-1.131870
44	1	0	1.808387	1.668027	0.832716
45	1	0	-1.397911	3.255931	0.434099

Sum of electronic and zero-point Energies= -975.446682
Sum of electronic and thermal Energies= -975.424562
Sum of electronic and thermal Enthalpies= -975.423618
Sum of electronic and thermal Free Energies= -975.499345

Table 9: Cartesian coordinates and energies for the structure '02b'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.977832	-0.182180	0.427460
2	6	0	-2.251781	-1.241769	1.312757
3	6	0	-3.342024	-2.058111	1.044438
4	7	0	-4.103308	-1.817714	-0.055136
5	6	0	-3.901918	-0.829610	-0.941599
6	6	0	-2.788827	0.053023	-0.731779
7	6	0	-1.395287	-1.536508	2.520798
8	6	0	-4.804273	-0.673895	-2.118117
9	8	0	-2.567104	1.001205	-1.572429
10	6	0	-0.742307	0.687594	0.625298
11	7	0	-1.084370	2.120753	0.123082
12	6	0	-1.879765	2.952688	1.063432
13	7	0	0.380966	0.113004	-0.027849
14	6	0	1.749274	0.618154	0.208565
15	6	0	2.734053	-0.464056	-0.274462
16	6	0	4.195601	-0.162603	0.060966
17	6	0	5.124320	-1.258191	-0.422704
18	8	0	6.406178	-1.003686	-0.078371
19	6	0	2.015210	1.958456	-0.451995
20	6	0	2.341568	3.085908	0.191961
21	8	0	4.786394	-2.243866	-1.042654
22	1	0	-1.424073	-0.713453	3.243832
23	1	0	-3.631174	-2.899233	1.659640
24	1	0	-4.889614	-2.438985	-0.224681
25	1	0	-4.232734	-0.773471	-3.047113

26	1	0	-5.613485	-1.409328	-2.116367
27	1	0	-5.233488	0.333303	-2.130110
28	1	0	-0.508239	0.812104	1.687742
29	1	0	-1.740493	-2.435405	3.035541
30	1	0	-0.352286	-1.692865	2.229310
31	1	0	1.949171	1.962860	-1.542338
32	1	0	2.440875	-1.417107	0.175668
33	1	0	2.630236	-0.592350	-1.359293
34	1	0	0.203507	-0.182438	-0.982762
35	1	0	4.345580	-0.049753	1.142172
36	1	0	4.533707	0.779871	-0.385355
37	1	0	6.956432	-1.731434	-0.416670
38	1	0	-2.828230	2.454141	1.267377
39	1	0	-1.330018	3.096979	1.996453
40	1	0	-2.077988	3.920637	0.600697
41	1	0	-1.660821	1.897820	-0.782633
42	1	0	2.448708	3.115109	1.274990
43	1	0	2.544902	4.009594	-0.342060
44	1	0	1.854739	0.735435	1.296568
45	1	0	-0.198041	2.583026	-0.103770

Sum of electronic and zero-point Energies=	-975.453770
Sum of electronic and thermal Energies=	-975.430851
Sum of electronic and thermal Enthalpies=	-975.429907
Sum of electronic and thermal Free Energies=	-975.508069

Table 10: Cartesian coordinates and energies for the structure '02TS03'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.943508	-0.062117	0.457639
2	6	0	-2.756514	-0.133562	1.607349
3	6	0	-3.907146	-0.906910	1.547546
4	7	0	-4.217409	-1.561403	0.392477
5	6	0	-3.505843	-1.528790	-0.741575
6	6	0	-2.289337	-0.744042	-0.766263
7	6	0	-2.418596	0.563377	2.906087
8	6	0	-3.948617	-2.295753	-1.939322
9	8	0	-1.592081	-0.670775	-1.819225
10	6	0	-0.678641	0.705294	0.455660
11	7	0	-1.235498	2.224662	-0.766550
12	6	0	-2.330863	3.128511	-0.379537
13	7	0	0.406316	0.164522	-0.108147
14	6	0	1.776904	0.693888	0.040353
15	6	0	2.751169	-0.499965	-0.007128
16	6	0	4.200226	-0.112208	0.291277
17	6	0	5.121162	-1.316023	0.268579

18	8	0	6.397742	-0.962110	0.533540
19	6	0	2.077677	1.734966	-1.017845
20	6	0	2.419502	3.001823	-0.761351
21	8	0	4.779493	-2.457334	0.044470
22	1	0	-2.341813	1.648335	2.777931
23	1	0	-4.588288	-1.041709	2.376140
24	1	0	-5.062154	-2.127230	0.393460
25	1	0	-3.177677	-3.019396	-2.225500
26	1	0	-4.890581	-2.824171	-1.768456
27	1	0	-4.063341	-1.621279	-2.794373
28	1	0	-0.479095	1.342978	1.311733
29	1	0	-3.189246	0.379662	3.657569
30	1	0	-1.468278	0.205712	3.316129
31	1	0	2.030049	1.383464	-2.049744
32	1	0	2.415733	-1.251001	0.714851
33	1	0	2.695414	-0.975448	-0.993893
34	1	0	0.211813	-0.458691	-0.894323
35	1	0	4.295543	0.361041	1.277022
36	1	0	4.585573	0.619098	-0.428147
37	1	0	6.943606	-1.767194	0.504976
38	1	0	-3.209561	2.535698	-0.115167
39	1	0	-2.027400	3.718361	0.488747
40	1	0	-2.602468	3.813383	-1.189803
41	1	0	-1.458961	1.665098	-1.592604
42	1	0	2.502545	3.379353	0.256053
43	1	0	2.657777	3.698255	-1.559795
44	1	0	1.828763	1.165066	1.030306
45	1	0	-0.368493	2.726979	-0.956679

Sum of electronic and zero-point Energies=	-975.443804
Sum of electronic and thermal Energies=	-975.420413
Sum of electronic and thermal Enthalpies=	-975.419469
Sum of electronic and thermal Free Energies=	-975.499215

Table 11: Cartesian coordinates and energies for the structure '03a'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.363170	0.648563	-1.018212
2	7	0	4.627438	-0.540456	-0.381678
3	6	0	3.753029	-1.273387	0.301643
4	6	0	2.380555	-0.788010	0.396574
5	6	0	2.083267	0.464741	-0.272678
6	6	0	3.094324	1.179740	-0.981936
7	6	0	4.157881	-2.549799	0.948808
8	8	0	1.534898	-1.463133	1.038410
9	6	0	0.741936	0.963483	-0.207192

10	7	0	-0.215589	0.342663	0.423787
11	6	0	-1.620411	0.798414	0.527104
12	6	0	-2.521349	-0.272896	-0.122630
13	6	0	-3.991818	0.146877	-0.177402
14	6	0	-4.841927	-0.892319	-0.882475
15	8	0	-6.143398	-0.535066	-0.892663
16	6	0	2.827486	2.486455	-1.688921
17	6	0	-1.941027	1.058060	1.981830
18	6	0	-2.278364	2.254252	2.467407
19	8	0	-4.425588	-1.915478	-1.381975
20	1	0	2.480578	3.255930	-0.991086
21	1	0	5.197976	1.109512	-1.527334
22	1	0	5.581058	-0.890497	-0.440399
23	1	0	5.214290	-2.778740	0.787407
24	1	0	3.957402	-2.500889	2.024546
25	1	0	3.545328	-3.371892	0.563037
26	1	0	0.484191	1.898026	-0.700125
27	1	0	3.735199	2.861859	-2.165067
28	1	0	2.070158	2.371646	-2.471700
29	1	0	-1.903642	0.188792	2.638532
30	1	0	-2.160902	-0.475742	-1.136271
31	1	0	-2.426993	-1.213411	0.432306
32	1	0	0.093400	-0.544124	0.876486
33	1	0	-4.120209	1.097604	-0.710765
34	1	0	-4.408434	0.307667	0.822818
35	1	0	-6.642830	-1.230277	-1.355665
36	1	0	-2.334578	3.138249	1.836115
37	1	0	-2.523361	2.388227	3.516292
38	1	0	-1.689377	1.736985	-0.035583

Sum of electronic and zero-point Energies=	-879.642018
Sum of electronic and thermal Energies=	-879.622156
Sum of electronic and thermal Enthalpies=	-879.621212
Sum of electronic and thermal Free Energies=	-879.693565

Table 12: Cartesian coordinates and energies for the structure '03TS04'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.172179	4.353661	0.103295
2	7	0	2.793660	3.331351	-0.898608
3	7	0	-5.023722	-0.452713	0.021318
4	6	0	-4.184232	-0.694085	-0.987015
5	6	0	-4.689235	-1.174734	-2.302220
6	6	0	-2.762820	-0.483414	-0.766570
7	8	0	-1.954041	-0.706318	-1.706838
8	6	0	-2.368965	-0.025951	0.554509

9	6	0	-0.970197	0.159867	0.823779
10	6	0	-3.341673	0.205941	1.569183
11	6	0	-2.976049	0.677538	2.956465
12	6	0	-4.668680	-0.016881	1.271668
13	8	0	3.799434	-3.466041	0.045188
14	6	0	4.338278	-2.404837	0.276468
15	8	0	5.662209	-2.291917	0.535261
16	6	0	3.652999	-1.055016	0.317771
17	6	0	2.158579	-1.157627	0.012772
18	6	0	1.433214	0.196911	0.112468
19	7	0	-0.032365	-0.074999	-0.052687
20	6	0	1.880126	1.203997	-0.910591
21	6	0	1.421629	2.647550	-0.786673
22	1	0	-6.013659	-0.608487	-0.150109
23	1	0	-4.392208	-0.478329	-3.093582
24	1	0	-5.776497	-1.288933	-2.310918
25	1	0	-4.222766	-2.133869	-2.551385
26	1	0	-5.478241	0.127724	1.973363
27	1	0	-2.456659	1.641430	2.929760
28	1	0	-2.325909	-0.041725	3.465972
29	1	0	-3.869329	0.804208	3.571436
30	1	0	3.832684	-0.623755	1.311434
31	1	0	4.158869	-0.391643	-0.390681
32	1	0	1.694421	-1.869850	0.702891
33	1	0	2.018761	-1.569298	-0.993522
34	1	0	2.497511	5.213234	0.065379
35	1	0	3.126948	3.900381	1.096275
36	1	0	4.194122	4.685217	-0.089270
37	1	0	2.950039	3.674678	-1.848633
38	1	0	-0.648393	0.503417	1.804263
39	1	0	-0.391806	-0.392677	-0.974647
40	1	0	1.534935	0.593035	1.133175
41	1	0	1.796717	0.811790	-1.929925
42	1	0	3.158304	2.173663	-0.811235
43	1	0	0.753817	3.048481	-1.555664
44	1	0	1.015383	2.896674	0.199089
45	1	0	6.048210	-3.184152	0.495624

Sum of electronic and zero-point Energies=	-975.391807
Sum of electronic and thermal Energies=	-975.368992
Sum of electronic and thermal Enthalpies=	-975.368048
Sum of electronic and thermal Free Energies=	-975.447529

Table 13: Cartesian coordinates and energies for the structure '03TS04_H_2O'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-5.219162	-0.434842	0.053679
2	6	0	-4.851317	0.154758	1.235270
3	6	0	-3.518731	0.384607	1.501556
4	6	0	-2.553857	-0.001931	0.527665
5	6	0	-2.961110	-0.626187	-0.718882
6	6	0	-4.387369	-0.829098	-0.912021
7	6	0	-1.149465	0.185020	0.770357
8	7	0	-0.220557	-0.198772	-0.062663
9	6	0	1.247276	0.059595	0.053963
10	6	0	1.962403	-1.304201	0.075381
11	6	0	3.400065	-1.209407	0.593784
12	6	0	4.119081	-2.539590	0.519077
13	8	0	5.339562	-2.473534	1.099694
14	6	0	-3.139917	1.026536	2.815185
15	8	0	-2.159049	-0.995973	-1.617946
16	6	0	-4.905839	-1.469062	-2.151914
17	6	0	1.677906	0.957266	-1.088049
18	6	0	1.149468	2.371060	-1.105838
19	7	0	2.239183	3.409835	-0.708827
20	6	0	2.382637	3.646305	0.753387
21	8	0	3.686505	-3.549631	0.005802
22	8	0	4.147317	1.796928	-1.191465
23	1	0	1.485980	0.462143	-2.045691
24	1	0	1.400617	-2.003168	0.704845
25	1	0	1.961706	-1.729329	-0.934154
26	1	0	3.428334	-0.872974	1.637981
27	1	0	3.991012	-0.478164	0.030888
28	1	0	5.757328	-3.347519	1.009082
29	1	0	0.848806	2.673310	-2.112277
30	1	0	0.306045	2.577791	-0.430673
31	1	0	1.372357	0.550825	1.029450
32	1	0	3.177143	4.374309	0.924214
33	1	0	1.441573	4.017332	1.165819
34	1	0	2.661742	2.705602	1.227571
35	1	0	3.176017	2.986975	-1.062757
36	1	0	2.054911	4.296384	-1.181112
37	1	0	3.169349	1.203881	-1.180366
38	1	0	4.693748	1.584509	-1.960511
39	1	0	-0.816734	0.647341	1.696821
40	1	0	-5.655523	0.409093	1.911494
41	1	0	-2.497736	0.370025	3.411979
42	1	0	-2.606882	1.971268	2.662587
43	1	0	-4.028574	1.244658	3.410821
44	1	0	-4.587032	-0.896341	-3.029263
45	1	0	-4.468927	-2.466985	-2.266165
46	1	0	-5.996080	-1.550480	-2.150312
47	1	0	-6.212855	-0.588409	-0.096855
48	1	0	-0.594640	-0.631979	-0.930940

Sum of electronic and zero-point Energies= -1051.832321
Sum of electronic and thermal Energies= -1051.807759
Sum of electronic and thermal Enthalpies= -1051.806815

Sum of electronic and thermal Free Energies= -1051.889972

Table 14: Cartesian coordinates and energies for the structure '04'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.503387	5.276792	0.385212
2	7	0	2.022824	4.044646	-0.206395
3	7	0	-4.776787	-0.837488	-0.165822
4	6	0	-3.961493	-0.503241	-1.162392
5	6	0	-4.464772	-0.366564	-2.555367
6	6	0	-2.555402	-0.275167	-0.849016
7	8	0	-1.765040	0.045254	-1.774470
8	6	0	-2.161158	-0.438761	0.537833
9	6	0	-0.784297	-0.235204	0.877905
10	6	0	-3.113337	-0.800248	1.537198
11	6	0	-2.744506	-0.981215	2.989855
12	6	0	-4.420344	-0.993423	1.151938
13	8	0	3.768552	-3.389696	-0.430545
14	6	0	4.396821	-2.379982	-0.194335
15	8	0	5.743055	-2.342700	-0.118302
16	6	0	3.792845	-1.012652	0.073138
17	6	0	2.302092	-0.977696	-0.279248
18	6	0	1.566388	0.260105	0.275671
19	7	0	0.124494	0.093201	0.002097
20	6	0	2.052617	1.593803	-0.311248
21	6	0	1.382929	2.835671	0.287705
22	1	0	-5.754847	-0.994100	-0.398589
23	1	0	-4.256519	0.642025	-2.928173
24	1	0	-5.536793	-0.565954	-2.629725
25	1	0	-3.921872	-1.052217	-3.214941
26	1	0	-5.216436	-1.269410	1.829125
27	1	0	-2.328353	-0.062144	3.415833
28	1	0	-2.006088	-1.779666	3.119526
29	1	0	-3.621741	-1.248395	3.582079
30	1	0	3.955743	-0.796157	1.138018
31	1	0	4.374996	-0.269014	-0.478948
32	1	0	1.828118	-1.880167	0.119184
33	1	0	2.177038	-1.018666	-1.367886
34	1	0	0.412686	5.404521	0.268141
35	1	0	1.733469	5.290988	1.455962
36	1	0	2.002016	6.134889	-0.072185
37	1	0	1.954676	4.091126	-1.220103
38	1	0	-0.454878	-0.354313	1.907551
39	1	0	-0.248034	0.185101	-0.966271
40	1	0	1.671927	0.281512	1.368457
41	1	0	1.913434	1.575149	-1.401673

42	1	0	3.129500	1.673749	-0.136196
43	1	0	0.291855	2.814567	0.092898
44	1	0	1.504125	2.820613	1.380317
45	1	0	6.079113	-3.242724	-0.274125

Sum of electronic and zero-point Energies= -975.469904
Sum of electronic and thermal Energies= -975.446958
Sum of electronic and thermal Enthalpies= -975.446014
Sum of electronic and thermal Free Energies= -975.525656

Table 15: Cartesian coordinates and energies for the structure '04_H_2O'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-4.798232	-0.969952	0.228689
2	6	0	-4.421188	-0.192714	1.295981
3	6	0	-3.108500	0.204736	1.425110
4	6	0	-2.177754	-0.208666	0.426933
5	6	0	-2.594585	-1.022542	-0.698577
6	6	0	-4.001516	-1.400661	-0.746628
7	6	0	-0.799217	0.176455	0.527007
8	7	0	0.095948	-0.179204	-0.354927
9	6	0	1.533781	0.144419	-0.281433
10	6	0	2.309157	-1.181660	-0.135309
11	6	0	3.799552	-0.990011	0.162043
12	6	0	4.467497	-2.295422	0.554722
13	8	0	5.808342	-2.152743	0.634067
14	6	0	-2.707343	1.042885	2.614228
15	8	0	-1.822869	-1.410310	-1.615194
16	6	0	-4.529744	-2.243062	-1.853655
17	6	0	1.941038	0.956286	-1.527189
18	6	0	1.278997	2.329148	-1.696487
19	7	0	1.680363	3.296832	-0.658493
20	6	0	1.176702	4.654261	-0.939714
21	8	0	3.893138	-3.337383	0.784160
22	8	0	0.535040	2.611253	1.812147
23	1	0	1.730336	0.358132	-2.423149
24	1	0	1.864514	-1.760877	0.679476
25	1	0	2.186368	-1.784527	-1.043397
26	1	0	3.951389	-0.290027	0.995033
27	1	0	4.351827	-0.575866	-0.687613
28	1	0	6.185517	-3.008017	0.904945
29	1	0	1.526707	2.705763	-2.701741
30	1	0	0.186326	2.237797	-1.662064
31	1	0	1.667962	0.746656	0.621747
32	1	0	1.563479	5.349528	-0.190347
33	1	0	1.462538	5.017335	-1.937454

34	1	0	0.084621	4.655629	-0.872736
35	1	0	1.003339	2.928860	0.992386
36	1	0	2.698812	3.333547	-0.626876
37	1	0	3.029423	1.087068	-1.503519
38	1	0	0.801919	3.186390	2.539430
39	1	0	-0.455892	0.810981	1.342962
40	1	0	-5.203744	0.065274	1.995766
41	1	0	-2.033654	0.486690	3.275331
42	1	0	-2.186097	1.955197	2.309489
43	1	0	-3.584076	1.328669	3.198832
44	1	0	-4.346084	-1.752123	-2.815337
45	1	0	-3.986539	-3.193490	-1.889156
46	1	0	-5.599367	-2.441960	-1.747732
47	1	0	-5.777428	-1.241565	0.181735
48	1	0	-0.279227	-0.766065	-1.126529

Sum of electronic and zero-point Energies= -1051.904579
Sum of electronic and thermal Energies= -1051.879151
Sum of electronic and thermal Enthalpies= -1051.878207
Sum of electronic and thermal Free Energies= -1051.962590

Table 16: Cartesian coordinates and energies for the structure '03r03'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.849681	-1.892359	0.143348
2	7	0	-4.577277	-0.774952	-0.192327
3	6	0	-4.095470	0.453528	-0.352100
4	6	0	-2.662148	0.657037	-0.159276
5	6	0	-1.879154	-0.511937	0.198025
6	6	0	-2.492685	-1.793214	0.346296
7	6	0	-4.983955	1.588541	-0.718184
8	8	0	-2.182278	1.808925	-0.307984
9	6	0	-0.470915	-0.352845	0.397441
10	7	0	0.143139	0.792939	0.269556
11	6	0	1.596660	1.057026	0.491356
12	6	0	2.456244	-0.025431	-0.189920
13	6	0	3.951728	0.142651	0.090802
14	6	0	4.739651	-1.067443	-0.374336
15	8	0	6.066033	-0.830804	-0.350729
16	6	0	-1.715179	-3.034362	0.712054
17	6	0	1.890667	2.449433	-0.010340
18	6	0	2.266804	3.459824	0.775484
19	8	0	4.255345	-2.127897	-0.711764
20	1	0	-1.221595	-2.926707	1.683729
21	1	0	-4.409052	-2.813335	0.229636
22	1	0	-5.577172	-0.903526	-0.330762

23	1	0	-6.027120	1.280475	-0.824428
24	1	0	-4.912882	2.374934	0.040960
25	1	0	-4.641466	2.040248	-1.655471
26	1	0	0.129039	-1.215508	0.670391
27	1	0	-2.376449	-3.900534	0.775509
28	1	0	-0.946961	-3.261346	-0.034679
29	1	0	2.485326	4.441095	0.366499
30	1	0	2.376193	3.342719	1.851256
31	1	0	1.794958	2.595747	-1.086568
32	1	0	1.760771	1.026132	1.576736
33	1	0	2.162409	-1.021421	0.154074
34	1	0	2.273442	-0.001800	-1.270562
35	1	0	-0.491066	1.578724	0.023964
36	1	0	4.144070	0.257595	1.166172
37	1	0	4.364447	1.037904	-0.383456
38	1	0	6.523865	-1.641792	-0.633700

Sum of electronic and zero-point Energies=	-879.639719
Sum of electronic and thermal Energies=	-879.620772
Sum of electronic and thermal Enthalpies=	-879.619828
Sum of electronic and thermal Free Energies=	-879.688474

Table 17: Cartesian coordinates and energies for the structure '03b'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.769958	-1.937309	0.251242
2	7	0	4.567076	-0.843056	0.015244
3	6	0	4.145585	0.397595	-0.212186
4	6	0	2.706963	0.642102	-0.213926
5	6	0	1.850300	-0.503216	0.030650
6	6	0	2.400745	-1.799346	0.264846
7	6	0	5.108276	1.504522	-0.457436
8	8	0	2.283708	1.807629	-0.424733
9	6	0	0.430823	-0.306567	0.029148
10	7	0	-0.122535	0.857420	-0.180474
11	6	0	-1.571661	1.194725	-0.180815
12	6	0	-2.453226	-0.057803	-0.113251
13	6	0	-3.940070	0.258950	-0.294257
14	6	0	-4.779039	-1.002352	-0.232055
15	8	0	-6.087127	-0.732788	-0.410480
16	6	0	1.546169	-3.016255	0.525615
17	6	0	-1.816729	2.173442	0.947705
18	6	0	-2.160089	3.450035	0.765424
19	8	0	-4.344384	-2.119907	-0.044848
20	1	0	0.877067	-3.225841	-0.315568
21	1	0	4.285775	-2.872709	0.417105

22	1	0	5.572528	-0.999291	0.014809
23	1	0	6.146661	1.165362	-0.421750
24	1	0	4.909119	1.960442	-1.433333
25	1	0	4.959601	2.297235	0.283659
26	1	0	-0.225342	-1.152556	0.203175
27	1	0	2.167958	-3.900614	0.676922
28	1	0	0.930947	-2.890591	1.422836
29	1	0	-2.338521	4.111208	1.607480
30	1	0	-2.281190	3.878323	-0.226964
31	1	0	-1.700509	1.770133	1.953626
32	1	0	-1.738436	1.710314	-1.135055
33	1	0	-2.152916	-0.765466	-0.894041
34	1	0	-2.317680	-0.566512	0.848397
35	1	0	0.568075	1.621812	-0.326443
36	1	0	-4.134953	0.748564	-1.256231
37	1	0	-4.305531	0.949485	0.473806
38	1	0	-6.580052	-1.570453	-0.359549

Sum of electronic and zero-point Energies= -879.641273
Sum of electronic and thermal Energies= -879.621579
Sum of electronic and thermal Enthalpies= -879.620634
Sum of electronic and thermal Free Energies= -879.691621

Table 18: Cartesian coordinates and energies for the structure '03TS05'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.114473	1.868053	0.139971
2	7	0	4.800334	0.694054	0.022797
3	6	0	4.242847	-0.521641	-0.099200
4	6	0	2.810816	-0.615714	-0.110973
5	6	0	2.060860	0.617696	0.011962
6	6	0	2.734255	1.864321	0.138170
7	6	0	5.100246	-1.734859	-0.226744
8	8	0	2.253385	-1.760283	-0.229334
9	6	0	0.623784	0.555669	-0.007560
10	7	0	0.011941	-0.605394	-0.152803
11	6	0	-1.357596	-0.899061	-0.165559
12	6	0	-2.247866	0.335550	-0.153546
13	6	0	-3.764678	0.147355	-0.225289
14	6	0	-4.476337	1.485939	-0.126236
15	8	0	-5.809807	1.339187	-0.263955
16	6	0	1.994895	3.174404	0.263331
17	6	0	-1.642211	-2.199008	-0.718484
18	6	0	-2.816293	-2.921569	-0.742969
19	8	0	-3.935686	2.555525	0.057852
20	1	0	1.347517	3.188077	1.146919

21	1	0	4.712102	2.765036	0.229050
22	1	0	5.814748	0.743265	0.024817
23	1	0	6.165510	-1.490835	-0.189163
24	1	0	4.867968	-2.445844	0.572871
25	1	0	4.885330	-2.250479	-1.168742
26	1	0	0.031926	1.456222	0.095950
27	1	0	2.693464	4.008660	0.355015
28	1	0	1.366350	3.365351	-0.613245
29	1	0	-2.801907	-3.914591	-1.179148
30	1	0	-3.796382	-2.469289	-0.626538
31	1	0	-0.747175	-2.764464	-0.986093
32	1	0	-1.746870	-1.692729	1.361230
33	1	0	-2.027244	0.932374	0.740983
34	1	0	-1.951626	0.976071	-0.998960
35	1	0	0.743191	-1.380304	-0.242803
36	1	0	-4.152598	-0.478305	0.587242
37	1	0	-4.077260	-0.324432	-1.161595
38	1	0	-6.221485	2.218007	-0.189735
39	8	0	-2.340301	-2.400225	1.905384
40	1	0	-1.804703	-2.938202	2.513286
41	1	0	-2.590686	-2.940643	1.017876

Sum of electronic and zero-point Energies= -955.984456
Sum of electronic and thermal Energies= -955.963303
Sum of electronic and thermal Enthalpies= -955.962359
Sum of electronic and thermal Free Energies= -956.035825

Table 19: Cartesian coordinates and energies for the structure '03TS05_2H_2O'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.420758	-1.716632	0.240846
2	7	0	-4.993329	-0.481143	0.184102
3	6	0	-4.322230	0.674526	0.012094
4	6	0	-2.901117	0.622871	-0.127106
5	6	0	-2.267534	-0.679655	-0.067194
6	6	0	-3.052500	-1.851673	0.118475
7	6	0	-5.062601	1.968860	-0.043146
8	8	0	-2.237292	1.708076	-0.300865
9	6	0	-0.840632	-0.763085	-0.210419
10	7	0	-0.133930	0.338748	-0.428198
11	6	0	1.238126	0.514833	-0.552182
12	6	0	2.049554	-0.764768	-0.501695
13	6	0	3.569242	-0.652378	-0.342154
14	6	0	4.176779	-1.978682	0.084083
15	8	0	5.524821	-1.938397	0.022259
16	6	0	-2.440002	-3.229788	0.178107

17	6	0	1.589680	1.758118	-1.193495
18	6	0	2.794396	2.265944	-1.603583
19	8	0	3.555460	-2.953065	0.450079
20	1	0	-1.721295	-3.315778	1.000598
21	1	0	-5.094146	-2.551425	0.381376
22	1	0	-6.002843	-0.426247	0.272941
23	1	0	-6.138198	1.832327	0.100873
24	1	0	-4.685346	2.653810	0.723147
25	1	0	-4.893184	2.461041	-1.006757
26	1	0	-0.331584	-1.716303	-0.151724
27	1	0	-3.207282	-3.991916	0.330575
28	1	0	-1.911963	-3.473300	-0.750448
29	1	0	2.800051	3.197827	-2.161744
30	1	0	3.711798	1.689538	-1.618894
31	1	0	0.734550	2.423128	-1.333344
32	1	0	1.481914	1.262458	1.116419
33	1	0	1.691389	-1.373304	0.337344
34	1	0	1.834188	-1.365259	-1.400785
35	1	0	-0.808134	1.175111	-0.477828
36	1	0	3.849638	0.079429	0.426104
37	1	0	4.068982	-0.342912	-1.263344
38	1	0	5.866285	-2.801223	0.315969
39	8	0	1.774601	1.753067	1.974700
40	1	0	0.994095	2.000835	2.496007
41	1	0	2.424953	2.658795	1.621205
42	1	0	3.079058	3.256254	0.062754
43	8	0	3.071586	3.544303	1.029205
44	1	0	3.972058	3.741063	1.329418

Sum of electronic and zero-point Energies=	-1032.430422
Sum of electronic and thermal Energies=	-1032.406572
Sum of electronic and thermal Enthalpies=	-1032.405628
Sum of electronic and thermal Free Energies=	-1032.486459

Table 20: Cartesian coordinates and energies for the structure '05a'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.829095	-1.908332	0.000175
2	7	0	-4.600099	-0.773902	-0.000125
3	6	0	-4.145505	0.479227	-0.000292
4	6	0	-2.707544	0.683225	-0.000196
5	6	0	-1.874552	-0.504291	0.000167
6	6	0	-2.455732	-1.807145	0.000335
7	6	0	-5.083053	1.635113	-0.000629
8	8	0	-2.250850	1.861467	-0.000373
9	6	0	-0.450995	-0.343146	0.000314

10	7	0	0.108455	0.846387	0.000112
11	6	0	1.491331	1.178152	0.000290
12	6	0	2.400307	-0.025939	0.000566
13	6	0	3.916232	0.169160	-0.000009
14	6	0	4.616485	-1.179449	-0.000450
15	8	0	5.955139	-1.032729	-0.000406
16	6	0	-1.627675	-3.069060	0.000632
17	6	0	1.730450	2.510990	0.000187
18	6	0	3.004063	3.291387	0.000524
19	8	0	4.058421	-2.256845	-0.000804
20	1	0	-0.985541	-3.128095	0.885889
21	1	0	-4.365264	-2.847150	0.000266
22	1	0	-5.609042	-0.902149	-0.000198
23	1	0	-6.129201	1.318444	-0.000223
24	1	0	-4.896116	2.266328	0.874670
25	1	0	-4.896565	2.265477	-0.876646
26	1	0	0.190269	-1.216008	0.000620
27	1	0	-2.268340	-3.952943	0.001075
28	1	0	-0.985889	-3.128690	-0.884841
29	1	0	3.025369	3.952159	-0.875343
30	1	0	3.911993	2.695368	0.000578
31	1	0	0.840946	3.141889	-0.000098
32	1	0	2.147177	-0.643835	0.872519
33	1	0	2.146741	-0.644507	-0.870772
34	1	0	-0.611384	1.609950	-0.000115
35	1	0	4.266010	0.718879	0.879592
36	1	0	4.265262	0.719032	-0.879823
37	1	0	6.360050	-1.917845	-0.000748
38	1	0	3.025058	3.951794	0.876682

Sum of electronic and zero-point Energies= -879.650811
Sum of electronic and thermal Energies= -879.631011
Sum of electronic and thermal Enthalpies= -879.630067
Sum of electronic and thermal Free Energies= -879.701027

Table 21: Cartesian coordinates and energies for the structure '05TS06'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.338682	-1.859722	-0.089599
2	7	0	4.940138	-0.635219	-0.080617
3	6	0	4.297618	0.543757	-0.035313
4	6	0	2.863670	0.537851	0.012408
5	6	0	2.201741	-0.751408	-0.006267
6	6	0	2.962029	-1.952538	-0.053660
7	6	0	5.068484	1.820255	-0.026380
8	8	0	2.228631	1.646224	0.070054

9	6	0	0.764206	-0.792581	0.033482
10	7	0	0.068229	0.327007	0.077912
11	6	0	-1.311912	0.560761	0.016695
12	6	0	-2.196165	-0.646126	0.287996
13	6	0	-3.621937	-0.561269	-0.274404
14	6	0	-4.346240	-1.892152	-0.166376
15	8	0	-5.672833	-1.747063	-0.370005
16	6	0	2.317863	-3.317847	-0.065417
17	6	0	-1.680743	1.953565	0.582979
18	6	0	-2.510241	2.073857	1.855331
19	8	0	-3.816148	-2.959829	0.051494
20	1	0	1.666154	-3.446915	-0.936362
21	1	0	4.997202	-2.716826	-0.126726
22	1	0	5.954950	-0.612127	-0.108802
23	1	0	6.147324	1.648488	-0.077206
24	1	0	4.766965	2.448116	-0.871261
25	1	0	4.840855	2.392177	0.879373
26	1	0	0.241887	-1.740885	0.015232
27	1	0	3.073897	-4.105040	-0.101545
28	1	0	1.712162	-3.483416	0.832101
29	1	0	-1.950651	1.660146	2.699691
30	1	0	-3.460775	1.537179	1.791819
31	1	0	-0.762307	2.538036	0.697654
32	1	0	-1.747043	-1.530126	-0.171116
33	1	0	-2.242457	-0.867399	1.365801
34	1	0	0.744856	1.151219	0.090370
35	1	0	-3.601917	-0.302973	-1.341854
36	1	0	-4.242190	0.194395	0.218188
37	1	0	-6.083978	-2.628204	-0.324216
38	1	0	-2.724841	3.122623	2.084868
39	1	0	-3.369449	2.408682	-0.620621
40	7	0	-2.353552	2.503876	-0.675022
41	1	0	-1.818379	1.414055	-1.119494
42	6	0	-1.979689	3.859223	-1.133928
43	1	0	-2.226358	4.614676	-0.380853
44	1	0	-0.905717	3.882568	-1.330471
45	1	0	-2.515296	4.083479	-2.058117

Sum of electronic and zero-point Energies= -975.409488
Sum of electronic and thermal Energies= -975.386757
Sum of electronic and thermal Enthalpies= -975.385813
Sum of electronic and thermal Free Energies= -975.463154

Table 22: Cartesian coordinates and energies for the structure '05TS06_H_2O'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.196581	0.418084	0.100664
2	6	0	1.615739	1.716041	-0.637597
3	1	0	0.784781	2.421749	-0.534472
4	1	0	3.692599	4.245758	0.513181
5	6	0	2.835895	3.874043	-0.051060
6	1	0	2.947335	4.140228	-1.103215
7	1	0	1.923847	4.316076	0.352178
8	7	0	2.756302	2.395431	0.120281
9	1	0	2.580612	2.139095	1.202583
10	1	0	3.644836	1.975352	-0.158301
11	1	0	1.440885	0.812342	1.404570
12	8	0	1.872400	1.556377	2.295601
13	1	0	2.238679	1.118592	3.075628
14	6	0	1.952672	1.567887	-2.123849
15	1	0	1.097822	1.129807	-2.646842
16	1	0	2.160081	2.533555	-2.594229
17	1	0	2.813758	0.913339	-2.290718
18	6	0	1.948576	-0.877368	-0.188479
19	1	0	1.547387	-1.665281	0.457385
20	1	0	1.772448	-1.223500	-1.219483
21	6	0	3.457999	-0.835786	0.076078
22	1	0	4.006323	-0.226838	-0.651749
23	1	0	3.675592	-0.416468	1.067168
24	6	0	4.073578	-2.224844	0.046965
25	8	0	5.422226	-2.160447	0.027358
26	1	0	5.768840	-3.069947	0.038199
27	8	0	3.453877	-3.265620	0.056633
28	7	0	-0.209856	0.281681	-0.011507
29	6	0	-0.954404	-0.802035	-0.053387
30	1	0	-0.469424	-1.769525	-0.093592
31	6	0	-2.391185	-0.710271	-0.028163
32	6	0	-3.002910	0.603005	0.005126
33	6	0	-3.193448	-1.883959	-0.039391
34	6	0	-4.439900	0.657831	0.048597
35	6	0	-4.566174	-1.743206	-0.005819
36	1	0	-5.256284	-2.575771	-0.008445
37	1	0	-0.832107	1.140033	0.028278
38	6	0	-2.600141	-3.271689	-0.081142
39	1	0	-1.992293	-3.422084	-0.979860
40	1	0	-1.962424	-3.461610	0.788941
41	1	0	-3.385283	-4.030640	-0.084890
42	6	0	-5.161970	1.960943	0.098084
43	1	0	-4.829679	2.540552	0.965567
44	1	0	-4.917124	2.561273	-0.784622
45	1	0	-6.246248	1.828465	0.149899
46	8	0	-2.331464	1.686169	-0.003466
47	7	0	-5.122271	-0.497006	0.038565
48	1	0	-6.135951	-0.439185	0.066707

Sum of electronic and zero-point Energies= -1051.850380
Sum of electronic and thermal Energies= -1051.825937
Sum of electronic and thermal Enthalpies= -1051.824993

Sum of electronic and thermal Free Energies= -1051.905528

Table 23: Cartesian coordinates and energies for the structure '06'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.281025	-1.752387	0.411077
2	7	0	4.947947	-0.616631	0.022648
3	6	0	4.387104	0.530346	-0.352567
4	6	0	2.931787	0.610548	-0.358134
5	6	0	2.210885	-0.581518	0.045431
6	6	0	2.904403	-1.766842	0.432303
7	6	0	5.218782	1.696022	-0.755972
8	8	0	2.377267	1.685679	-0.708407
9	6	0	0.776376	-0.549941	0.037957
10	7	0	0.094662	0.503703	-0.319770
11	6	0	-1.375397	0.677958	-0.380971
12	6	0	-2.099870	-0.640109	-0.097071
13	6	0	-3.607687	-0.623709	-0.371862
14	6	0	-4.162229	-2.034986	-0.436585
15	8	0	-5.508330	-2.030275	-0.509373
16	6	0	2.193651	-3.028756	0.858633
17	6	0	-1.744036	1.921879	0.501898
18	6	0	-1.674891	1.643983	2.009935
19	8	0	-3.498331	-3.051303	-0.430769
20	1	0	1.552605	-3.418733	0.060995
21	1	0	4.899365	-2.596214	0.683508
22	1	0	5.964469	-0.658638	0.021215
23	1	0	6.288664	1.479211	-0.701286
24	1	0	4.962402	1.999845	-1.776590
25	1	0	4.989996	2.555387	-0.116572
26	1	0	0.223027	-1.434495	0.332770
27	1	0	2.912226	-3.810330	1.112498
28	1	0	1.568004	-2.859161	1.741281
29	1	0	-0.702065	1.241617	2.314012
30	1	0	-2.447423	0.933065	2.323409
31	1	0	-0.986222	2.679775	0.262329
32	1	0	-1.673281	-1.421113	-0.735931
33	1	0	-1.928419	-0.960658	0.937503
34	1	0	0.705037	1.303445	-0.587528
35	1	0	-3.839515	-0.126608	-1.320911
36	1	0	-4.173044	-0.079338	0.389252
37	1	0	-5.811969	-2.953056	-0.567925
38	1	0	-1.833826	2.573109	2.564948
39	1	0	-3.778315	2.145196	0.665962
40	7	0	-3.029821	2.464660	0.058292
41	1	0	-1.582166	0.985089	-1.413335

42	6	0	-3.081529	3.927984	-0.049539
43	1	0	-2.799243	4.457307	0.874926
44	1	0	-2.417222	4.260827	-0.853078
45	1	0	-4.097686	4.226717	-0.318442

Sum of electronic and zero-point Energies= -975.466854
Sum of electronic and thermal Energies= -975.444694
Sum of electronic and thermal Enthalpies= -975.443750
Sum of electronic and thermal Free Energies= -975.520345

Table 24: Cartesian coordinates and energies for the structure '05br05a'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.856262	-0.485953	0.133341
2	6	0	2.460862	-1.772195	0.255945
3	6	0	3.826725	-1.867322	0.108480
4	7	0	4.568300	-0.742468	-0.148408
5	6	0	4.090404	0.495460	-0.277372
6	6	0	2.658431	0.691789	-0.137392
7	6	0	1.664448	-3.022958	0.537839
8	6	0	4.997436	1.641804	-0.557121
9	8	0	2.179642	1.855568	-0.254392
10	6	0	0.438949	-0.332756	0.274964
11	7	0	-0.142341	0.840079	0.158984
12	6	0	-1.517259	1.176389	0.278710
13	6	0	-2.460137	0.011684	0.474030
14	6	0	-3.892584	0.149898	-0.062086
15	6	0	-4.488943	-1.218101	-0.356523
16	8	0	-5.816543	-1.136725	-0.561380
17	6	0	-1.766700	2.505741	0.225234
18	6	0	-3.054794	3.242539	0.396971
19	8	0	-3.863163	-2.256171	-0.421545
20	1	0	0.925099	-3.214267	-0.247131
21	1	0	4.378713	-2.794025	0.181877
22	1	0	5.572850	-0.865504	-0.248957
23	1	0	6.042561	1.331672	-0.636230
24	1	0	4.696226	2.137078	-1.486382
25	1	0	4.902822	2.393702	0.233670
26	1	0	-0.177936	-1.197487	0.487734
27	1	0	2.318720	-3.895172	0.591907
28	1	0	1.131677	-2.952108	1.492137
29	1	0	-2.902154	4.075734	1.092445
30	1	0	-3.871501	2.631365	0.775425
31	1	0	-0.903578	3.148415	0.051109
32	1	0	-2.046010	-0.860258	-0.040318
33	1	0	-2.489014	-0.262915	1.537728

34	1	0	0.560729	1.597903	-0.026358
35	1	0	-3.915540	0.713419	-1.002619
36	1	0	-4.565874	0.665197	0.626182
37	1	0	-6.148449	-2.026771	-0.774035
38	1	0	-3.369142	3.693266	-0.553802

Sum of electronic and zero-point Energies= -879.650667
Sum of electronic and thermal Energies= -879.631636
Sum of electronic and thermal Enthalpies= -879.630692
Sum of electronic and thermal Free Energies= -879.699116

Table 25: Cartesian coordinates and energies for the structure '05b'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.526848	-0.305215	-0.286816
2	6	0	-2.191958	-1.548153	-0.502816
3	6	0	-3.548760	-1.610006	-0.272330
4	7	0	-4.222858	-0.493282	0.151368
5	6	0	-3.683908	0.704476	0.381135
6	6	0	-2.255839	0.861770	0.171018
7	6	0	-1.467158	-2.786405	-0.970376
8	6	0	-4.521358	1.845304	0.842585
9	8	0	-1.718830	1.984647	0.391467
10	6	0	-0.116933	-0.194162	-0.514840
11	7	0	0.523256	0.933128	-0.304450
12	6	0	1.894901	1.234517	-0.488188
13	6	0	2.814744	0.207979	-1.118934
14	6	0	3.740370	-0.549820	-0.147058
15	6	0	3.069652	-1.646475	0.651977
16	8	0	3.851489	-2.073946	1.655780
17	6	0	2.272716	2.475253	-0.105340
18	6	0	3.637860	3.072561	-0.208069
19	8	0	1.973208	-2.124871	0.417844
20	1	0	-0.648715	-3.051727	-0.293929
21	1	0	-4.143858	-2.502813	-0.404909
22	1	0	-5.223509	-0.589501	0.305024
23	1	0	-5.573506	1.568652	0.949073
24	1	0	-4.147255	2.218619	1.801884
25	1	0	-4.436799	2.678838	0.137207
26	1	0	0.456818	-1.056765	-0.827663
27	1	0	-2.149416	-3.637083	-1.024484
28	1	0	-1.040291	-2.642182	-1.968990
29	1	0	3.591763	4.022270	-0.754699
30	1	0	4.364100	2.425971	-0.703719
31	1	0	1.510130	3.121603	0.328290
32	1	0	2.245255	-0.511204	-1.712923

33	1	0	3.451523	0.737250	-1.832980
34	1	0	-0.121810	1.687738	0.034301
35	1	0	4.242610	0.130132	0.547160
36	1	0	4.541286	-1.037923	-0.717682
37	1	0	3.404124	-2.811307	2.107232
38	1	0	4.022946	3.314125	0.790966

Sum of electronic and zero-point Energies= -879.660185
Sum of electronic and thermal Energies= -879.640626
Sum of electronic and thermal Enthalpies= -879.639682
Sum of electronic and thermal Free Energies= -879.709384

Table 26: Cartesian coordinates and energies for the structure '05TS07'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.300176	-1.262191	-1.046574
2	6	0	-3.683935	-1.236386	-1.144144
3	7	0	-4.380026	-0.229293	-0.545437
4	6	0	-3.846019	0.777291	0.159107
5	6	0	-2.407618	0.827959	0.307438
6	6	0	-1.658832	-0.230035	-0.329882
7	6	0	-4.716485	1.824145	0.764388
8	8	0	-1.869236	1.761750	0.971395
9	6	0	-0.185975	-0.190229	-0.206609
10	7	0	0.036573	-0.843212	1.678526
11	6	0	-0.577327	-2.108870	2.108222
12	6	0	-1.548882	-2.377130	-1.739276
13	7	0	0.416890	1.011957	-0.237064
14	6	0	1.782530	1.332282	-0.490760
15	6	0	2.238048	2.500132	0.003933
16	6	0	3.557642	3.154096	-0.284793
17	6	0	2.569334	0.433664	-1.432056
18	6	0	3.868580	-0.175028	-0.878543
19	6	0	3.685778	-1.200076	0.213254
20	8	0	2.614936	-1.593948	0.651783
21	8	0	4.860719	-1.662897	0.662711
22	1	0	-0.933905	-2.951600	-1.039246
23	1	0	-4.265896	-1.971620	-1.682177
24	1	0	-5.391621	-0.241320	-0.643993
25	1	0	-5.777214	1.645383	0.567138
26	1	0	-4.553769	1.867710	1.846492
27	1	0	-4.439781	2.810327	0.376459
28	1	0	0.375684	-1.010739	-0.634468
29	1	0	-2.240931	-3.075232	-2.215086
30	1	0	-0.888503	-1.986268	-2.520719
31	1	0	3.407671	4.220021	-0.488269

32	1	0	4.071660	2.724058	-1.148142
33	1	0	1.569962	3.061696	0.656406
34	1	0	1.935046	-0.369193	-1.815479
35	1	0	2.844314	1.030085	-2.310066
36	1	0	-0.173780	1.756146	0.151090
37	1	0	4.546398	0.592811	-0.493682
38	1	0	4.421126	-0.667497	-1.688553
39	1	0	4.694498	-2.331688	1.350061
40	1	0	4.235507	3.096615	0.577012
41	1	0	-1.647313	-2.089395	1.887785
42	1	0	-0.112742	-2.933138	1.563248
43	1	0	-0.444085	-2.281850	3.181610
44	1	0	-0.311644	-0.043134	2.205926
45	1	0	1.053927	-0.885333	1.735149

Sum of electronic and zero-point Energies= -975.459100
Sum of electronic and thermal Energies= -975.435883
Sum of electronic and thermal Enthalpies= -975.434938
Sum of electronic and thermal Free Energies= -975.513102

Table 27: Cartesian coordinates and energies for the structure '07'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.725274	-0.346250	-0.234035
2	6	0	-2.315210	-1.125868	-1.243497
3	6	0	-3.689659	-1.035510	-1.425279
4	7	0	-4.414960	-0.201396	-0.633861
5	6	0	-3.920159	0.572971	0.344900
6	6	0	-2.502134	0.539470	0.589473
7	6	0	-1.516355	-2.033289	-2.149279
8	6	0	-4.820447	1.458185	1.137381
9	8	0	-1.994134	1.276089	1.504030
10	6	0	-0.218625	-0.321649	-0.031188
11	7	0	0.338074	0.817429	-0.695602
12	6	0	1.741065	1.083745	-0.806944
13	6	0	2.562902	0.002250	-1.492859
14	6	0	3.882482	-0.406163	-0.819713
15	6	0	3.749602	-1.000176	0.559976
16	8	0	4.936768	-1.363095	1.062932
17	6	0	2.193286	2.309666	-0.480952
18	6	0	3.534720	2.910522	-0.803806
19	8	0	2.706225	-1.155801	1.180645
20	7	0	0.067369	-0.282669	1.488035
21	6	0	-0.246454	-1.533006	2.232172
22	1	0	-1.024007	-2.833362	-1.585547
23	1	0	-4.237191	-1.589530	-2.175258

24	1	0	-5.416818	-0.156135	-0.798582
25	1	0	-5.870446	1.337824	0.856285
26	1	0	-4.707002	1.246784	2.205601
27	1	0	-4.532324	2.506396	1.002404
28	1	0	0.260605	-1.237299	-0.379988
29	1	0	-2.159039	-2.506971	-2.894376
30	1	0	-0.743519	-1.471809	-2.683758
31	1	0	3.406574	3.947582	-1.131755
32	1	0	4.057797	2.383325	-1.606235
33	1	0	1.491545	2.981871	0.013783
34	1	0	1.948114	-0.890636	-1.636726
35	1	0	2.808265	0.347863	-2.505310
36	1	0	-0.200993	1.659673	-0.523144
37	1	0	4.578222	0.433822	-0.736558
38	1	0	4.403081	-1.146639	-1.439366
39	1	0	4.802428	-1.738163	1.951085
40	1	0	4.196526	2.942400	0.071716
41	1	0	-1.307412	-1.758442	2.124548
42	1	0	0.362090	-2.347849	1.838812
43	1	0	-0.012631	-1.379765	3.286515
44	1	0	-0.555829	0.512282	1.812698
45	1	0	1.069290	-0.083694	1.584213

Sum of electronic and zero-point Energies=	-975.468623
Sum of electronic and thermal Energies=	-975.445797
Sum of electronic and thermal Enthalpies=	-975.444853
Sum of electronic and thermal Free Energies=	-975.521626

Table 28: Cartesian coordinates and energies for the structure '07TS08'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.599761	0.035760	1.627203
2	7	0	4.247674	0.303288	0.460502
3	6	0	3.700367	0.273582	-0.764734
4	6	0	2.305002	-0.072305	-0.876342
5	6	0	1.612232	-0.368323	0.349753
6	6	0	2.253488	-0.308337	1.600262
7	6	0	4.518954	0.590126	-1.969309
8	8	0	1.725165	-0.111132	-2.006544
9	6	0	0.165692	-0.739966	0.194101
10	7	0	-0.686236	0.236265	-0.601291
11	6	0	-1.404322	1.326617	0.031826
12	6	0	-2.462603	0.950367	1.046140
13	6	0	-3.859887	0.659346	0.463630
14	6	0	-3.989411	-0.699768	-0.186276
15	8	0	-5.181857	-0.855116	-0.783003

16	6	0	1.553151	-0.599408	2.908999
17	6	0	-1.123755	2.577585	-0.371145
18	6	0	-1.793232	3.848215	0.059772
19	8	0	-3.140823	-1.575219	-0.166831
20	1	0	1.156242	-1.619497	2.938077
21	1	0	4.186770	0.106509	2.532413
22	1	0	5.232209	0.548015	0.522008
23	1	0	5.554751	0.831588	-1.714468
24	1	0	4.508715	-0.257071	-2.663305
25	1	0	4.077458	1.432766	-2.511947
26	1	0	-0.329835	-0.927841	1.144029
27	1	0	2.241481	-0.494322	3.750296
28	1	0	0.720300	0.090619	3.080439
29	1	0	-1.051800	4.560930	0.439265
30	1	0	-2.550961	3.701569	0.832078
31	1	0	-0.336365	2.700358	-1.115511
32	1	0	-2.145356	0.080190	1.629788
33	1	0	-2.562418	1.772102	1.758585
34	1	0	-0.080656	0.571482	-1.364018
35	1	0	-4.163616	1.423092	-0.259794
36	1	0	-4.609917	0.692676	1.264268
37	1	0	-5.228996	-1.753145	-1.155533
38	1	0	-2.277425	4.331524	-0.797699
39	6	0	-0.358155	-3.223398	-0.134067
40	1	0	0.536158	-3.586368	0.383921
41	1	0	-1.203410	-3.178187	0.553998
42	1	0	-0.605001	-3.915519	-0.940957
43	7	0	-0.143190	-1.888900	-0.718580
44	1	0	0.542837	-1.889560	-1.479574
45	1	0	-1.062472	-0.945293	-1.038637

Sum of electronic and zero-point Energies= -975.426650
Sum of electronic and thermal Energies= -975.403969
Sum of electronic and thermal Enthalpies= -975.403025
Sum of electronic and thermal Free Energies= -975.480307

Table 29: Cartesian coordinates and energies for the structure '07TS08_H_2O'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.948455	-0.265325	1.738511
2	6	0	-3.181443	-0.879359	1.930697
3	7	0	-4.060215	-0.960059	0.895289
4	6	0	-3.854473	-0.495148	-0.347593
5	6	0	-2.596957	0.148697	-0.627089
6	6	0	-1.664779	0.250373	0.462505
7	6	0	-4.901647	-0.646840	-1.397532

8	8	0	-2.329630	0.603631	-1.787006
9	6	0	-0.369640	0.948709	0.112771
10	7	0	0.379823	0.231264	-0.991117
11	6	0	1.063862	-1.008213	-0.611251
12	6	0	0.616087	-2.163330	-1.125868
13	6	0	1.218869	-3.526012	-0.953331
14	6	0	-0.984525	-0.187364	2.901153
15	6	0	2.270837	-0.824772	0.275995
16	6	0	3.551716	-0.425624	-0.480592
17	6	0	4.671577	-0.072266	0.478620
18	8	0	4.530573	0.149283	1.663468
19	8	0	5.862857	-0.008877	-0.150830
20	7	0	-0.594180	2.345877	-0.387553
21	6	0	-0.892126	3.335532	0.674133
22	1	0	-0.740120	0.849160	3.156054
23	1	0	-3.502119	-1.307677	2.870362
24	1	0	-4.951960	-1.412351	1.078282
25	1	0	-4.504337	-1.213727	-2.246233
26	1	0	-5.796860	-1.148947	-1.020125
27	1	0	-5.181674	0.335446	-1.792545
28	1	0	0.300667	1.022165	0.968321
29	1	0	-1.412599	-0.648772	3.793541
30	1	0	-0.046720	-0.707324	2.681029
31	1	0	-0.268888	-2.123988	-1.761978
32	1	0	2.083877	-0.063810	1.040751
33	1	0	2.455713	-1.747876	0.829911
34	1	0	-0.328447	0.047102	-1.715322
35	1	0	3.386541	0.458713	-1.108247
36	1	0	3.889891	-1.222922	-1.149746
37	1	0	6.536684	0.246057	0.503705
38	1	0	-1.761966	3.041093	1.268420
39	1	0	-0.020201	3.441094	1.323913
40	1	0	-1.094012	4.298323	0.201734
41	1	0	-1.367085	2.279463	-1.063732
42	1	0	1.525329	-3.931196	-1.925157
43	1	0	0.478729	-4.223735	-0.544316
44	1	0	1.142246	1.158576	-1.463544
45	1	0	1.678808	2.639981	-2.484794
46	1	0	0.491772	2.598285	-1.058886
47	8	0	1.541681	2.307893	-1.586516
48	1	0	2.091478	-3.532496	-0.297423

Sum of electronic and zero-point Energies= -1051.866370
Sum of electronic and thermal Energies= -1051.841783
Sum of electronic and thermal Enthalpies= -1051.840838
Sum of electronic and thermal Free Energies= -1051.922820

Table 30: Cartesian coordinates and energies for the structure '08a'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.352737	0.605492	1.359816
2	6	0	-3.627646	0.050245	1.349424
3	7	0	-4.055794	-0.626547	0.252268
4	6	0	-3.336265	-0.839335	-0.863645
5	6	0	-2.006549	-0.301725	-0.923632
6	6	0	-1.549335	0.444858	0.217001
7	6	0	-3.920780	-1.600916	-2.004857
8	8	0	-1.276724	-0.492220	-1.958444
9	6	0	-0.205100	1.138464	0.059723
10	7	0	-0.205426	2.260161	-0.852532
11	6	0	-0.622940	3.551194	-0.300807
12	6	0	-1.900190	1.349526	2.597347
13	7	0	0.811459	0.145690	-0.523337
14	6	0	1.346635	-0.891591	0.377238
15	6	0	0.846115	-2.130061	0.280362
16	6	0	1.255970	-3.327186	1.083635
17	6	0	2.449974	-0.422130	1.301954
18	6	0	3.886210	-0.613974	0.769722
19	6	0	4.234305	0.245821	-0.424519
20	8	0	3.450170	0.947865	-1.046520
21	8	0	5.529974	0.159245	-0.744791
22	1	0	-1.671868	2.397675	2.381928
23	1	0	-4.324106	0.124956	2.173406
24	1	0	-4.998536	-1.004917	0.275316
25	1	0	-4.940083	-1.938554	-1.796807
26	1	0	-3.927385	-0.980873	-2.907560
27	1	0	-3.296545	-2.470107	-2.237323
28	1	0	0.187119	1.476864	1.020095
29	1	0	-2.677657	1.335692	3.364297
30	1	0	-1.004124	0.894424	3.032663
31	1	0	0.384279	-3.767798	1.581309
32	1	0	2.006934	-3.105047	1.844341
33	1	0	0.073594	-2.303811	-0.467175
34	1	0	2.305116	0.635320	1.551280
35	1	0	2.376498	-0.967964	2.246118
36	1	0	0.258244	-0.267655	-1.330037
37	1	0	4.064285	-1.658347	0.486976
38	1	0	4.611645	-0.391432	1.560432
39	1	0	5.699267	0.720994	-1.522319
40	1	0	1.661097	-4.103638	0.423704
41	1	0	-1.661454	3.571989	0.062728
42	1	0	0.044401	3.831360	0.520388
43	1	0	-0.519971	4.307418	-1.081868
44	1	0	-0.718886	2.031213	-1.700838
45	1	0	1.603106	0.705906	-0.890377

Sum of electronic and zero-point Energies= -975.462935
Sum of electronic and thermal Energies= -975.440115

Sum of electronic and thermal Enthalpies= -975.439171
Sum of electronic and thermal Free Energies= -975.516330

Table 31: Cartesian coordinates and energies for the structure '08b'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.674145	0.521683	0.154036
2	6	0	-2.605741	0.913819	1.133027
3	6	0	-3.892713	0.396940	1.066076
4	7	0	-4.217772	-0.459391	0.062735
5	6	0	-3.383469	-0.876161	-0.903828
6	6	0	-2.034857	-0.380905	-0.901416
7	6	0	-2.269943	1.894720	2.230659
8	6	0	-3.863103	-1.808799	-1.963989
9	8	0	-1.221293	-0.759226	-1.819889
10	6	0	-0.287885	1.149561	0.134714
11	7	0	-0.292472	2.350483	-0.619088
12	6	0	0.873371	3.235429	-0.564309
13	7	0	0.736718	0.081606	-0.408123
14	6	0	1.285972	-0.860416	0.580279
15	6	0	2.462060	-0.334117	1.376483
16	6	0	3.852615	-0.654971	0.788516
17	6	0	4.165026	0.044120	-0.514894
18	8	0	5.423119	-0.171682	-0.911761
19	6	0	0.728657	-2.075042	0.679628
20	6	0	1.130666	-3.174465	1.616005
21	8	0	3.385151	0.735566	-1.156248
22	1	0	-1.914508	2.840292	1.809915
23	1	0	-4.678652	0.643279	1.766866
24	1	0	-5.171319	-0.809529	0.036489
25	1	0	-4.897291	-2.123868	-1.798895
26	1	0	-3.787839	-1.332683	-2.947631
27	1	0	-3.219667	-2.693560	-2.004552
28	1	0	0.058858	1.368560	1.148170
29	1	0	-3.145287	2.107069	2.848140
30	1	0	-1.488256	1.504522	2.892185
31	1	0	0.268312	-3.506584	2.205755
32	1	0	1.926075	-2.890427	2.308126
33	1	0	-0.089985	-2.307758	0.000927
34	1	0	2.372685	0.751162	1.502194
35	1	0	2.429556	-0.757808	2.383534
36	1	0	0.149778	-0.407903	-1.170428
37	1	0	3.968779	-1.732149	0.620286
38	1	0	4.636330	-0.379647	1.503825
39	1	0	5.571691	0.290117	-1.756345
40	1	0	1.472479	-4.048190	1.048103

41	1	0	0.628741	4.163053	-1.085906
42	1	0	1.083267	3.489110	0.480159
43	1	0	1.785345	2.818031	-1.012719
44	1	0	-0.691225	2.246158	-1.545896
45	1	0	1.531923	0.574222	-0.843703

Sum of electronic and zero-point Energies= -975.466396
Sum of electronic and thermal Energies= -975.443564
Sum of electronic and thermal Enthalpies= -975.442620
Sum of electronic and thermal Free Energies= -975.519425

Table 32: Cartesian coordinates and energies for the structure '08TS09'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.213006	-0.044803	1.607069
2	6	0	-3.423147	-0.703996	1.435248
3	7	0	-3.994129	-0.745822	0.199840
4	6	0	-3.482132	-0.210274	-0.917615
5	6	0	-2.219976	0.487855	-0.826958
6	6	0	-1.624454	0.566248	0.483658
7	6	0	-4.209120	-0.323285	-2.213662
8	8	0	-1.679305	0.986083	-1.859153
9	6	0	-0.367349	1.344970	0.595940
10	7	0	-0.330052	2.576347	0.052038
11	6	0	0.762887	3.516822	0.285164
12	6	0	-1.607348	0.010677	2.991061
13	7	0	0.840334	0.242686	-0.503517
14	6	0	1.201298	-1.090955	-0.115572
15	6	0	0.532473	-2.140001	-0.627911
16	6	0	0.744548	-3.594461	-0.327362
17	6	0	2.329049	-1.164734	0.894550
18	6	0	3.755579	-1.185166	0.304392
19	6	0	4.232208	0.129981	-0.271644
20	8	0	3.550089	1.134344	-0.422873
21	8	0	5.526419	0.086691	-0.609133
22	1	0	-1.516776	1.041978	3.347652
23	1	0	-3.966390	-1.187946	2.234981
24	1	0	-4.887689	-1.223311	0.117526
25	1	0	-5.139304	-0.890553	-2.118525
26	1	0	-4.436554	0.674365	-2.604545
27	1	0	-3.569905	-0.803135	-2.962246
28	1	0	0.187062	1.252920	1.525173
29	1	0	-2.226258	-0.531855	3.708900
30	1	0	-0.610248	-0.441691	3.011633
31	1	0	-0.192628	-4.063983	-0.004786
32	1	0	1.493716	-3.773923	0.446789

33	1	0	-0.239165	-1.923803	-1.366630
34	1	0	2.250599	-0.325629	1.596424
35	1	0	2.213619	-2.072571	1.490440
36	1	0	0.285755	0.294208	-1.364518
37	1	0	3.843612	-1.942011	-0.484397
38	1	0	4.476403	-1.477638	1.076581
39	1	0	5.782892	0.948396	-0.983234
40	1	0	1.063874	-4.129771	-1.230015
41	1	0	0.401008	4.530777	0.105060
42	1	0	1.089446	3.447903	1.325988
43	1	0	1.623874	3.328026	-0.367279
44	1	0	-0.865389	2.676882	-0.807779
45	1	0	1.678683	0.829684	-0.580591

Sum of electronic and zero-point Energies= -975.461243
Sum of electronic and thermal Energies= -975.438173
Sum of electronic and thermal Enthalpies= -975.437228
Sum of electronic and thermal Free Energies= -975.515322

Table 33: Cartesian coordinates and energies for the structure '09'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.389430	-0.760538	-0.388117
2	6	0	5.258347	0.264998	-0.093354
3	7	0	4.766980	1.493129	0.280275
4	6	0	3.483703	1.816432	0.397008
5	6	0	2.481382	0.789704	0.104958
6	6	0	2.985287	-0.511773	-0.295904
7	6	0	3.071962	3.184872	0.809270
8	8	0	1.268126	1.071891	0.208820
9	6	0	2.059532	-1.559857	-0.599501
10	7	0	0.758309	-1.479148	-0.579422
11	6	0	-0.129217	-2.595391	-0.893805
12	6	0	4.963818	-2.096546	-0.796450
13	1	0	4.642855	-2.381886	-1.803825
14	1	0	6.334867	0.177766	-0.134734
15	1	0	5.450722	2.218422	0.484473
16	1	0	3.929096	3.839557	0.986654
17	1	0	2.431017	3.627132	0.038979
18	1	0	2.462723	3.131520	1.717968
19	1	0	2.460284	-2.531044	-0.879125
20	1	0	6.054939	-2.062697	-0.799112
21	1	0	4.662849	-2.891926	-0.106375
22	1	0	-0.763597	-2.318858	-1.739387
23	1	0	0.453850	-3.484386	-1.139991
24	1	0	-0.769077	-2.792081	-0.030048

25	1	0	0.278842	-0.591003	-0.330167
26	1	0	-1.546178	0.038863	2.592529
27	6	0	-3.276062	-1.204143	3.152462
28	1	0	-4.076863	-1.780247	2.681299
29	1	0	-2.691946	-1.896826	3.771736
30	1	0	-3.750003	-0.495460	3.843998
31	6	0	-2.398346	-0.489696	2.161750
32	6	0	-2.555767	-0.407939	0.825530
33	7	0	-1.602245	0.260115	0.003676
34	1	0	-2.044699	0.692567	-0.806551
35	1	0	-1.066424	0.960714	0.508550
36	6	0	-3.694641	-1.051186	0.055653
37	1	0	-4.023921	-1.951385	0.580090
38	1	0	-3.330614	-1.374825	-0.926522
39	6	0	-4.937770	-0.161690	-0.147158
40	1	0	-5.789360	-0.772257	-0.472340
41	1	0	-5.249707	0.302775	0.795256
42	6	0	-4.776950	0.936898	-1.174515
43	8	0	-3.771625	1.174974	-1.821777
44	8	0	-5.910836	1.648292	-1.321399
45	1	0	-5.754525	2.330778	-1.997174

Sum of electronic and zero-point Energies= -975.476673
Sum of electronic and thermal Energies= -975.453106
Sum of electronic and thermal Enthalpies= -975.452162
Sum of electronic and thermal Free Energies= -975.533038

Table 34: Cartesian coordinates and energies for the structure '09TS10'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.189034	-1.048874	-0.463282
2	6	0	-4.230021	-0.283072	-0.965714
3	7	0	-4.200256	1.070022	-0.825244
4	6	0	-3.219756	1.768051	-0.230924
5	6	0	-2.095603	1.049333	0.309436
6	6	0	-2.118749	-0.387400	0.180288
7	6	0	-3.302712	3.253814	-0.139175
8	8	0	-1.139781	1.689531	0.857664
9	6	0	-1.004714	-1.150458	0.777639
10	7	0	-0.538430	-0.772800	1.978784
11	6	0	0.351145	-1.614642	2.761784
12	6	0	-3.278838	-2.553607	-0.585759
13	1	0	-3.326955	-3.028359	0.400158
14	1	0	-5.098416	-0.697787	-1.458853
15	1	0	-4.985805	1.595745	-1.198031
16	1	0	-4.217669	3.644667	-0.593250

17	1	0	-3.260348	3.567997	0.908924
18	1	0	-2.436408	3.709901	-0.629899
19	1	0	-0.974501	-2.220533	0.599477
20	1	0	-4.176822	-2.844849	-1.134874
21	1	0	-2.420264	-2.975542	-1.116349
22	1	0	0.560781	-1.125685	3.713628
23	1	0	-0.118755	-2.582717	2.961691
24	1	0	1.299692	-1.787853	2.238892
25	1	0	-0.614725	0.217981	2.195963
26	1	0	-0.103666	0.030216	-1.176784
27	6	0	0.567639	-1.991984	-1.725791
28	1	0	0.893167	-2.901186	-1.208648
29	1	0	-0.427329	-2.189231	-2.134722
30	1	0	1.231735	-1.850785	-2.588476
31	6	0	0.526701	-0.778199	-0.822081
32	6	0	1.649399	-0.329248	-0.095455
33	7	0	1.563833	0.786608	0.630241
34	1	0	2.408662	1.169199	1.048089
35	1	0	0.689416	1.325230	0.642874
36	6	0	2.965591	-1.083730	-0.041921
37	1	0	2.798438	-2.115030	-0.356142
38	1	0	3.339781	-1.110145	0.986306
39	6	0	4.064201	-0.481614	-0.944735
40	1	0	4.852902	-1.223543	-1.112109
41	1	0	3.682321	-0.225146	-1.939963
42	6	0	4.725642	0.751287	-0.361394
43	8	0	4.401744	1.303015	0.676270
44	8	0	5.741364	1.176256	-1.126723
45	1	0	6.136771	1.962275	-0.709555

Sum of electronic and zero-point Energies= -975.461441
Sum of electronic and thermal Energies= -975.438612
Sum of electronic and thermal Enthalpies= -975.437668
Sum of electronic and thermal Free Energies= -975.513735

Table 35: Cartesian coordinates and energies for the structure '10'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.250105	-0.875683	-0.517818
2	6	0	-4.309638	-0.017606	-0.784959
3	7	0	-4.168179	1.311993	-0.559461
4	6	0	-3.056453	1.899929	-0.082931
5	6	0	-1.925214	1.075592	0.218833
6	6	0	-2.047272	-0.332392	-0.024061
7	6	0	-3.028679	3.374858	0.140671
8	8	0	-0.872643	1.637194	0.701637

9	6	0	-0.865538	-1.220312	0.339600
10	7	0	-0.677988	-1.199789	1.764547
11	6	0	0.215166	-2.192315	2.332162
12	6	0	-3.461202	-2.356155	-0.744522
13	1	0	-3.337027	-2.919856	0.185657
14	1	0	-5.269809	-0.345383	-1.159661
15	1	0	-4.964133	1.910922	-0.758009
16	1	0	-3.963171	3.854394	-0.164623
17	1	0	-2.846036	3.592321	1.198351
18	1	0	-2.198546	3.824779	-0.413219
19	1	0	-1.106556	-2.255042	0.084236
20	1	0	-4.469545	-2.551624	-1.116396
21	1	0	-2.758405	-2.762290	-1.478950
22	1	0	0.248263	-2.072146	3.417424
23	1	0	-0.161397	-3.198428	2.115886
24	1	0	1.253476	-2.139216	1.956706
25	1	0	-0.570128	-0.269378	2.150979
26	1	0	0.092685	-0.031136	-1.240182
27	6	0	0.642928	-2.069243	-1.610909
28	1	0	0.891130	-2.995858	-1.082714
29	1	0	-0.271822	-2.254893	-2.181012
30	1	0	1.433126	-1.863801	-2.339513
31	6	0	0.413190	-0.896579	-0.648876
32	6	0	1.644314	-0.411897	0.072486
33	7	0	1.519800	0.669914	0.769939
34	1	0	2.352731	1.068380	1.209593
35	1	0	0.555141	1.150314	0.789471
36	6	0	2.994992	-1.093269	-0.004596
37	1	0	2.867178	-2.115644	-0.359116
38	1	0	3.418702	-1.145934	1.002967
39	6	0	4.011155	-0.377547	-0.924057
40	1	0	4.829191	-1.065471	-1.162796
41	1	0	3.573335	-0.093097	-1.888174
42	6	0	4.623573	0.861387	-0.298804
43	8	0	4.287539	1.349320	0.767031
44	8	0	5.599363	1.367729	-1.061539
45	1	0	5.964825	2.156701	-0.622430

Sum of electronic and zero-point Energies= -975.471971
Sum of electronic and thermal Energies= -975.449764
Sum of electronic and thermal Enthalpies= -975.448820
Sum of electronic and thermal Free Energies= -975.523281

Table 36: NBO charges on heavy atoms

	C1	C2	C3	N4	C5	C6	O7	C8	N9	C10	C11	C12	C13	C14	C15	C16	O17	O18	N19
EP01 + V01	-0.203	0.412	0.263	-0.459	-0.054	0.016	-0.638	0.172	-0.496	-0.504	-0.443	-0.214	-0.124	-0.481	-0.574	0.817	-0.611	-0.731	-0.913
pre-reaction complex	-0.21	0.413	0.262	-0.468	-0.046	0.01	-0.647	0.17	-0.507	-0.502	-0.429	-0.257	-0.126	-0.47	-0.579	0.862	-0.689	-0.693	-0.915
00TS01	-0.155	0.373	0.217	-0.457	-0.034	-0.027	-0.722	0.168	-0.608	-0.502	-0.400	-0.270	-0.103	-0.487	-0.568	0.821	-0.624	-0.711	-0.779
01	-0.090	0.346	0.220	-0.462	-0.015	-0.021	-0.722	0.111	-0.708	-0.503	-0.390	-0.276	-0.092	-0.493	-0.570	0.818	-0.614	-0.713	-0.708
01TS02	-0.144	0.367	0.209	-0.462	-0.036	-0.025	-0.734	0.109	-0.725	-0.496	-0.393	-0.260	-0.091	-0.484	-0.570	0.819	-0.622	-0.709	-0.718
01TS02_H_2O	-0.132	0.354	0.209	-0.452	-0.027	-0.036	-0.735	0.116	-0.729	-0.498	-0.391	-0.268	-0.090	-0.486	-0.570	0.817	-0.619	-0.711	-0.727
02a	-0.120	0.347	0.209	-0.463	-0.017	-0.034	-0.727	0.114	-0.656	-0.503	-0.418	-0.237	-0.097	-0.483	-0.571	0.820	-0.628	-0.709	-0.710
02b	-0.105	0.352	0.218	-0.463	-0.027	-0.022	-0.722	0.114	-0.713	-0.502	-0.436	-0.273	-0.106	-0.478	-0.572	0.814	-0.602	-0.721	-0.697
02TS03	-0.158	0.378	0.217	-0.463	-0.045	-0.022	-0.710	0.173	-0.803	-0.504	-0.432	-0.257	-0.102	-0.482	-0.572	0.814	-0.600	-0.720	-0.590
03a	-0.200	0.410	0.259	0.459	-0.054	0.014	-0.639	0.178			-0.395	-0.261	-0.101	-0.484	-0.574	0.815	-0.602	-0.718	-0.482
03TS04	-0.189	0.401	0.239	-0.464	-0.055	-0.002	-0.658	0.138	-0.721	-0.499	-0.286	-0.630	-0.088	-0.479	-0.567	0.814	-0.602	-0.725	-0.482
03TS04_H_2O	-0.190	0.400	0.240	-0.464	-0.054	-0.003	-0.657	0.131	-0.693	-0.497	-0.279	-0.643	-0.079	-0.479	-0.572	0.815	-0.604	-0.723	-0.480
04	-0.200	0.411	0.258	-0.458	-0.053	0.012	-0.645	0.177	-0.719	-0.495	-0.268	-0.492	-0.072	-0.483	-0.572	0.815	-0.602	-0.717	-0.487
04_H_2O	-0.201	0.408	0.25	-0.459	-0.058	0.02	-0.651	0.178	-0.749	-0.499	-0.275	-0.49	-0.087	-0.485	-0.57	0.815	-0.599	-0.72	-0.497
03r03	-0.202	0.411	0.260	-0.459	-0.056	0.017	-0.634	0.182			-0.383	-0.276	-0.107	-0.484	-0.573	0.817	-0.610	-0.713	-0.494
03b	-0.207	0.410	0.257	-0.459	-0.055	0.016	-0.639	0.183			-0.387	-0.265	-0.107	-0.499	-0.570	0.817	-0.610	-0.714	-0.492
03TS05	-0.155	0.374	0.212	-0.472	-0.035	-0.019	-0.696	0.059			-0.681	-0.159	-0.101	-0.516	-0.569	0.817	-0.604	-0.717	-0.479
03TS05_2H_2O	-0.143	0.365	0.197	-0.478	-0.031	-0.03	-0.712	0.02			-0.641	-0.222	-0.033	-0.52	-0.561	0.816	-0.602	-0.72	-0.489
05a	-0.189	0.402	0.247	-0.462	-0.048	0.007	-0.654	0.143			-0.739	-0.144	0.138	-0.525	-0.566	0.818	-0.609	-0.713	-0.486
05TS06	-0.152	0.375	0.209	-0.472	-0.036	-0.020	-0.699	0.069	-0.702	-0.498	-0.716	-0.088	-0.109	-0.508	-0.564	0.816	-0.599	-0.719	-0.470
05TS06_H_2O	-0.160	0.379	0.216	-0.470	-0.040	-0.017	-0.688	0.082	-0.688	-0.496	-0.720	-0.083	-0.149	-0.508	-0.566	0.817	-0.598	-0.721	-0.468
06	-0.204	0.408	0.255	-0.458	-0.054	0.013	-0.647	0.183	-0.728	-0.493	-0.718	-0.084	-0.078	-0.508	-0.563	0.816	-0.611	-0.716	-0.490
05br05a	-0.189	0.402	0.246	-0.462	-0.048	0.007	-0.654	0.146			-0.741	-0.144	0.137	-0.525	-0.565	0.818	-0.611	-0.712	-0.484
05b	-0.183	0.402	0.243	-0.462	-0.051	0.011	-0.658	0.149			-0.743	-0.148	0.125	-0.516	-0.570	0.828	-0.647	-0.702	-0.485
05TS07	-0.148	0.379	0.214	-0.464	-0.047	-0.025	-0.707	0.153	-0.789	-0.502	-0.735	-0.222	0.133	-0.509	-0.569	0.843	-0.674	-0.698	-0.587
07	-0.111	0.354	0.212	-0.464	-0.034	-0.026	-0.727	0.114	-0.696	-0.499	-0.733	-0.262	0.135	-0.508	-0.571	0.849	-0.684	-0.696	-0.677
07TS08	-0.138	0.371	0.209	-0.465	-0.044	-0.026	-0.728	0.113	-0.718	-0.494	-0.735	-0.190	0.122	-0.507	-0.570	0.829	-0.651	-0.701	-0.720
07TS08_H_2O	-0.131	0.357	0.21	-0.463	-0.036	-0.029	-0.734	0.116	-0.73	-0.498	-0.732	-0.203	0.131	-0.513	-0.566	0.814	-0.608	-0.715	-0.722
08a	-0.114	0.353	0.203	-0.466	-0.030	-0.039	-0.728	0.117	-0.711	-0.497	-0.736	-0.182	0.114	-0.515	-0.569	0.834	-0.643	-0.696	-0.696
08b	-0.094	0.348	0.210	-0.465	-0.029	-0.023	-0.724	0.116	-0.704	-0.506	-0.735	-0.184	0.111	-0.515	-0.570	0.839	-0.655	-0.694	-0.719
08TS09	-0.142	0.373	0.207	-0.463	-0.043	-0.021	-0.717	0.151	-0.610	-0.501	-0.731	-0.217	0.125	-0.508	-0.572	0.837	-0.654	-0.696	-0.781
09	-0.206	0.419	0.255	-0.459	-0.063	0.014	-0.643	0.171	-0.484	-0.499	-0.721	-0.297	0.139	-0.506	-0.569	0.827	-0.64	-0.71	-0.915
09TS10	-0.128	0.372	0.210	-0.467	-0.034	-0.030	-0.738	0.080	-0.586	-0.494	-0.720	-0.376	0.299	-0.522	-0.568	0.827	-0.635	-0.703	-0.774
10	-0.053	0.363	0.204	-0.467	-0.022	-0.038	-0.761	-0.058	-0.696	-0.489	-0.706	-0.365	0.435	-0.545	-0.567	0.827	-0.634	-0.698	-0.700

Table 37: NBO charges on oxygen and hydrogen atoms of water molecules

	H_{N4}	H_{C8}	$H1_{N9}$	$H2_{N9}$	$H3_{C11}$	$H2_{C12}$	H_{C13}	$H1_{N19}$	$H2_{N19}$	O_W	$H1_W$	$H2_W$
EP01 + V01	0.471	0.251	0.494				0.237	0.39	0.396			
pre-reaction complex	0.495	0.247	0.493				0.245	0.41	0.39			
00TS01	0.466	0.263	0.466				0.246	0.438	0.462			
01	0.467	0.26	0.425				0.251	0.497	0.456			
01TS02	0.465	0.271	0.478				0.25	0.473	0.496			
01TS02_H_2O	0.465	0.27	0.47				0.254	0.47	0.515	-1.037	0.536	0.514
02a	0.467	0.265	0.504	0.473			0.239	0.429				
02b	0.467	0.261	0.499	0.467			0.245	0.428				
02TS03	0.466	0.263	0.453	0.441			0.249	0.47				
03a	0.47	0.248					0.248	0.49				
03TS04	0.466	0.239	0.45	0.419			0.238	0.488				
03TS04_H_2O	0.466	0.232	0.45	0.509			0.232	0.489		-1.083	0.515	0.443
04	0.47	0.249	0.397			0.275	0.25	0.49				
04_H_2O	0.468	0.283	0.409			0.257	0.273	0.484		-1.066	0.513	0.514
03r03	0.47	0.25					0.268	0.492				
03b	0.478	0.255					0.275	0.493				
03TS05	0.464	0.248					0.527	0.485		-0.921	0.567	0.532
03TS05_$2H_2O$	0.462	0.245					0.529	0.485		-0.953	0.559	0.557
05a	0.469	0.255			0.279			0.488				
05TS06	0.463	0.242	0.444	0.403	0.263			0.484				
05TS06_H_2O	0.463	0.245	0.445	0.512	0.257			0.486		-1.078	0.518	0.432
06	0.469	0.255	0.398		0.265		0.288	0.487				
05br05a	0.469	0.253			0.279			0.488				
05b	0.468	0.267			0.278			0.488				
05TS07	0.464	0.27	0.444	0.459	0.264			0.474				
07	0.465	0.266	0.498	0.487	0.258			0.434				
07TS08	0.464	0.271	0.469	0.499	0.271			0.477				
07TS08_H_2O	0.465	0.271	0.472	0.514	0.271			0.472		-1.041	0.534	0.509
08a	0.464	0.261	0.426		0.275			0.498	0.501			
08b	0.464	0.259	0.427		0.273			0.497	0.484			
08TS09	0.463	0.261	0.463		0.269			0.463	0.465			
09	0.468	0.244	0.497		0.255			0.441	0.426			
09TS10	0.464	0.261	0.468		0.26			0.465	0.461			
10	0.463	0.258	0.424		0.254			0.481	0.465			

Table 38: NBO Energetic analysis with hyperconjugative delocalizations involving the acceptor and donor NBOs

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol
EP01		
43. LP (1) O 7	/290. BD*(1) N 9 - H	6.48
44. LP (2) O 7	/290. BD*(1) N 9 - H	21.19
00TS01		
72. LP (1) O 7	/495. BD*(1) N 9 - H	0.94
73. LP (2) O 7	/495. BD*(1) N 9 - H	2.42
72. LP (1) O 7	/500. BD*(1) N 19 - H	1.40
73. LP (2) O 7	/500. BD*(1) N 19 - H	2.36
01		
74. LP (1) O 7	/500. BD*(1) N 19 - H	10.60
75. LP (2) O 7	/500. BD*(1) N 19 - H	76.01
01TS02		
77. LP (1) O 7	/519. BD*(1) N 19 – H	1.75
77. LP (1) O 7	/542. BD*(1) N 9 - H	1.21
78. LP (2) O 7	/519. BD*(1) N 19 - H	3.93
78. LP (2) O 7	/542. BD*(1) N 9- H	3.14
02a		
74. LP (1) O 7	/495. BD*(1) N 9 - H 9	8.32
75. LP (2) O 7	/495. BD*(1) N 9 - H 9	40.84
02b		
46. BD (2) C 11 - C 12	/496. BD*(1) N 9 - H1	5.60
74. LP (1) O 7	/495. BD*(1) N 9 - H2	9.39
75. LP (2) O 7	/495. BD*(1) N 9 - H2	52.61
02TS03		
72. LP (1) O 7	/501. BD*(1) N 19 - H	2.00
73. LP (2) O 7	/501. BD*(1) N 19 - H	4.38
46. BD (2) C 11- C 12	/496. BD*(1) N 9 - H	2.28
03a		
65. LP (1) O 7	/435. BD*(1) N 19 - H	6.45
66. LP (2) O 7	/435. BD*(1) N 19 - H	21.07
03TS04_H_2O		
78. LP (1) O 7	/516. BD*(1) N 19 - H	6.03
79. LP (2) O 7	/516. BD*(1) N 19- H	18.73
04_H_2O		
75. LP (1) O 7	/489. BD*(1) N 19 - H	5.96
76. LP (2) O 7	/489. BD*(1) N 19- H	19.19
03b		
41. BD (2) C 11 - C 12	/432. BD*(1) N 19 - C 13	5.55
65. LP (1) O 7	/433. BD*(1) N 19 - H	6.23
66. LP (2) O 7	/433. BD*(1) N 19 - H	19.98

03TS05_2H_2O		
39. BD (1) C 11 - C 12	/481. BD*(1) N 19 - C 13	1.86
70. LP (1) O 7	/482. BD*(1) N 19 - H	7.26
71. LP (2) O 7	/482. BD*(1) N 19 - H	41.54
05b		
28. BD (1) C 11 - C 12	/434. BD*(1) C 13 - N 19	3.35
29. BD (2) C 11 - C 12	/435. BD*(2) C 13 - N 19	15.44
65. LP (1) O 7	/438. BD*(1) N 19 - H	6.96
66. LP (2) O 7	/438. BD*(1) N 19 - H	27.70
435. BD*(2) C 13 - N 19	/441. BD*(2) C 11 - C 12	9.15
05a		
25. BD (1) C 11 - C 12	/429. BD*(1) C 13- N 19	3.20
26. BD (2) C 11 - C 12	/430. BD*(2) C 13 - N 19	16.50
65. LP (1) O 7	/433. BD*(1) N 19	7.12
66. LP (2) O 7	/433. BD*(1) N 19	28.28
430. BD*(2) C 13- N 19	/436. BD*(2) C 11 - C 12	8.43
05TS06_H_2O		
83. LP (1) O 7	/525. BD*(1) N 19 - H	7.57
84. LP (2) O 7	/525. BD*(1) N 19 - H	36.86
06		
73. LP (1) O 7	/490. BD*(1) N 19 - H	6.26
74. LP (2) O 7	/490. BD*(1) N 19 - H	21.18
05TS07		
73. LP (1) O 7	/501. BD*(1) N 19	3.78
74. LP (2) O 7	/501. BD*(1) N 19	9.35
34. BD (2) C 12 - C 13	/488. BD*(1) C 9 - N 19	0.75
34. BD (2) C 12 - C 13	/489. BD*(2) C 9 - N 19	7.70
76. LP (1) O 17	/492. BD*(1) N 9 - H 1	0.10
76. LP (1) O 17	/493. BD*(1) N 9 - H 2	4.98
77. LP (2) O 17	/493. BD*(1) N 9- H 2	0.29
75. LP (1) N 9	/488. BD*(1) C 9 - N 19	0.15
75. LP (1) N 9	/489. BD*(2) C 9 - N 19	95.49
33. BD (1) C 12 - C 13	/488. BD*(1) C 9 - N 19	3.07
07		
73. LP (1) O 7	/515. BD*(1) N 19 - H1	7.35
74. LP (2) O 7	/515. BD*(1) N 19 - H1	28.07
79. LP (1) O 17	/516. BD*(1) N 19 - H2	5.53
80. LP (2) O 17	/516. BD*(1) N 19 - H3	1.82
76. LP (1) N 9	/497. BD*(1) C 12 - C 13	3.00
76. LP (1) N 9	/498. BD*(2) C 12 - C 13	16.38
07TS08_H2O		
77. LP (1) O 7	/519. BD*(1) N 19 - H	1.54
77. LP (1) O 7	/543. BD*(1) N 9 - H	1.57
78. LP (2) O 7	/519. BD*(1) N 19 - H	4.00
78. LP (2) O 7	/543. BD*(1) N 9 - H	3.77

25. BD (2) C 12 - C 13	/515. BD*(1) C 8 - N 19	4.12
24. BD (1) C 12 - C 13	/515. BD*(1) C 8 - N 19	0.86
08a		
73. LP (1) O 7	/500. BD*(1) N 19 - H	6.91
74. LP (2) O 7	/500. BD*(1) N 19 - H	26.75
76. LP (1) N 9	/489. BD*(1) C 8 - N 19	6.69
76. LP (1) N 9	/501. BD*(1) N 19 - H	1.24
77. LP (1) O 17	/501. BD*(1) N 19 - H	7.65
78. LP (2) O 17	/501. BD*(1) N 19 - H	10.75
33. BD (2) C 12 - C 13	/489. BD*(1) C 8 - N 19	3.98
32. BD (1) C 12 - C 13	/489. BD*(1) C 8 - N 19	0.61
08b		
80. LP (2) O 17	/501. BD*(1) N 19 - H	10.34
79. LP (1) O 17	/501. BD*(1) N 19 - H	6.83
74. LP (1) O 7	/500. BD*(1) N 19 - H	8.65
75. LP (2) O 7	/500. BD*(1) N 19 - H	42.10
08TS09		
34. BD (2) C 12 - C 13	/489. BD*(1) C 8 - N 19	6.75
74. LP (2) O 7	/492. BD*(1) N 10 - H	2.57
74. LP (2) O 7	/500. BD*(1) N 19 - H1	2.57
76. LP (1) O 17	/501. BD*(1) N 19 - H2	5.79
77. LP (2) O 17	/501. BD*(1) N 19 - H2	8.79
75. LP (1) N 9	/489. BD*(1) C 8 - N 19	69.55
09TS10		
73. LP (1) O 7	/492. BD*(1) N 9 - H	1.17
73. LP (1) O 7	/509. BD*(1) N 19 – H 1	6.72
74. LP (2) O 7	/492. BD*(1) N 9 - H	4.33
74. LP (2) O 7	/509. BD*(1) N 19 - H1	7.22
77. LP (1) O 17	/508. BD*(1) N 19 - H2	3.41
78. LP (2) O 17	/508. BD*(1) N 19 - H2	4.33
10		
73. LP (1) O 7	/509. BD*(1) N 19 – H1	12.25
74. LP (2) O 7	/492. BD*(1) N 9 - H	0.53
74. LP (2) O 7	/509. BD*(1) N 19 – H1	49.38
78. LP (2) O 17	/508. BD*(1) N 19 – H2	4.97
77. LP (1) O 17	/508. BD*(1) N 19 – H2	3.92

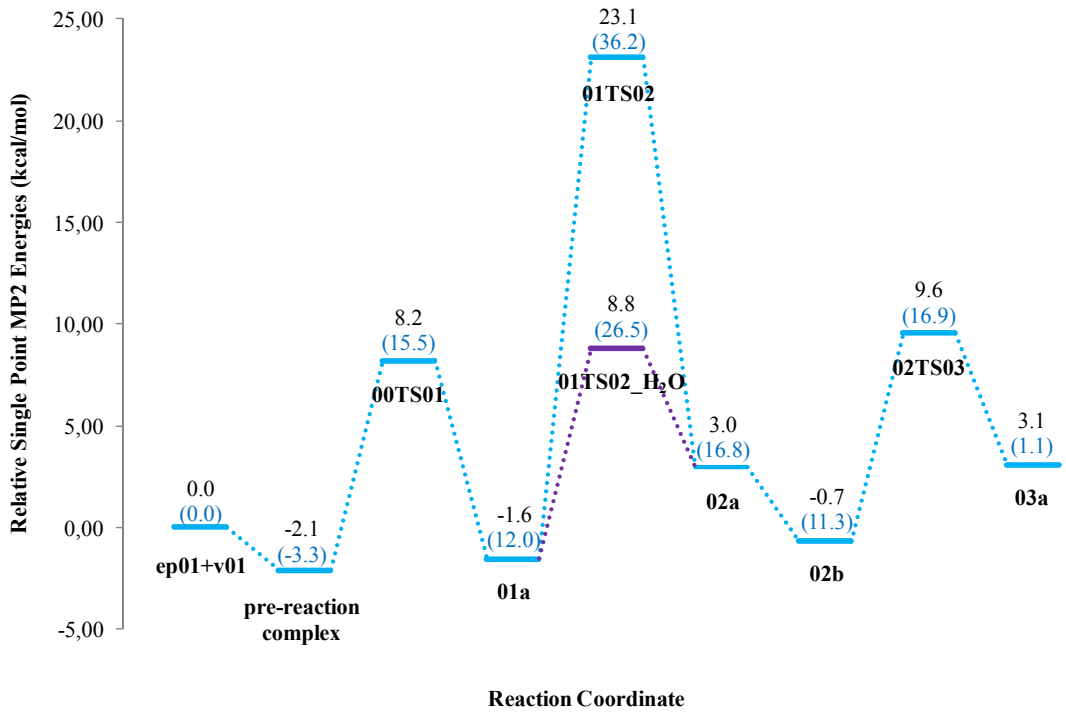

Figure 1: Single point relative MP2 energies for External Aldimine Formation Pathway (Relative Gibbs free energies from gas phase optimization calculations are written in parantheses, energies are given in kcal/mol)

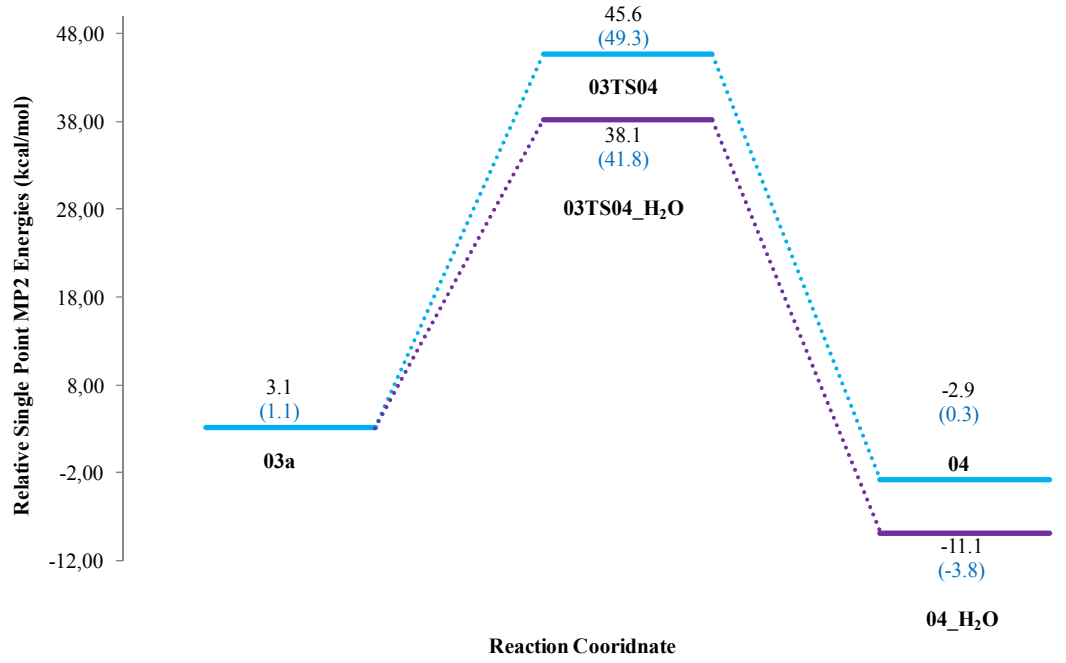

Figure 2: Single point relative MP2 energies for Michael Addition Pathway (Relative Gibbs free energies from gas phase optimization calculations are written in parantheses, energies are given in kcal/mol)

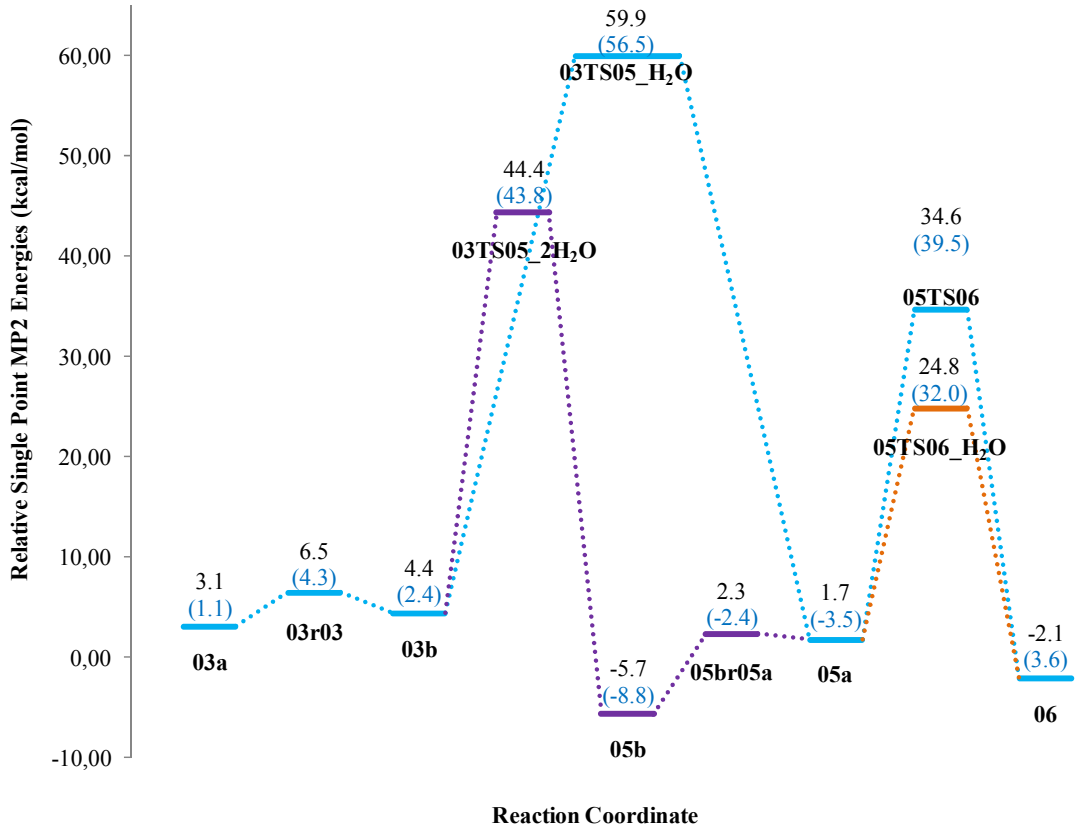

Figure 3: Single point relative MP2 energies for Enamine Michael Addition Pathway (Relative Gibbs free energies from gas phase optimization calculations are written in parantheses, energies are given in kcal/mol)

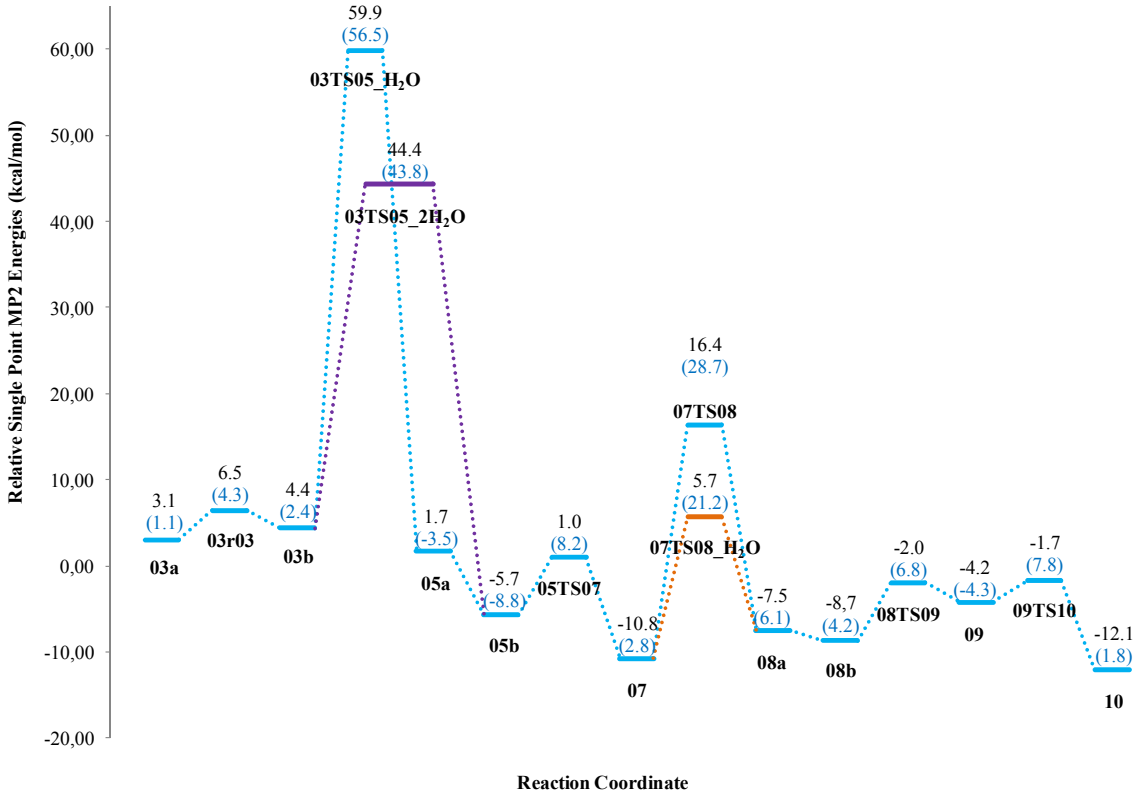

Figure 4: Single point relative MP2 energies for Enamine Pathway (Relative Gibbs free energies from gas phase optimization calculations are written in parantheses, energies are given in kcal/mol)