Supplementary Materials for

The kinetics of polyurethane moisture curing reaction: A combined experimental and DFT mechanistic study

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In order to perform in-situ transmission infrared studies, nitrogen gas is usually used as the driving force, and by setting up a bubbler in the middle section of the gas circuit, the gas is mixed with water vapor so that it reacts with the -NCO groups in the polyurethane. This enables the process of gradually increasing the ambient humidity from near zero to the experimentally specified humidity. The purpose of this design is to achieve the specified humidity quickly during the initial reaction phase, thus reducing the effect of experimental error.

In wet-curing polyurethane hot melt adhesives, the reaction between isocyanate groups and water molecules is very fast. By controlling the humidity of the reaction environment, the amount of water molecules can be adjusted and the rate of reaction can be regulated. This control enables the rapid attainment of a specified humidity level at an early stage, resulting in more accurate and reliable experimental data.

However, precise control of humidity is difficult to achieve with the equipment configuration of a bubbler and gas flow meter alone. In the process of debugging the gas circuit, this paper found that there is a nonlinear variation relationship between gas velocity and gas circuit humidity. As the gas velocity increases, the humidity will first rise and then decline in the trend. When the gas velocity reaches a certain value, the humidity will instead begin to decline. The reason for this phenomenon is that too fast air velocity will cause the bubbler to produce too many large bubbles, and these bubbles fail to stay in the water long enough to carry water vapor effectively, preventing the humidity of the air path from rising further. When the experimental humidity is relatively low, the air velocity will also decrease, which will limit the rate of change of the airway humidity, thus increasing the possibility of experimental error. Therefore, the interrelationship between gas velocity and humidity needs to be considered comprehensively in the experimental design to determine the optimal operating parameters.

Notably, the selection of an appropriate experimental humidity range is also critical to the accuracy and reliability of the study results. Humidity conditions that are either too low or too high may adversely affect the conduct of the polyurethane wet curing reaction. Too low a humidity may result in a reaction rate that is too slow to achieve the intended degree of cure. Too much humidity, on the other hand, may cause unwanted side reactions or material failure. Therefore, the characteristics of the polyurethane hot melt adhesive under study and the required curing conditions need to be fully considered in the experimental design in order to select a suitable humidity range.

In this paper, a gas circuit configuration consisting of a drying gas circuit in parallel with a humidifying gas circuit is designed to achieve joint control of the humidity of the gas entering the in-situ cell. This gas path configuration consists of one branch set up with a bubbler and the other branch set up with a drying tube, and the flow rates of the branch gases are separately controlled by flow meters (Fig. S1). With this gas path configuration, the humidity of the gas in the humidified gas section can be increased while the flow rate of the gas in the drying gas section is increased, thereby realizing precise control of the humidity of the combined gas to maintain it at a predetermined target humidity condition. At the same time, increasing the flow rate of the drying gas section can increase the rate of change of humidity in the in-situ cell, effectively reducing the error generated by the experimental operation.

The design of this parallel air path has several advantages. Firstly, the humidity of the gas can be accurately controlled by the humidification gas path to ensure that the humidity change in the experiment meets the predetermined requirements. Secondly, by increasing the flow rate of the drying gas path, the rate of change of humidity in the in-situ cell can be increased, effectively reducing the experimental error. In addition, the design provides simultaneous control of humidity and temperature, allowing researchers to conduct experiments over a wider range of conditions to investigate the effects of different humidity and temperature on the wet-curing reaction of polyurethane.

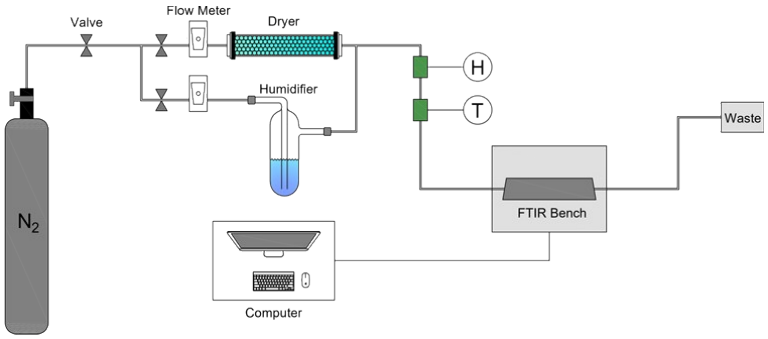
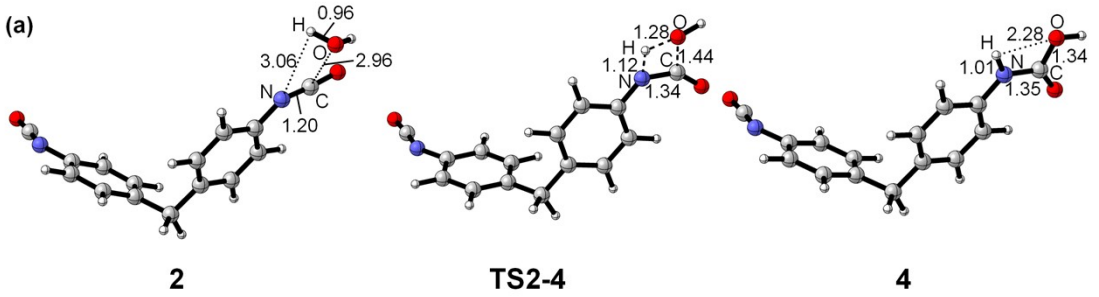
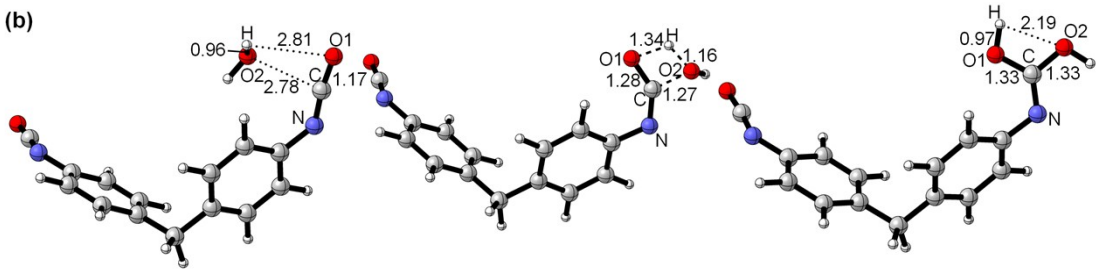


Fig. S1 In-situ infrared reaction cell

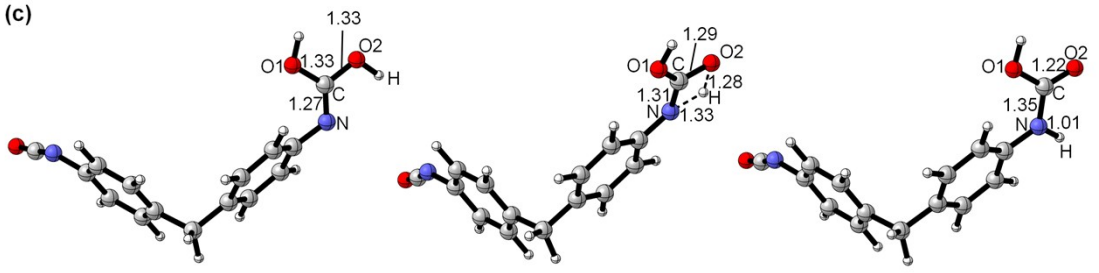
T: Thermometer; H: Hygrometer



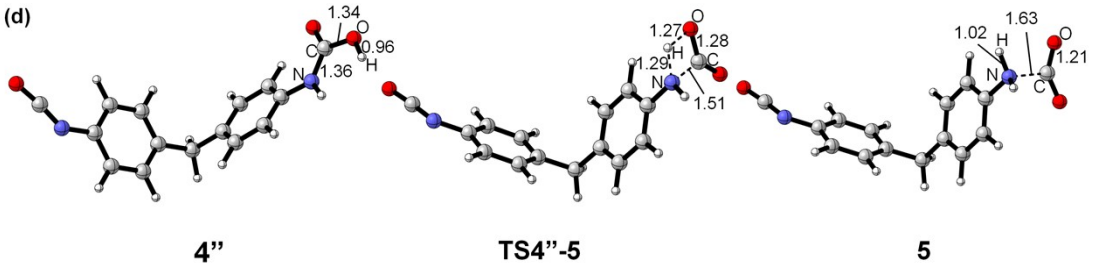
2 **TS2-4** **4**



2' **TS2'-3** **3**



3' **TS3'-4'** **4'**



4'' **TS4''-5** **5**

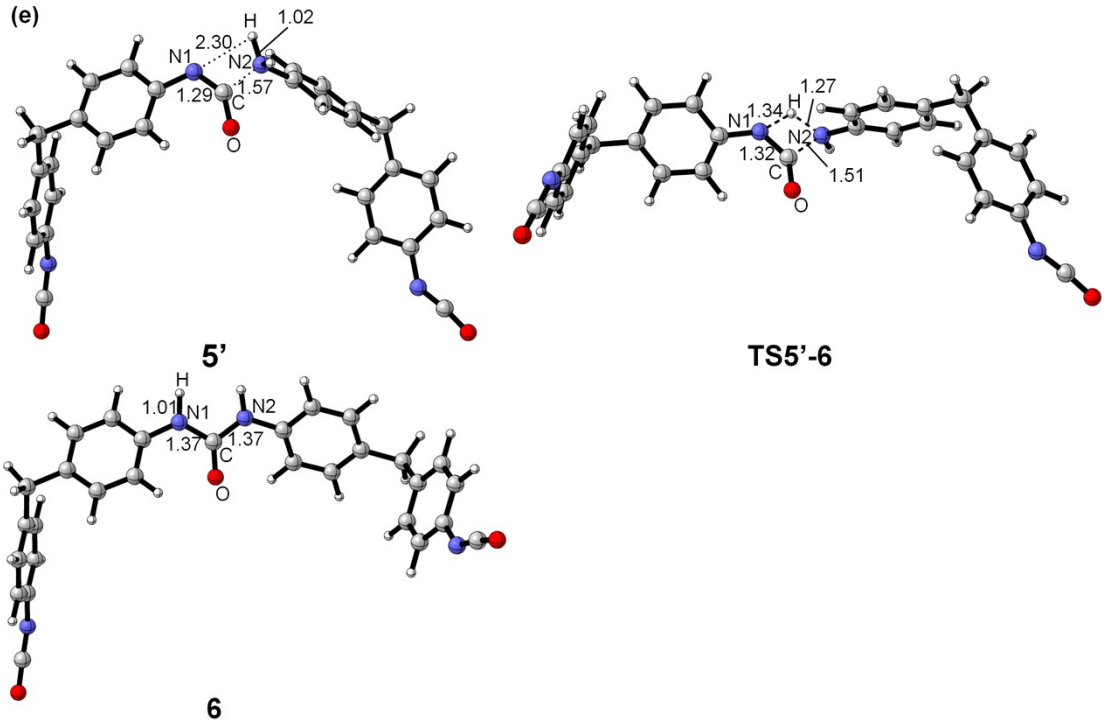
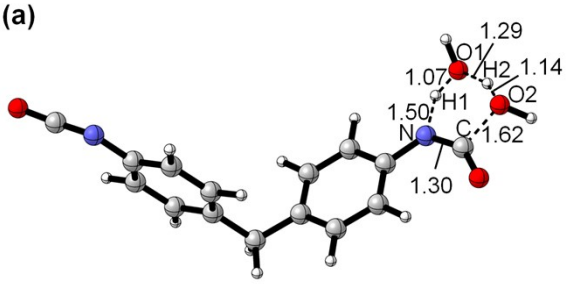
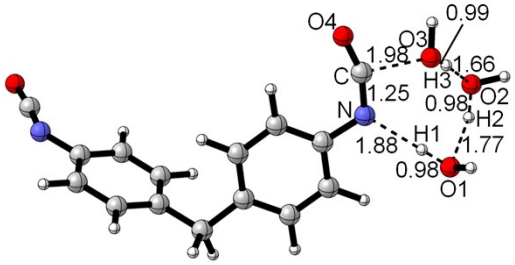


Fig. S2 Optimized structure for PUR moisture curing reaction without the involvement of additional water molecules. (a) breakage of C=N bond; (b) breakage of C=O bond; (c) H-transfer; (d) carbamic acid decomposition; (e) reaction of amine with isocyanate.

(a)

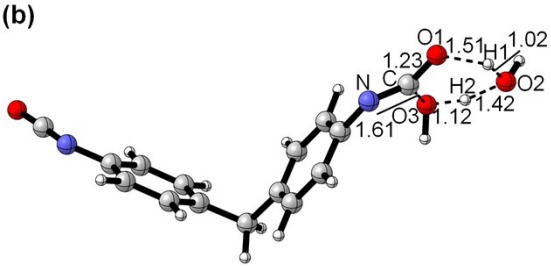


TS2-4-I

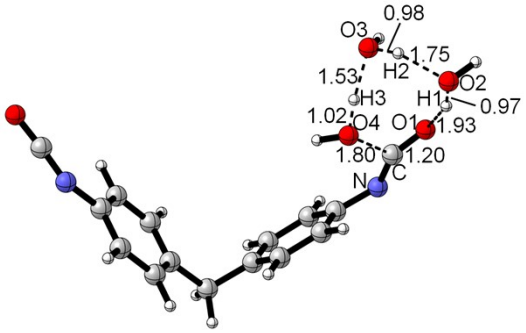


TS2-4-II

(b)

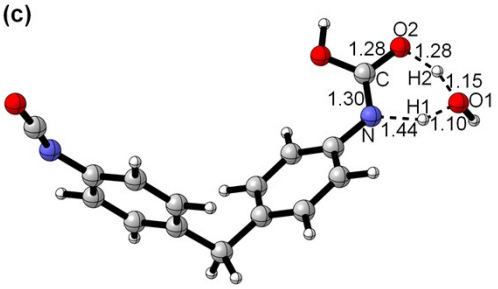


TS2'-3-I

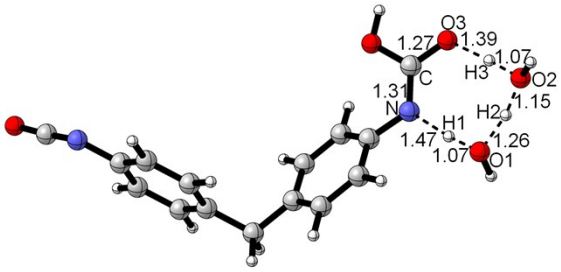


TS2'-3-II

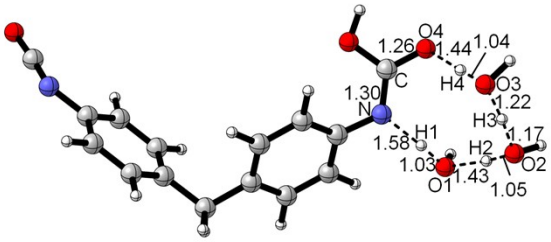
(c)



TS3'-4'-I



TS3'-4'-II



TS3'-4'-III

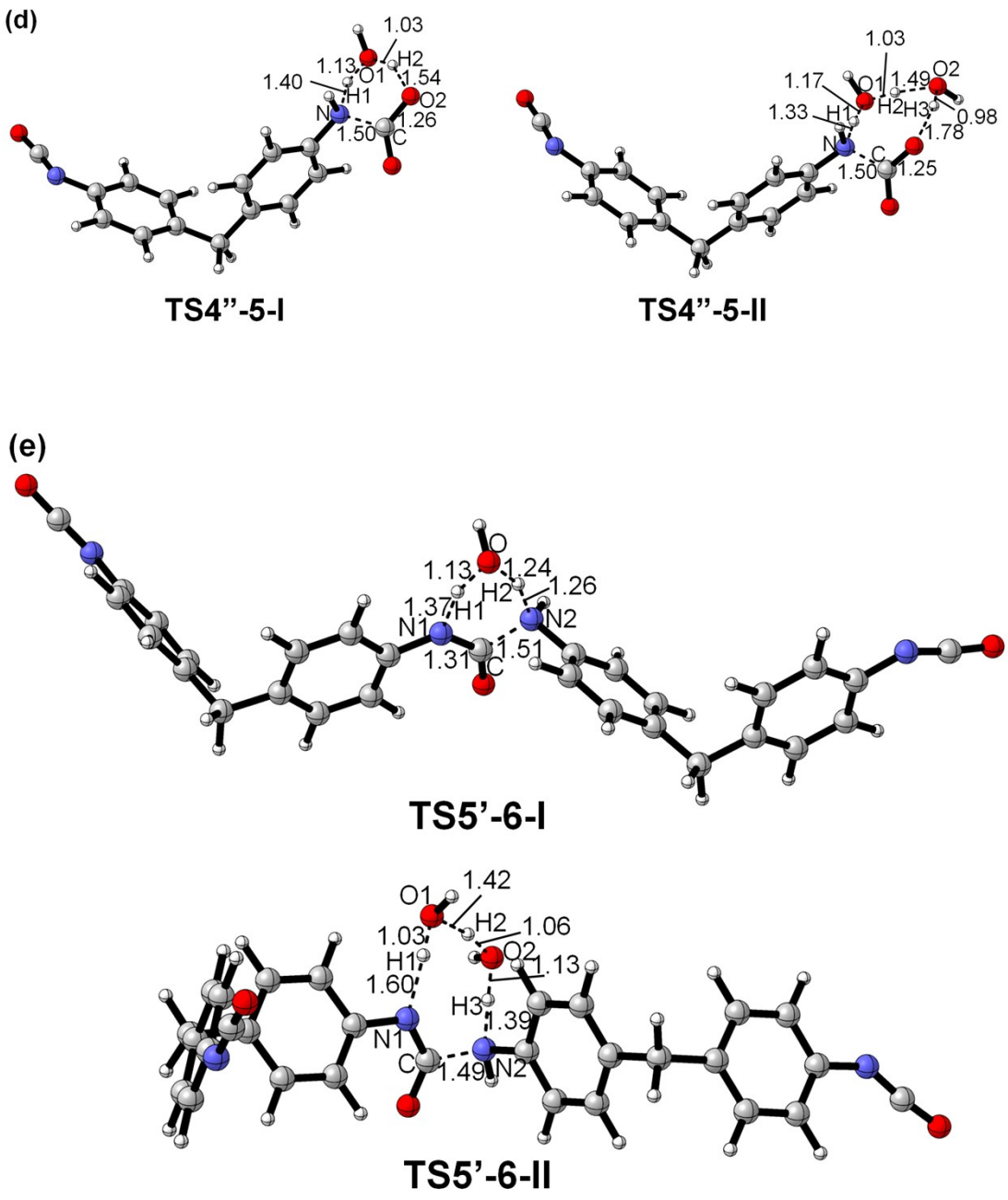


Fig. S3 Optimized structure for PUR moisture curing reaction with the involvement of additional water molecules. (a) breakage of C=N bond; (b) breakage of C=O bond; (c) H-transfer; (d) carbamic acid decomposition; (e) reaction of amine with isocyanate. * The Greek numbers indicate the number of additional water molecules involved in the reaction

2p-I

Geometry with 35 atoms:

Total energy: -990.048750652

N	-3.769037	-1.494557	0.042576
C	-4.905072	-1.591500	-0.340717
O	-5.300758	0.362461	2.103231
H	-5.943815	-0.359100	2.132460
O	-6.017149	-1.840094	-0.634719
H	-5.440569	0.949809	0.369168
H	-4.446826	-0.085963	2.172162
O	-5.525121	1.149560	-0.583640
H	-6.332239	0.686257	-0.840393
C	-2.680563	-0.612768	-0.032934
C	-2.458199	0.167139	-1.167396
C	-1.797232	-0.557576	1.046667
C	-1.355528	1.015102	-1.205208
H	-3.151203	0.111798	-2.000571
C	-0.703001	0.296162	0.992790
H	-1.981167	-1.179486	1.916928
C	-0.467559	1.094624	-0.130813
H	-1.183047	1.625997	-2.087011
H	-0.016246	0.340865	1.834361
C	0.743765	1.999554	-0.183364
H	0.675875	2.633222	-1.073953
H	0.748480	2.662444	0.687865
C	2.041849	1.220117	-0.214735
C	3.010362	1.388632	0.776607
C	2.288779	0.302888	-1.241420
C	4.200427	0.668255	0.748913
H	2.834444	2.095719	1.582375
C	3.471229	-0.423616	-1.284624
H	1.540838	0.153932	-2.016176
C	4.427207	-0.239697	-0.285085
H	4.951539	0.803203	1.521300
H	3.662254	-1.134304	-2.081401
N	5.611813	-0.989923	-0.349918
C	6.627704	-1.128792	0.281574
O	7.657684	-1.359948	0.799222

2p-II

Geometry with 38 atoms:

Total energy: -1066.460508810

N	-4.250041	0.072035	-0.156671
C	-4.790810	0.855038	0.586726

O	-0.283421	1.310196	-0.452331
H	-0.201450	0.354616	-0.324529
O	-5.428507	1.616144	1.212202
H	-1.520212	1.895503	0.844386
H	-2.829160	2.387981	-0.715572
O	-2.331229	2.348759	1.148419
H	-2.635377	1.841030	1.911019
H	-1.021233	1.416709	-1.083517
O	-2.647441	2.233680	-1.660109
H	-3.328330	1.604172	-1.930677
C	-3.054381	-0.665665	-0.153009
C	-2.373562	-0.936483	1.037887
C	-2.566260	-1.140208	-1.367684
C	-1.190139	-1.661385	0.996262
H	-2.772277	-0.572992	1.980761
C	-1.378351	-1.866452	-1.393162
H	-3.110525	-0.926913	-2.282016
C	-0.674394	-2.135255	-0.217411
H	-0.651557	-1.860708	1.919347
H	-0.992447	-2.227353	-2.342272
C	0.659095	-2.849603	-0.249729
H	0.771931	-3.358116	-1.212336
H	0.696829	-3.608648	0.537330
C	1.796668	-1.868405	-0.051921
C	2.040871	-0.878971	-1.012310
C	2.586480	-1.892269	1.097760
C	3.040019	0.066556	-0.830961
H	1.428595	-0.842198	-1.910616
C	3.596835	-0.953694	1.292823
H	2.411180	-2.652998	1.853086
C	3.818372	0.026709	0.329750
H	3.221935	0.835191	-1.575933
H	4.209848	-0.971814	2.187324
N	4.834645	0.967302	0.555753
C	5.306400	1.936529	0.019315
O	5.856716	2.890288	-0.392604

2-I

Geometry with 35 atoms:

Total energy: -990.044539507

N	-4.022527	-0.026822	-0.039016
C	-4.926462	-0.033816	-0.837508
O	-5.872447	0.031738	-1.529052
H	-4.465771	1.423364	1.572195

O	-5.341508	2.925424	-0.791239
H	-6.166680	2.428907	-0.849528
H	-5.077903	2.829449	0.141130
O	-4.356300	2.349494	1.834715
H	-3.438258	2.538920	1.595870
C	-2.769015	-0.644085	0.123160
C	-2.308838	-1.601332	-0.780918
C	-1.993691	-0.278706	1.223617
H	-2.921955	-1.878418	-1.633058
C	-1.066685	-2.191849	-0.573379
C	-0.754197	-0.876469	1.413524
H	-2.368718	0.463375	1.920846
C	-0.275250	-1.841470	0.522946
H	-0.708575	-2.940878	-1.274212
H	-0.148530	-0.590477	2.269610
C	1.094358	-2.454665	0.723297
H	1.226967	-2.722592	1.775887
H	1.166043	-3.372846	0.132396
C	2.192732	-1.497308	0.311737
C	2.941804	-0.807179	1.267315
C	2.447063	-1.254206	-1.041341
C	3.924341	0.101884	0.890064
H	2.757218	-0.985428	2.323171
C	3.425916	-0.350798	-1.435206
H	1.870082	-1.780551	-1.797550
C	4.164274	0.327706	-0.465627
H	4.505683	0.634871	1.636444
H	3.626357	-0.164980	-2.484856
N	5.148085	1.234359	-0.890594
C	5.968479	1.970963	-0.406742
O	6.804776	2.724906	-0.068261

2-II

Geometry with 38 atoms:

Total energy: -1066.460985050

N	-3.998070	-0.576652	0.148684
C	-4.733351	0.061870	-0.552975
O	-5.567850	0.661920	-1.129939
H	-3.394929	2.219316	1.360572
O	-4.686187	3.112248	0.294437
H	-5.493139	2.596708	0.166309
O	-2.537590	1.790947	1.549705
H	-2.388679	1.730786	-0.346730
H	-1.961608	2.524368	1.802299

O	-2.718272	1.870133	-1.256667
H	-4.120477	2.845601	-0.456183
H	-2.077330	2.468370	-1.662219
C	-2.710835	-1.128956	0.164356
C	-2.198182	-1.581169	1.376886
C	-1.955834	-1.234745	-1.007941
C	-0.921605	-2.135175	1.417021
H	-2.797072	-1.490809	2.276710
C	-0.684416	-1.787122	-0.949325
H	-2.368233	-0.875445	-1.945029
C	-0.149741	-2.245909	0.260169
H	-0.521253	-2.487422	2.363523
H	-0.091841	-1.860967	-1.857967
C	1.254953	-2.807015	0.304595
H	1.419466	-3.284081	1.276032
H	1.371495	-3.575907	-0.465552
C	2.294378	-1.728054	0.084986
C	2.461355	-0.708998	1.030610
C	3.082718	-1.706363	-1.065322
C	3.393354	0.300402	0.839566
H	1.849367	-0.707653	1.929334
C	4.022106	-0.699137	-1.273721
H	2.964134	-2.487902	-1.810365
C	4.175506	0.302457	-0.320046
H	3.523574	1.086680	1.576972
H	4.635312	-0.684882	-2.168174
N	5.128760	1.306463	-0.550839
C	5.547469	2.295699	-0.006582
O	6.043540	3.275733	0.412699

3p-I

Geometry with 35 atoms:

Total energy: -990.070845667

N	-4.048360	0.242901	-0.074572
C	-4.128950	1.481876	0.237420
O	-5.281816	2.136479	0.280890
H	-6.018503	1.496705	0.033714
O	-3.076128	2.256466	0.524410
H	-3.386751	3.159313	0.698404
O	-6.862239	0.200241	-0.436344
H	-6.012701	-0.280675	-0.463768
H	-7.311739	-0.145695	0.347029
C	-2.790684	-0.401347	-0.064325
C	-2.414528	-1.158214	-1.175933

C	-1.942411	-0.379759	1.052549
C	-1.206303	-1.851859	-1.185174
H	-3.074168	-1.191993	-2.037513
C	-0.741974	-1.077013	1.035768
H	-2.233989	0.186035	1.932047
C	-0.352860	-1.823372	-0.082413
H	-0.926108	-2.428127	-2.063174
H	-0.091272	-1.044879	1.906939
C	0.972310	-2.555266	-0.088300
H	1.052135	-3.139765	-1.011233
H	1.013007	-3.261725	0.747553
C	2.147936	-1.607150	0.015756
C	2.351469	-0.628867	-0.965700
C	3.034743	-1.666022	1.090296
C	3.411319	0.261675	-0.882592
H	1.663562	-0.563868	-1.805239
C	4.103407	-0.777993	1.190745
H	2.890777	-2.416363	1.862467
C	4.288599	0.185216	0.203995
H	3.566188	1.017602	-1.646530
H	4.790226	-0.824252	2.028908
N	5.369129	1.072894	0.328327
C	5.838757	2.008820	-0.266324
O	6.396307	2.927162	-0.744019

3p-II

Geometry with 38 atoms:

Total energy: -1066.480690570

N	-3.747449	0.346838	0.079536
C	-3.904421	1.621587	0.098559
O	-5.078623	2.209554	0.060986
O	-2.881717	2.484921	0.133606
H	-3.235251	3.388874	0.119997
O	-5.657787	-1.495695	-0.645117
H	-4.939364	-0.862039	-0.376864
H	-6.730785	-0.211240	-0.279296
O	-7.090145	0.677618	-0.032295
H	-5.863905	1.540841	0.027945
H	-7.583796	0.974861	-0.809138
H	-5.721645	-2.111808	0.096783
C	-2.462817	-0.235432	0.167132
C	-1.496941	0.162221	1.103373
C	-2.184997	-1.327811	-0.658895
C	-0.280773	-0.503866	1.180154

H	-1.708472	0.988474	1.773806
C	-0.961088	-1.986979	-0.575591
H	-2.940475	-1.656500	-1.366683
C	0.008555	-1.587884	0.343917
H	0.460029	-0.180759	1.908353
H	-0.760841	-2.830481	-1.231291
C	1.338955	-2.302223	0.445785
H	1.342826	-3.145303	-0.253774
H	1.459586	-2.720209	1.450884
C	2.516439	-1.397969	0.151362
C	3.523105	-1.193783	1.097004
C	2.614607	-0.742483	-1.080458
C	4.608216	-0.366043	0.826262
H	3.459887	-1.691117	2.060917
C	3.691525	0.085485	-1.368168
H	1.834293	-0.883068	-1.824115
C	4.690018	0.271518	-0.411291
H	5.388122	-0.211214	1.565638
H	3.769983	0.589870	-2.325263
N	5.768435	1.112237	-0.729195
C	6.783978	1.509613	-0.218712
O	7.797866	1.970049	0.158708

3p-III

Geometry with 41 atoms:

Total energy: -1142.877435970

N	-3.261815	0.298707	0.259403
C	-3.361396	1.577689	0.186921
O	-4.501471	2.219599	0.298099
O	-2.315295	2.382078	-0.048426
H	-2.624343	3.302011	-0.042402
O	-5.106606	-1.164909	-1.267273
H	-4.556244	-0.629609	-0.644960
H	-6.725924	-0.606475	-1.101079
O	-7.585780	-0.201259	-0.832682
H	-6.884293	0.454808	0.533525
O	-6.324348	0.809980	1.275450
H	-5.253253	1.602089	0.666461
H	-6.894755	1.421386	1.761125
H	-7.690044	0.556365	-1.422986
H	-4.820284	-0.864352	-2.140170
C	-1.988404	-0.313942	0.210166
C	-1.794814	-1.394733	-0.654013
C	-0.937925	0.063671	1.057779

C	-0.572761	-2.061079	-0.690163
H	-2.612472	-1.708171	-1.295812
C	0.275933	-0.610630	1.017703
H	-1.082585	0.885127	1.752573
C	0.480616	-1.683169	0.143074
H	-0.438730	-2.893054	-1.376756
H	1.079683	-0.299913	1.681154
C	1.794508	-2.439513	0.128968
H	1.842222	-3.104707	0.998802
H	1.820034	-3.079328	-0.759613
C	3.006716	-1.537012	0.141452
C	3.265633	-0.683524	-0.938276
C	3.878662	-1.515994	1.229633
C	4.367779	0.158907	-0.938465
H	2.592114	-0.681395	-1.791550
C	4.988796	-0.674664	1.247567
H	3.689358	-2.167766	2.077898
C	5.231760	0.160043	0.161526
H	4.568569	0.815620	-1.779744
H	5.664911	-0.660601	2.095529
N	6.357811	0.997307	0.198209
C	6.895495	1.817258	-0.500775
O	7.517309	2.630266	-1.079400

3-I

Geometry with 35 atoms:

Total energy: -990.061513569

N	3.601493	1.057801	0.957856
C	4.650669	0.926306	0.240182
O	5.698784	1.757358	0.399613
H	5.468684	2.397281	1.091438
O	4.868045	0.006821	-0.682959
H	5.798198	0.105958	-1.073026
H	7.481984	1.168654	-1.261423
O	7.239297	0.312948	-1.644207
H	7.817784	-0.321416	-1.197912
C	2.505130	0.198394	0.735236
C	1.947492	-0.008956	-0.535499
C	1.893979	-0.407737	1.836475
C	0.828206	-0.816430	-0.690844
H	2.398413	0.470816	-1.398577
C	0.776407	-1.222126	1.671103
H	2.310365	-0.240506	2.825211
C	0.228891	-1.442695	0.406878

H	0.407111	-0.963064	-1.683223
H	0.323538	-1.694745	2.539230
C	-1.009442	-2.294858	0.222588
H	-0.863588	-2.982598	-0.616475
H	-1.167179	-2.897756	1.122521
C	-2.236856	-1.448521	-0.037877
C	-2.847475	-0.754008	1.012780
C	-2.759778	-1.307155	-1.323905
C	-3.952935	0.054779	0.791845
H	-2.448712	-0.851209	2.019521
C	-3.866524	-0.496986	-1.563929
H	-2.298245	-1.839928	-2.150738
C	-4.461467	0.181720	-0.504272
H	-4.429092	0.587006	1.609832
H	-4.274307	-0.388993	-2.563214
N	-5.578922	0.989016	-0.769635
C	-6.344280	1.699751	-0.170867
O	-7.155508	2.417112	0.287543

3-II

Geometry with 38 atoms:

Total energy: -1066.461848500

N	-3.748389	-1.154103	-0.502977
C	-4.138059	-0.031132	-0.033486
O	-3.376262	0.914124	0.567713
H	-2.450236	0.620579	0.608082
O	-5.401291	0.332740	-0.126143
H	-5.569337	1.249528	0.291836
H	-5.153893	3.150730	0.388454
O	-5.845610	2.642018	0.872597
H	-6.686345	2.940286	0.499331
H	-3.366543	2.672256	-0.382544
O	-3.733841	3.553418	-0.561188
H	-4.052202	3.496216	-1.471932
C	-2.400041	-1.535500	-0.345522
C	-1.796040	-1.639550	0.916763
C	-1.655002	-1.898736	-1.473254
C	-0.477037	-2.067833	1.036369
H	-2.373849	-1.397838	1.805434
C	-0.338960	-2.328354	-1.343071
H	-2.120826	-1.838115	-2.451915
C	0.271223	-2.417829	-0.089025
H	-0.025041	-2.140112	2.022896
H	0.224141	-2.604758	-2.231054

C	1.720584	-2.835087	0.047017
H	2.008057	-3.432105	-0.823884
H	1.842128	-3.459371	0.937393
C	2.629096	-1.629016	0.156146
C	2.985092	-0.905148	-0.987323
C	3.084672	-1.182879	1.397683
C	3.776729	0.231528	-0.898899
H	2.636801	-1.239221	-1.961376
C	3.877855	-0.044059	1.504488
H	2.818850	-1.735094	2.294909
C	4.221249	0.661843	0.354526
H	4.054924	0.789048	-1.788214
H	4.234133	0.301203	2.468988
N	5.022091	1.807496	0.486391
C	5.508453	2.655176	-0.216817
O	6.037559	3.539260	-0.783464

4pp-I

Geometry with 35 atoms:

Total energy: -990.074520440

N	-3.941035	0.547432	-0.029673
C	-5.151858	0.111094	-0.488949
O	-5.347123	-0.977882	-1.011288
O	-6.156228	0.977994	-0.339842
O	-5.397326	3.165343	0.885306
H	-5.874446	1.824169	0.112431
H	-4.675288	3.635828	0.445904
H	-3.933837	1.419667	0.487406
H	-5.073951	2.988317	1.779645
C	-2.745669	-0.199903	0.010124
C	-2.466533	-1.248726	-0.867928
C	-1.784124	0.176250	0.956072
C	-1.249235	-1.920514	-0.769383
H	-3.186169	-1.535013	-1.621952
C	-0.573380	-0.496269	1.031634
H	-1.997081	0.999539	1.632541
C	-0.289264	-1.566765	0.176880
H	-1.044637	-2.738761	-1.454875
H	0.162389	-0.188221	1.770661
C	1.017087	-2.324749	0.289428
H	1.025869	-2.904150	1.219306
H	1.077581	-3.044481	-0.533931
C	2.233209	-1.426619	0.265739
C	2.521985	-0.656342	-0.867729

C	3.085361	-1.337783	1.365898
C	3.636275	0.168940	-0.908758
H	1.862623	-0.707010	-1.730699
C	4.207515	-0.512649	1.342937
H	2.872213	-1.924491	2.254988
C	4.482476	0.236240	0.203081
H	3.861457	0.759906	-1.791596
H	4.870591	-0.447551	2.198842
N	5.622526	1.054724	0.198940
C	6.194258	1.806255	-0.547864
O	6.847381	2.559095	-1.171755

4pp-II

Geometry with 38 atoms:

Total energy: -1066.488423760

N	-3.846602	0.010176	0.431434
C	-4.930452	-0.012191	-0.403114
O	-5.111644	-0.837710	-1.288007
O	-5.834113	0.942017	-0.167234
O	-2.644327	2.776368	-0.600835
H	-3.894046	2.932192	0.614175
H	-3.048812	2.185485	-1.251564
H	-3.835556	0.742316	1.133249
O	-4.615504	2.732845	1.256578
H	-5.463674	1.671901	0.421543
H	-1.938856	2.243302	-0.208118
H	-5.121812	3.549312	1.359574
C	-2.622580	-0.665654	0.262698
C	-2.411181	-1.699155	-0.653392
C	-1.562790	-0.254214	1.083409
C	-1.150344	-2.286943	-0.743205
H	-3.213670	-2.036678	-1.292350
C	-0.317825	-0.857607	0.983670
H	-1.726025	0.548137	1.798757
C	-0.087728	-1.887641	0.065691
H	-0.997419	-3.083654	-1.466471
H	0.489262	-0.517582	1.627528
C	1.262088	-2.570654	-0.027408
H	1.303751	-3.133553	-0.966176
H	1.358196	-3.302754	0.782726
C	2.428538	-1.612437	0.043772
C	2.607650	-0.638121	-0.946658
C	3.337425	-1.660989	1.100221
C	3.666889	0.255681	-0.890391

H	1.904861	-0.580663	-1.774089
C	4.405783	-0.770231	1.173637
H	3.211084	-2.407174	1.879403
C	4.568067	0.186900	0.177061
H	3.804585	1.006885	-1.662325
H	5.110613	-0.810760	1.997017
N	5.650756	1.075682	0.270842
C	6.109067	2.002627	-0.346628
O	6.657189	2.913485	-0.848626

4p-I

Geometry with 35 atoms:

Total energy: -990.091286453

N	-4.056503	0.323390	0.038737
C	-4.353357	1.605665	0.347468
O	-5.481382	2.082380	0.221644
H	-6.611938	0.758784	-0.659747
O	-3.319428	2.323703	0.800482
H	-3.648303	3.219764	0.980197
O	-6.752249	-0.118479	-1.057107
H	-4.820883	-0.156290	-0.436468
H	-7.138749	-0.635070	-0.338317
C	-2.794323	-0.317832	0.056011
C	-2.519192	-1.233419	-0.959558
C	-1.859671	-0.116487	1.076154
C	-1.314533	-1.930398	-0.964891
H	-3.251027	-1.392973	-1.746002
C	-0.655001	-0.807599	1.047777
H	-2.076608	0.567951	1.887001
C	-0.363227	-1.726189	0.034427
H	-1.112732	-2.640781	-1.761829
H	0.071661	-0.639034	1.838981
C	0.950112	-2.480989	0.038277
H	0.999443	-3.108648	-0.857581
H	0.984337	-3.151231	0.904086
C	2.149342	-1.560727	0.085519
C	2.420234	-0.698307	-0.983929
C	2.992471	-1.530073	1.196050
C	3.505882	0.164563	-0.951854
H	1.768517	-0.704568	-1.854099
C	4.085481	-0.668110	1.246174
H	2.794165	-2.190133	2.035795
C	4.340309	0.176902	0.170771
H	3.715954	0.829014	-1.784715

H	4.739492	-0.646116	2.111115
N	5.448342	1.035823	0.241623
C	5.986199	1.870345	-0.439958
O	6.605489	2.698741	-0.998965

4p-II

Geometry with 38 atoms:

Total energy: -1066.498218490

N	-3.688842	0.422256	0.071405
C	-3.989184	1.734853	0.111431
O	-5.134474	2.175862	-0.006097
O	-2.937819	2.546577	0.280428
H	-3.276667	3.456582	0.294241
O	-5.665271	-1.541039	-0.694719
H	-4.459982	-0.195229	-0.209934
H	-6.390513	-0.905762	-0.500268
O	-7.374105	0.510619	-0.127224
H	-6.608343	1.115542	-0.055790
H	-7.765821	0.729299	-0.982766
H	-5.590107	-2.071648	0.109007
C	-2.416110	-0.188511	0.181987
C	-1.432997	0.265194	1.067627
C	-2.179900	-1.332327	-0.581088
C	-0.221315	-0.408211	1.151686
H	-1.619453	1.132008	1.689600
C	-0.966428	-2.005989	-0.472337
H	-2.949617	-1.689089	-1.258823
C	0.031817	-1.553805	0.390093
H	0.541433	-0.043436	1.835532
H	-0.793623	-2.895483	-1.072116
C	1.355760	-2.277300	0.509942
H	1.348106	-3.143196	-0.160878
H	1.474133	-2.663304	1.528095
C	2.540532	-1.393991	0.183802
C	3.552782	-1.172261	1.119312
C	2.638899	-0.774484	-1.066535
C	4.643479	-0.361246	0.821502
H	3.489080	-1.641442	2.097155
C	3.721207	0.036686	-1.381057
H	1.854756	-0.929220	-1.803275
C	4.724461	0.242046	-0.433196
H	5.427821	-0.192639	1.553107
H	3.800035	0.513941	-2.351928
N	5.806387	1.067265	-0.777677

C	6.819566	1.485079	-0.279152
O	7.831735	1.960735	0.083715

4p-III

Geometry with 41 atoms:

Total energy: -1142.895050810

N	3.190869	0.640806	0.102422
C	3.434296	1.926173	-0.220092
O	4.532643	2.463671	-0.057136
O	2.389103	2.589913	-0.726585
H	2.687348	3.493042	-0.922973
O	5.152739	-0.603639	1.797488
H	3.933204	0.207557	0.666819
H	5.507208	-1.127057	1.046388
O	6.049156	-1.691421	-0.565589
H	6.367518	-0.769450	-0.691747
O	6.831898	0.928323	-0.507032
H	6.025142	1.426083	-0.269537
H	7.354757	0.912529	0.305076
H	6.854214	-2.200181	-0.404785
H	5.748335	0.156154	1.849455
C	1.969083	-0.068880	0.023853
C	1.702571	-0.998663	1.029521
C	1.071956	0.074178	-1.039148
C	0.541765	-1.765057	0.983746
H	2.409340	-1.116044	1.845416
C	-0.090061	-0.686829	-1.061675
H	1.284139	0.768540	-1.842786
C	-0.374194	-1.617911	-0.057663
H	0.346540	-2.484982	1.773775
H	-0.789552	-0.561858	-1.884903
C	-1.647346	-2.437042	-0.111742
H	-1.636087	-3.077131	-1.000405
H	-1.682477	-3.095787	0.762183
C	-2.886117	-1.569526	-0.148945
C	-3.218903	-0.769266	0.951070
C	-3.702208	-1.521653	-1.278949
C	-4.337078	0.051302	0.928804
H	-2.588477	-0.789223	1.836616
C	-4.827476	-0.701519	-1.319350
H	-3.456313	-2.133550	-2.142222
C	-5.142312	0.083434	-0.214515
H	-4.594664	0.667569	1.784936
H	-5.460500	-0.665981	-2.199329

N	-6.280303	0.902603	-0.277373
C	-6.859165	1.698254	0.416742
O	-7.517101	2.488645	0.986698

4-I

Geometry with 35 atoms:

Total energy: -990.090070387

N	-3.944400	0.550309	-0.089321
C	-5.015861	0.150210	-0.810516
O	-5.161438	-0.911798	-1.397603
H	-4.038190	1.463449	0.363197
O	-5.966398	1.113711	-0.808215
H	-6.718730	0.781572	-1.323424
H	-5.145000	2.894562	1.795847
O	-4.777242	3.144355	0.937824
H	-5.496480	2.952881	0.318409
C	-2.763038	-0.172206	0.157960
C	-2.434197	-1.373982	-0.472202
C	-1.871112	0.382478	1.086994
H	-3.104680	-1.814100	-1.196145
C	-1.230179	-2.005003	-0.160065
C	-0.677447	-0.258310	1.380174
H	-2.125969	1.319768	1.574947
C	-0.337742	-1.468064	0.764996
H	-0.985655	-2.941451	-0.654902
H	0.005333	0.186787	2.100187
C	0.981520	-2.142314	1.076396
H	1.093352	-2.255689	2.159601
H	0.981829	-3.145272	0.637832
C	2.155306	-1.351647	0.539958
C	3.008157	-0.652777	1.396604
C	2.383300	-1.277181	-0.837699
C	4.065033	0.102619	0.899052
H	2.845455	-0.700286	2.469843
C	3.435793	-0.530673	-1.351103
H	1.724162	-1.811948	-1.517227
C	4.275655	0.161421	-0.478411
H	4.726132	0.645116	1.568230
H	3.615353	-0.476134	-2.419429
N	5.330049	0.912160	-1.022535
C	6.219728	1.628375	-0.641459
O	7.124335	2.341956	-0.406763

4-II

Geometry with 38 atoms:

Total energy: -1066.491730110

N	-3.663418	0.256990	-0.421151
C	-3.929821	1.502741	-0.864349
O	-3.138408	2.318720	-1.312630
H	-4.445171	-0.267928	-0.006505
O	-5.256645	1.770388	-0.755618
H	-5.399426	2.671204	-1.089318
O	-5.781576	-1.256165	0.789381
H	-6.126405	-0.457973	1.244411
H	-6.370110	-1.371417	0.032184
O	-6.493181	1.195566	1.815402
H	-6.078923	1.588175	1.029520
H	-7.440548	1.293187	1.652025
C	-2.389608	-0.340336	-0.339172
C	-2.246789	-1.411553	0.547568
C	-1.296930	0.058137	-1.115607
C	-1.026709	-2.065890	0.664189
H	-3.098078	-1.722283	1.146126
C	-0.081416	-0.605465	-0.980204
H	-1.395869	0.873122	-1.819396
C	0.077850	-1.674515	-0.095536
H	-0.931293	-2.892980	1.362527
H	0.762090	-0.282825	-1.585469
C	1.395065	-2.416505	0.013938
H	1.391141	-2.997908	0.942454
H	1.475883	-3.138851	-0.806652
C	2.605878	-1.512732	-0.014012
C	2.789746	-0.542972	0.980013
C	3.555738	-1.610851	-1.030261
C	3.892804	0.297834	0.966783
H	2.054637	-0.445432	1.774858
C	4.669256	-0.774183	-1.059502
H	3.426572	-2.353598	-1.812259
C	4.835886	0.178257	-0.059244
H	4.032663	1.046394	1.740812
H	5.407052	-0.854932	-1.850402
N	5.965931	1.009897	-0.105877
C	6.447741	1.907653	0.536512
O	7.023066	2.785004	1.066913

5p-I

Geometry with 61 atoms:

Total energy: -1638.824609610

N	-0.860482	0.231985	-0.560397
C	-0.085626	-0.349184	-1.425865
O	-0.073217	-1.387144	-2.087506
N	1.181980	0.527714	-1.646466
H	1.016379	1.472898	-1.250098
H	1.326141	0.602381	-2.659283
O	0.223728	2.699936	-0.030779
H	-0.345828	1.890485	-0.045068
H	-0.234752	3.324817	-0.607765
C	-2.070793	-0.356586	-0.152197
C	-2.547590	-1.620719	-0.527730
C	-2.856857	0.412803	0.723921
C	-3.770173	-2.082585	-0.039439
H	-1.967745	-2.242568	-1.195865
C	-4.070857	-0.056483	1.199929
H	-2.488880	1.391001	1.021875
C	-4.549068	-1.318469	0.827344
H	-4.121389	-3.066148	-0.342174
H	-4.662601	0.562922	1.870585
C	2.346232	-0.089050	-1.016931
C	3.102175	-1.008274	-1.729512
C	2.621596	0.218667	0.309728
C	4.178017	-1.622469	-1.094253
H	2.855661	-1.235408	-2.762081
C	3.700151	-0.403773	0.927310
H	2.005716	0.938504	0.840717
C	4.487716	-1.329047	0.235555
H	4.782880	-2.340639	-1.640302
H	3.933366	-0.168469	1.962037
C	-5.885960	-1.812760	1.337025
H	-6.017350	-2.858102	1.037883
H	-5.901299	-1.782649	2.431568
C	5.695772	-1.952213	0.903336
H	5.931754	-2.901313	0.413809
H	5.465026	-2.158925	1.952485
C	-7.039815	-0.987117	0.809423
C	-7.832147	-0.219827	1.665481
C	-7.319179	-0.962690	-0.560935
C	-8.882225	0.550557	1.175748
H	-7.627694	-0.225397	2.732547
C	-8.364939	-0.201892	-1.066386
H	-6.705471	-1.549239	-1.240177
C	-9.146328	0.556191	-0.193587
H	-9.495953	1.146306	1.844636

H	-8.584451	-0.186613	-2.128525
C	6.891020	-1.025949	0.823763
C	7.746883	-1.060926	-0.281225
C	7.126297	-0.078649	1.822520
C	8.812011	-0.176096	-0.391263
H	7.578821	-1.793153	-1.066552
C	8.186763	0.816053	1.726489
H	6.473296	-0.041290	2.690250
C	9.027539	0.766473	0.616835
H	9.477075	-0.208283	-1.249005
H	8.369153	1.550925	2.503021
N	-10.196104	1.318715	-0.729978
N	10.090004	1.680833	0.542673
C	-11.056856	2.069887	-0.350654
C	10.984491	1.963190	-0.212689
O	11.894083	2.339313	-0.855500
O	-11.936987	2.814003	-0.116939

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Geometry with 64 atoms:

Total energy: -1715.234084520

N	0.946280	-2.653947	0.002682
C	0.143146	-2.714599	-1.020444
O	0.252203	-2.620732	-2.246264
N	-1.307361	-2.944223	-0.566832
H	-1.381632	-3.538091	0.309730
H	-1.762606	-3.447316	-1.335256
O	-1.760336	-4.334147	1.727101
H	-1.025770	-3.938912	2.254112
H	-1.500041	-5.255096	1.591390
O	0.403259	-3.065948	2.671763
H	0.573251	-2.857342	1.710745
H	0.234698	-2.210819	3.088691
C	2.317509	-2.387501	-0.197066
C	2.875953	-1.795388	-1.344143
C	3.179698	-2.703914	0.863109
C	4.243178	-1.552802	-1.414970
H	2.239833	-1.524147	-2.175871
C	4.546315	-2.461827	0.776992
H	2.760705	-3.145753	1.761880
C	5.103626	-1.887104	-0.366165
H	4.652818	-1.090156	-2.310719
H	5.190009	-2.726405	1.612326
C	-1.985850	-1.668582	-0.352480

C	-1.965971	-1.104815	0.914851
C	-2.587510	-1.028590	-1.430076
C	-2.579152	0.130789	1.106984
H	-1.474984	-1.624127	1.732057
C	-3.197266	0.202276	-1.219378
H	-2.577810	-1.491486	-2.412297
C	-3.198521	0.795593	0.047016
H	-2.572794	0.583954	2.094084
H	-3.681633	0.710642	-2.048885
C	6.585281	-1.589356	-0.460790
H	7.107474	-2.110915	0.347668
H	6.980454	-1.968611	-1.408559
C	-3.905683	2.116674	0.263813
H	-3.585050	2.542357	1.219232
H	-3.623463	2.816897	-0.528099
C	6.865074	-0.104828	-0.368649
C	7.231831	0.634814	-1.493334
C	6.718481	0.563496	0.852697
C	7.452373	2.007454	-1.409946
H	7.351357	0.132569	-2.449295
C	6.937179	1.929674	0.954150
H	6.428229	0.001622	1.737152
C	7.304646	2.651930	-0.185479
H	7.738677	2.581272	-2.284744
H	6.826858	2.444054	1.904137
C	-5.408936	1.939141	0.260709
C	-6.051321	1.356028	1.356809
C	-6.176220	2.308234	-0.846489
C	-7.424666	1.147531	1.354430
H	-5.466688	1.060968	2.224471
C	-7.552067	2.105283	-0.865659
H	-5.692382	2.764818	-1.705532
C	-8.173742	1.522254	0.238959
H	-7.923823	0.696857	2.205407
H	-8.145937	2.394877	-1.727194
N	7.534116	4.035757	-0.124871
N	-9.559162	1.298535	0.261034
C	7.516536	4.915926	0.696806
C	-10.515316	1.464535	-0.451398
O	7.536611	5.863465	1.392663
O	-11.526546	1.568794	-1.042247

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Geometry with 35 atoms:

Total energy: -990.058970833

N	3.865182	0.830506	-0.714931
C	5.128658	-0.154714	-0.909873
O	4.803684	-1.291765	-1.204157
O	6.182123	0.452403	-0.735843
O	5.322649	2.483656	1.054249
H	5.996502	1.948444	0.601780
H	4.191449	1.586304	-0.078837
H	3.694645	1.245002	-1.637665
H	5.411735	3.361787	0.660707
C	2.666888	0.190892	-0.211474
C	2.440411	0.178265	1.157240
C	1.795048	-0.432368	-1.097429
C	1.308393	-0.469041	1.647054
H	3.136965	0.672593	1.828275
C	0.670288	-1.072322	-0.593764
H	1.998076	-0.410143	-2.163907
C	0.416083	-1.103402	0.782216
H	1.119446	-0.481420	2.716414
H	-0.024156	-1.553688	-1.277475
C	-0.816851	-1.807051	1.311973
H	-0.776489	-2.865379	1.033861
H	-0.814638	-1.754064	2.404822
C	-2.093580	-1.202802	0.771278
C	-2.543142	0.036951	1.241275
C	-2.827081	-1.844492	-0.226818
C	-3.696320	0.619147	0.735014
H	-1.980680	0.550953	2.016734
C	-3.983942	-1.272135	-0.749094
H	-2.491606	-2.807523	-0.601268
C	-4.416589	-0.040852	-0.265577
H	-4.047544	1.577272	1.106004
H	-4.552845	-1.772422	-1.525222
N	-5.588068	0.515486	-0.803020
C	-6.259806	1.504960	-0.659275
O	-6.999880	2.417471	-0.621128

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Geometry with 38 atoms:

Total energy: -1066.466989430

N	3.491066	0.321025	-0.675070
C	4.812792	-0.514385	-0.456152
O	4.691906	-1.458613	0.307014
O	5.747758	-0.029092	-1.102267

O	3.964641	2.473846	0.850446
H	4.906401	2.607691	0.580846
H	3.639746	1.220495	-0.111028
H	3.475764	0.578286	-1.666165
O	6.486308	2.493289	-0.106187
H	6.324590	1.631135	-0.535049
H	3.489821	3.233692	0.487579
H	7.072624	2.283257	0.632617
C	2.255245	-0.320676	-0.277347
C	1.900020	-0.313313	1.064846
C	1.463611	-0.950672	-1.231228
C	0.723355	-0.947056	1.455264
H	2.536550	0.183553	1.790773
C	0.290456	-1.576233	-0.827298
H	1.763463	-0.946047	-2.275106
C	-0.091305	-1.585310	0.518093
H	0.436790	-0.948109	2.503037
H	-0.340254	-2.063937	-1.566120
C	-1.392173	-2.239941	0.931962
H	-1.397100	-2.374664	2.017744
H	-1.467517	-3.229703	0.471626
C	-2.585185	-1.406080	0.515966
C	-2.895195	-0.228671	1.205932
C	-3.370728	-1.765058	-0.579776
C	-3.962817	0.568902	0.819493
H	-2.290224	0.065927	2.059870
C	-4.444372	-0.974951	-0.982129
H	-3.144181	-2.676534	-1.125810
C	-4.738153	0.190992	-0.281041
H	-4.203823	1.479179	1.360248
H	-5.055496	-1.255423	-1.833132
N	-5.826837	0.969096	-0.704130
C	-6.378295	1.993997	-0.395072
O	-7.005649	2.969456	-0.202333

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Geometry with 61 atoms:

Total energy: -1638.866812290

N	-0.409208	-2.348458	-0.251618
C	-0.276264	-3.189434	-1.324238
O	-1.228972	-3.703269	-1.916702
N	1.010193	-3.445041	-1.731626
H	2.087305	-0.804159	1.157143
H	1.066048	-3.815527	-2.672310

O	1.635944	-0.202722	0.547442
H	0.372999	-1.735442	-0.021382
H	2.160967	-0.278500	-0.263587
C	-1.645960	-1.992493	0.324582
C	-2.713028	-2.888139	0.430183
C	-1.775034	-0.707135	0.864144
C	-3.896603	-2.483067	1.042244
H	-2.616910	-3.893659	0.041668
C	-2.957911	-0.323566	1.481439
H	-0.940439	-0.016011	0.795193
C	-4.040805	-1.202147	1.575852
H	-4.720540	-3.188148	1.117110
H	-3.045899	0.680031	1.891098
C	2.204954	-2.969176	-1.136262
C	3.101781	-2.205661	-1.888680
C	2.506449	-3.279549	0.190252
C	4.278835	-1.745744	-1.309040
H	2.866428	-1.972330	-2.922704
C	3.680021	-2.796670	0.765677
H	1.820111	-3.890735	0.767984
C	4.581310	-2.025851	0.028762
H	4.967063	-1.146735	-1.899805
H	3.902455	-3.032767	1.802704
C	-5.343017	-0.750135	2.201663
H	-5.954108	-1.627969	2.434303
H	-5.140201	-0.227943	3.141951
C	5.862131	-1.517434	0.651237
H	6.715932	-2.046328	0.213157
H	5.857109	-1.766031	1.718573
C	-6.110485	0.172944	1.279154
C	-6.174318	1.546822	1.521446
C	-6.737272	-0.334231	0.136907
C	-6.847876	2.399203	0.652612
H	-5.693810	1.957871	2.405071
C	-7.415758	0.502238	-0.739946
H	-6.691800	-1.400811	-0.068721
C	-7.469184	1.871501	-0.479240
H	-6.897226	3.466767	0.844967
H	-7.904664	0.107751	-1.624209
C	6.081864	-0.028265	0.484179
C	7.346569	0.468294	0.159205
C	5.037574	0.882094	0.675555
C	7.574906	1.833987	0.034886
H	8.167454	-0.225218	-0.000679

C	5.249060	2.250209	0.554431
H	4.040013	0.519922	0.909845
C	6.520254	2.725026	0.234841
H	8.559649	2.213372	-0.220714
H	4.438683	2.955905	0.702047
N	-8.162180	2.695237	-1.380322
N	6.705216	4.111439	0.114950
C	-8.440097	3.859044	-1.512843
C	7.592996	4.883513	-0.142013
O	8.362770	5.741176	-0.374553
O	-8.779160	4.956987	-1.762478

6-II

Geometry with 64 atoms:

Total energy: -1715.264140900

N	0.849334	-2.226725	-0.038183
C	0.091528	-2.890059	-0.956134
O	0.549125	-3.553278	-1.883239
N	-1.298993	-2.814086	-0.769885
H	-1.523569	-3.922317	0.897313
H	-1.733034	-3.300040	-1.550756
O	-1.487584	-4.326077	1.784192
H	-0.370541	-3.204932	2.579599
H	-0.960883	-5.126418	1.657274
O	0.270607	-2.512151	2.852594
H	0.460050	-2.082057	0.894866
H	-0.233646	-1.926235	3.430996
C	2.259410	-2.142904	-0.136142
C	2.884753	-1.871276	-1.357005
C	3.030733	-2.271653	1.019080
C	4.267200	-1.748211	-1.411304
H	2.288977	-1.754827	-2.255085
C	4.414723	-2.135127	0.950110
H	2.542233	-2.480173	1.965436
C	5.053711	-1.878339	-0.262989
H	4.746212	-1.535673	-2.364085
H	5.006044	-2.238866	1.856268
C	-1.957568	-1.565798	-0.494969
C	-1.980279	-1.023531	0.785943
C	-2.619692	-0.910459	-1.536936
C	-2.629219	0.189467	1.012665
H	-1.495978	-1.541207	1.606894
C	-3.284258	0.284309	-1.294428
H	-2.605490	-1.342482	-2.533601

C	-3.287425	0.857852	-0.018763
H	-2.631592	0.613881	2.013001
H	-3.801566	0.786450	-2.108344
C	6.552782	-1.674689	-0.331229
H	7.025615	-2.177997	0.517774
H	6.944960	-2.123223	-1.248885
C	-4.034540	2.149999	0.235016
H	-3.718354	2.563145	1.197679
H	-3.781341	2.879100	-0.540862
C	6.904734	-0.202108	-0.306400
C	7.220110	0.483675	-1.480204
C	6.868956	0.511287	0.896806
C	7.495712	1.848229	-1.462047
H	7.254133	-0.055935	-2.422695
C	7.142627	1.871396	0.932972
H	6.622923	-0.008507	1.819341
C	7.455269	2.539472	-0.254466
H	7.742862	2.380825	-2.374042
H	7.118987	2.421842	1.868649
C	-5.532546	1.932191	0.240695
C	-6.147113	1.287413	1.318420
C	-6.323091	2.329464	-0.839889
C	-7.515510	1.049124	1.324846
H	-5.544249	0.968774	2.165078
C	-7.694317	2.096329	-0.850774
H	-5.860514	2.831479	-1.685183
C	-8.288114	1.454802	0.236521
H	-7.993865	0.553154	2.162434
H	-8.305563	2.407226	-1.692608
N	7.737498	3.914600	-0.261502
N	-9.668345	1.201467	0.268021
C	7.794050	4.830259	0.518203
C	-10.638619	1.378044	-0.422230
O	7.884452	5.806356	1.167563
O	-11.660765	1.486807	-0.993336

TS2P-3-I

Geometry with 35 atoms:

Total energy: -990.013048273

N	-3.648264	-0.501363	0.952506
C	-4.536808	-0.804921	0.060063
O	-5.600564	-1.607302	0.657072
H	-5.608431	-1.501400	1.623327
O	-4.735118	-0.613526	-1.146829

H	-7.054150	-0.790548	-1.454026
H	-6.608764	-1.392723	0.097219
O	-7.528840	-1.137903	-0.677198
H	-8.062946	-0.401895	-0.336875
C	-2.512779	0.239442	0.596804
C	-2.131254	0.624588	-0.701566
C	-1.666096	0.616867	1.655476
C	-0.959746	1.349144	-0.911362
H	-2.749565	0.356597	-1.547212
C	-0.501077	1.337481	1.435108
H	-1.947701	0.327379	2.663588
C	-0.125629	1.719849	0.143370
H	-0.690422	1.633102	-1.926603
H	0.130113	1.609134	2.278453
C	1.180142	2.446318	-0.104759
H	1.102061	3.033320	-1.025200
H	1.380056	3.138593	0.718981
C	2.331399	1.470462	-0.228512
C	3.120227	1.145159	0.878672
C	2.587156	0.826408	-1.442030
C	4.137555	0.202667	0.783814
H	2.937626	1.637665	1.830154
C	3.601095	-0.117698	-1.554740
H	1.983433	1.068559	-2.312760
C	4.374075	-0.430594	-0.437559
H	4.748813	-0.046445	1.646127
H	3.800284	-0.614976	-2.497988
N	5.390015	-1.389767	-0.575394
C	6.224980	-1.924745	0.107486
O	7.078007	-2.518895	0.657134

TS2p-3

Geometry with 32 atoms:

Total energy: -913.580487960

N	4.410611	0.329517	-0.569371
C	4.678710	1.341047	0.145503
O	5.934640	2.054413	-0.060762
H	6.025787	2.426290	-0.960088
O	4.186072	2.056653	1.087879
H	5.330745	2.670048	0.723794
C	3.187305	-0.348719	-0.355108
C	2.541208	-0.430998	0.886861
C	2.627909	-1.016025	-1.448215
C	1.354725	-1.144238	1.010625

H	2.973648	0.056678	1.753552
C	1.437578	-1.723647	-1.314540
H	3.136930	-0.969754	-2.405871
C	0.781731	-1.797364	-0.084607
H	0.862215	-1.198059	1.979102
H	1.015145	-2.231711	-2.177722
C	-0.536469	-2.527127	0.061036
H	-0.676135	-3.191593	-0.797828
H	-0.520174	-3.148618	0.961625
C	-1.700530	-1.562846	0.148926
C	-2.387596	-1.366225	1.346667
C	-2.086039	-0.819631	-0.973378
C	-3.438947	-0.456661	1.431178
H	-2.101223	-1.934139	2.227431
C	-3.132128	0.089102	-0.907320
H	-1.557244	-0.956966	-1.913452
C	-3.809372	0.268841	0.302884
H	-3.972947	-0.305545	2.363114
H	-3.430756	0.661548	-1.780567
N	-4.873560	1.177968	0.411227
C	-5.472413	1.953537	-0.288577
O	-6.135636	2.740828	-0.856827

TS2p-3-II

Geometry with 38 atoms:

Total energy: -1066.437456760

N	-3.719090	-1.258599	-0.534117
C	-4.269239	-0.158853	-0.288117
O	-3.059754	1.093196	0.196737
H	-2.193253	0.934568	-0.210412
O	-5.325594	0.415529	-0.265066
H	-5.837611	1.787649	1.006696
H	-4.863045	3.235126	0.026738
O	-5.971049	2.711230	1.280425
H	-6.856516	2.924098	0.957108
H	-3.432412	1.969961	-0.179339
O	-4.142295	3.244441	-0.647531
H	-4.579976	2.987336	-1.471162
C	-2.371256	-1.597002	-0.334220
C	-1.732459	-1.403651	0.898960
C	-1.670661	-2.220074	-1.369434
C	-0.412745	-1.801106	1.070339
H	-2.280741	-0.945341	1.716165
C	-0.349033	-2.616618	-1.184915

H	-2.169405	-2.386902	-2.318773
C	0.299535	-2.412990	0.033927
H	0.074161	-1.638795	2.029315
H	0.184222	-3.096997	-2.001119
C	1.748993	-2.804229	0.230605
H	2.056858	-3.464079	-0.586476
H	1.858930	-3.359692	1.167201
C	2.649859	-1.588316	0.268449
C	2.917037	-0.874024	-0.905282
C	3.194517	-1.129065	1.467844
C	3.711372	0.263520	-0.887800
H	2.494990	-1.217082	-1.846765
C	3.991731	0.012277	1.503935
H	2.996151	-1.671354	2.388235
C	4.249064	0.705687	0.325043
H	3.921501	0.813342	-1.800272
H	4.415565	0.368374	2.436707
N	5.057973	1.850618	0.386179
C	5.506593	2.688628	-0.351926
O	6.006011	3.564426	-0.957405

TS2-4

Geometry with 32 atoms:

Total energy: -913.596040931

N	4.236467	0.782930	0.634942
C	5.247630	0.990202	-0.176183
O	5.633728	0.772865	-1.299280
H	5.109479	1.547464	1.388514
O	6.102515	1.738803	0.810344
H	6.263535	2.659248	0.526552
C	3.094625	0.029975	0.326926
C	2.119441	-0.110331	1.323752
C	2.887917	-0.578616	-0.916071
C	0.967327	-0.843111	1.080463
H	2.280079	0.363367	2.287184
C	1.725307	-1.311664	-1.144536
H	3.629707	-0.477086	-1.699386
C	0.752086	-1.461046	-0.156777
H	0.217830	-0.939251	1.862795
H	1.576050	-1.779502	-2.114320
C	-0.508919	-2.262021	-0.407255
H	-0.533637	-3.129663	0.260966
H	-0.486194	-2.644535	-1.432852
C	-1.764085	-1.445107	-0.196316

C	-2.071862	-0.390521	-1.064677
C	-2.622223	-1.699392	0.873502
C	-3.207395	0.383484	-0.877902
H	-1.408420	-0.175138	-1.898689
C	-3.765163	-0.929921	1.077875
H	-2.396980	-2.512590	1.557872
C	-4.055445	0.109656	0.200069
H	-3.447186	1.198286	-1.554477
H	-4.431997	-1.129210	1.909852
N	-5.213244	0.872488	0.422368
C	-5.784524	1.805546	-0.081351
O	-6.439134	2.701819	-0.469100

TS2-4-I

Geometry with 35 atoms:

Total energy: -990.034695271

N	-3.903669	0.506612	-0.073276
C	-4.775877	0.035173	-0.844443
O	-5.261346	-0.769489	-1.565172
H	-4.376341	2.076818	1.069812
O	-6.043405	1.477943	-0.868006
H	-6.917131	1.075726	-0.748422
H	-5.869872	2.039474	-0.069623
O	-5.048220	2.758416	1.262673
H	-4.670914	3.571978	0.901367
C	-2.713347	-0.230355	0.163351
C	-2.367040	-1.401438	-0.514824
C	-1.843777	0.282507	1.132128
H	-3.029122	-1.813912	-1.269268
C	-1.164304	-2.041492	-0.223318
C	-0.649389	-0.365542	1.413555
H	-2.120633	1.192929	1.655995
C	-0.290468	-1.538047	0.740461
H	-0.903249	-2.950913	-0.758209
H	0.021010	0.046199	2.164470
C	1.038021	-2.205835	1.027051
H	1.156109	-2.348542	2.105981
H	1.051312	-3.194655	0.558033
C	2.195354	-1.379449	0.508150
C	3.026387	-0.671967	1.379212
C	2.425133	-1.276150	-0.867260
C	4.063315	0.120486	0.897531
H	2.862031	-0.741904	2.450989
C	3.457915	-0.492315	-1.364947

H	1.782918	-1.817544	-1.557609
C	4.275598	0.208285	-0.478271
H	4.707712	0.669930	1.577289
H	3.638563	-0.414647	-2.431674
N	5.309290	0.997928	-1.006733
C	6.179140	1.729823	-0.609912
O	7.064006	2.462526	-0.359478

TS2-4-II

Geometry with 38 atoms:

Total energy: -1066.441943580

N	-3.666812	0.275592	-0.373099
C	-3.813231	1.388623	-0.926392
O	-3.513783	2.371553	-1.507453
H	-5.059069	-0.774110	0.336524
O	-5.768853	1.614298	-0.672748
H	-5.938333	2.544276	-0.882616
O	-5.711001	-1.278390	0.868129
H	-6.188788	0.199573	1.724728
H	-6.434201	-1.459353	0.253327
O	-6.312265	1.160444	1.894980
H	-5.974628	1.513882	0.298594
H	-7.269243	1.274272	1.967248
C	-2.374209	-0.317676	-0.320612
C	-2.258446	-1.506823	0.402188
C	-1.243994	0.216577	-0.945793
C	-1.028114	-2.144924	0.503268
H	-3.138893	-1.920565	0.883829
C	-0.020078	-0.436607	-0.841296
H	-1.315130	1.139077	-1.513458
C	0.110420	-1.624553	-0.117369
H	-0.951537	-3.066364	1.074503
H	0.849471	-0.007628	-1.332014
C	1.429222	-2.368947	-0.033837
H	1.428206	-2.971862	0.881031
H	1.496674	-3.075379	-0.869540
C	2.648009	-1.477385	-0.051307
C	2.854025	-0.535921	0.965228
C	3.585828	-1.560443	-1.079895
C	3.966999	0.292017	0.961454
H	2.128557	-0.449932	1.770162
C	4.709677	-0.737534	-1.099193
H	3.439705	-2.281447	-1.879043
C	4.898294	0.186715	-0.076730

H	4.123430	1.019543	1.752166
H	5.438618	-0.807434	-1.899291
N	6.038467	1.004674	-0.113754
C	6.545548	1.870796	0.552117
O	7.143887	2.719357	1.103446

TS3p-4p

Geometry with 32 atoms:

Total energy: -913.609868630

N	-4.261293	-0.760446	-0.694387
C	-5.193978	-1.171068	0.131174
O	-6.043717	-1.867500	-0.549601
H	-5.146682	-1.485040	-1.379470
O	-5.283677	-0.947898	1.421319
H	-6.075030	-1.389156	1.774777
C	-3.115801	0.014275	-0.473017
C	-2.202836	0.134973	-1.529331
C	-2.851619	0.676605	0.731341
C	-1.048777	0.889621	-1.378080
H	-2.411977	-0.372770	-2.465572
C	-1.687231	1.429434	0.867083
H	-3.548722	0.611712	1.558030
C	-0.770927	1.551028	-0.177352
H	-0.347856	0.968168	-2.206059
H	-1.494493	1.939065	1.807815
C	0.512676	2.336444	-0.013041
H	0.663224	2.986565	-0.880598
H	0.431380	2.976234	0.871395
C	1.709593	1.421203	0.133245
C	2.621832	1.249297	-0.910260
C	1.898841	0.695693	1.313264
C	3.699169	0.378223	-0.785851
H	2.489956	1.805780	-1.834262
C	2.970455	-0.176093	1.455275
H	1.193002	0.815109	2.131468
C	3.870424	-0.334165	0.401110
H	4.408134	0.248763	-1.598167
H	3.120095	-0.735222	2.372669
N	4.944725	-1.222544	0.568254
C	5.889475	-1.625536	-0.059978
O	6.843292	-2.098086	-0.559543

TS3p-4p-I

Geometry with 35 atoms:

Total energy: -990.059952837

N	-4.035255	0.297365	-0.180911
C	-4.330770	1.429951	0.407187
O	-5.493517	1.965107	0.291177
H	-6.127386	1.173736	-0.493106
O	-3.420030	2.094453	1.130958
H	-3.833611	2.914138	1.446883
O	-6.267116	0.275755	-1.200472
H	-5.241632	-0.010688	-0.920996
H	-6.874900	-0.353072	-0.781611
C	-2.788077	-0.346506	-0.074923
C	-2.309281	-1.020979	-1.202478
C	-2.046664	-0.419760	1.114049
C	-1.111658	-1.728051	-1.154387
H	-2.889902	-0.985413	-2.119505
C	-0.848897	-1.122987	1.149091
H	-2.416035	0.065591	2.010148
C	-0.360960	-1.788179	0.020392
H	-0.758579	-2.245442	-2.042932
H	-0.283022	-1.164843	2.077291
C	0.960886	-2.524903	0.076049
H	1.049983	-3.168663	-0.804912
H	0.988200	-3.168711	0.960884
C	2.132980	-1.568659	0.126558
C	2.496320	-0.837667	-1.010851
C	2.846752	-1.363387	1.307324
C	3.547303	0.067371	-0.976183
H	1.946074	-0.982296	-1.937441
C	3.902499	-0.456808	1.360611
H	2.577412	-1.922370	2.199148
C	4.251039	0.256035	0.217246
H	3.829775	0.630059	-1.861071
H	4.457331	-0.298493	2.279134
N	5.321447	1.161282	0.293130
C	5.909209	1.925330	-0.428419
O	6.564270	2.702328	-1.019795

TS3p-4p-II

Geometry with 38 atoms:

Total energy: -1066.471772400

N	-3.752916	0.298046	0.050446
C	-3.994811	1.583569	0.147786
O	-5.151656	2.106837	0.115447
O	-2.953166	2.441185	0.263953

H	-3.326586	3.335823	0.292271
O	-5.657491	-1.266046	-0.586614
H	-4.815365	-0.651671	-0.310945
H	-6.525031	-0.362974	-0.418913
O	-7.086201	0.619355	-0.209490
H	-6.267845	1.293824	-0.061297
H	-7.543448	0.894672	-1.018158
H	-5.758678	-1.922770	0.117666
C	-2.460956	-0.254028	0.151674
C	-1.506608	0.145739	1.101345
C	-2.154326	-1.338691	-0.677828
C	-0.283786	-0.507052	1.187173
H	-1.732051	0.962976	1.777054
C	-0.927300	-1.989600	-0.579975
H	-2.893099	-1.668189	-1.403114
C	0.027760	-1.586165	0.352763
H	0.443938	-0.179153	1.926589
H	-0.711758	-2.828644	-1.236796
C	1.362668	-2.289208	0.469689
H	1.374175	-3.143276	-0.216518
H	1.483850	-2.691063	1.481336
C	2.536723	-1.383837	0.164325
C	3.547349	-1.172724	1.104196
C	2.629733	-0.736924	-1.072438
C	4.631448	-0.347047	0.823193
H	3.488148	-1.663172	2.071890
C	3.705588	0.088845	-1.370506
H	1.846355	-0.882622	-1.811880
C	4.708179	0.281490	-0.419264
H	5.414438	-0.187047	1.558197
H	3.780305	0.586407	-2.331478
N	5.785468	1.119507	-0.747883
C	6.803384	1.521207	-0.245804
O	7.819078	1.984989	0.122726

TS3p-4p-III

Geometry with 41 atoms:

Total energy: -1142.864759360

N	-3.275429	0.358199	-0.131955
C	-3.403391	1.661428	-0.125926
O	-4.515612	2.272047	-0.080679
O	-2.288607	2.437335	-0.217972
H	-2.589103	3.358530	-0.190635
O	-5.138717	-1.091030	-1.268584

H	-4.434433	-0.493728	-0.808896
H	-6.324751	-0.921760	-0.478665
O	-7.112830	-0.715944	0.188029
H	-6.730656	0.229292	0.779345
O	-6.230038	1.181358	1.361337
H	-5.520397	1.617668	0.732151
H	-6.909760	1.851688	1.522140
H	-7.877142	-0.451875	-0.345110
H	-5.292276	-0.681605	-2.131293
C	-2.011760	-0.259022	-0.081604
C	-1.755695	-1.333309	-0.941575
C	-1.026140	0.083198	0.858463
C	-0.547652	-2.023783	-0.883032
H	-2.517549	-1.620596	-1.660574
C	0.175521	-0.610997	0.909642
H	-1.213756	0.896494	1.552237
C	0.437597	-1.676729	0.041346
H	-0.370064	-2.848996	-1.568336
H	0.925727	-0.324294	1.643586
C	1.739824	-2.447776	0.126989
H	1.733693	-3.085958	1.018017
H	1.809928	-3.114978	-0.739071
C	2.958439	-1.554477	0.179766
C	3.259318	-0.705657	-0.892843
C	3.794446	-1.536956	1.296028
C	4.365712	0.130190	-0.858352
H	2.613706	-0.700944	-1.767420
C	4.908248	-0.701979	1.349068
H	3.572996	-2.184959	2.139380
C	5.191624	0.129843	0.270663
H	4.598524	0.783346	-1.694015
H	5.555467	-0.689882	2.219291
N	6.318644	0.963295	0.345298
C	6.879071	1.786730	-0.331165
O	7.520351	2.602218	-0.884674

TS4pp-5

Geometry with 32 atoms:

Total energy: -913.613436992

N	4.292018	0.689262	-0.968111
C	5.227318	1.197672	0.105613
O	5.774777	0.530059	0.946291
H	4.806124	0.161509	-1.678891
O	5.194900	2.457534	-0.158452

H	4.394050	1.977699	-1.031123
C	3.134146	-0.029844	-0.504457
C	2.822695	-1.275192	-1.031735
C	2.326621	0.555700	0.470747
C	1.685330	-1.942722	-0.579327
H	3.463261	-1.718429	-1.788608
C	1.202824	-0.124007	0.917208
H	2.577114	1.536250	0.867520
C	0.867246	-1.381029	0.399743
H	1.437969	-2.916974	-0.991489
H	0.567245	0.328815	1.674019
C	-0.381267	-2.090122	0.881270
H	-0.401231	-3.101339	0.463722
H	-0.352572	-2.181898	1.971670
C	-1.634902	-1.344676	0.478176
C	-2.059107	-1.351165	-0.854085
C	-2.366730	-0.604611	1.409395
C	-3.186020	-0.642739	-1.250653
H	-1.496512	-1.918638	-1.591268
C	-3.495991	0.112923	1.028561
H	-2.051342	-0.590633	2.449048
C	-3.902659	0.091739	-0.305736
H	-3.517335	-0.650283	-2.283393
H	-4.063329	0.686176	1.755594
N	-5.035347	0.801758	-0.733159
C	-5.880093	1.523216	-0.269139
O	-6.759253	2.234875	0.051986

TS4pp-5-I

Geometry with 35 atoms:

Total energy: -990.037559402

N	3.893632	0.802345	-0.541842
C	5.223569	0.117180	-0.382938
O	5.240062	-1.104290	-0.281433
O	6.182935	0.940069	-0.358653
O	4.828495	2.752758	0.644593
H	5.643635	2.237778	0.271745
H	4.139116	1.977269	0.196285
H	3.860891	1.166378	-1.498242
H	4.740538	3.586048	0.153582
C	2.720685	0.030832	-0.254686
C	2.551341	-0.503890	1.020050
C	1.734379	-0.142768	-1.222784
C	1.394525	-1.217376	1.317876

H	3.321963	-0.359189	1.771568
C	0.577977	-0.849096	-0.910503
H	1.874096	0.278454	-2.214581
C	0.394317	-1.401274	0.360261
H	1.264965	-1.635925	2.312081
H	-0.192234	-0.975002	-1.667252
C	-0.861570	-2.185888	0.684520
H	-0.864239	-3.120444	0.113135
H	-0.845137	-2.455474	1.745257
C	-2.124667	-1.416675	0.370575
C	-2.479460	-0.298278	1.134939
C	-2.941979	-1.778490	-0.700196
C	-3.620636	0.435354	0.844771
H	-1.850418	0.000241	1.969827
C	-4.089197	-1.051026	-1.007756
H	-2.679987	-2.642952	-1.303672
C	-4.426237	0.054864	-0.233329
H	-3.895304	1.299955	1.441634
H	-4.722588	-1.333498	-1.841606
N	-5.587042	0.772982	-0.560692
C	-6.197623	1.729258	-0.156722
O	-6.885738	2.638052	0.130930

TS4pp-5-II

Geometry with 38 atoms:

Total energy: -1066.454059760

N	3.543986	0.309500	-0.668411
C	4.825522	-0.440920	-0.436929
O	4.786881	-1.376668	0.361892
O	5.782147	0.040631	-1.085864
O	3.953601	2.373469	0.683582
H	4.958941	2.528860	0.492977
H	3.703603	1.430526	0.031704
H	3.532666	0.587758	-1.650896
O	6.386864	2.461201	0.047775
H	6.326026	1.604642	-0.432832
H	3.466253	3.138069	0.339217
H	6.937399	2.275111	0.821223
C	2.314154	-0.334937	-0.293479
C	2.004375	-0.478725	1.055362
C	1.430927	-0.788879	-1.270772
C	0.813063	-1.098661	1.423527
H	2.695437	-0.109578	1.806789
C	0.239318	-1.395391	-0.891333

H	1.680506	-0.666581	-2.321087
C	-0.079955	-1.568184	0.458717
H	0.574808	-1.219734	2.476669
H	-0.452048	-1.746494	-1.653554
C	-1.381690	-2.234174	0.854650
H	-1.381369	-2.402940	1.935842
H	-1.454240	-3.212125	0.367997
C	-2.584647	-1.401649	0.468992
C	-2.898672	-0.241140	1.185907
C	-3.381827	-1.748262	-0.622248
C	-3.982121	0.549706	0.830911
H	-2.284667	0.044300	2.036490
C	-4.470693	-0.963955	-0.994324
H	-3.151950	-2.646247	-1.188853
C	-4.769293	0.183355	-0.265371
H	-4.226993	1.445960	1.393045
H	-5.090306	-1.235431	-1.842084
N	-5.874891	0.955240	-0.655407
C	-6.438761	1.960510	-0.306296
O	-7.078985	2.918687	-0.073611

TS5p-6

Geometry with 58 atoms:

Total energy: -1562.386832350

N	1.249474	-3.122444	-0.675206
H	1.592238	-3.645160	-1.485358
H	0.191519	-3.607992	-0.155966
N	-0.872648	-2.865525	-0.497702
C	0.117715	-2.200575	-1.078202
O	0.263107	-1.178384	-1.728956
C	-2.235713	-2.543559	-0.561131
C	-2.742123	-1.485788	-1.332459
C	-3.125768	-3.328536	0.178244
C	-4.108805	-1.236597	-1.351787
H	-2.067178	-0.867525	-1.911282
C	-4.491459	-3.065742	0.147889
H	-2.735015	-4.145181	0.777531
C	-5.006241	-2.020192	-0.619900
H	-4.488755	-0.411419	-1.950359
H	-5.167925	-3.685873	0.730178
C	2.333605	-2.529426	0.059730
C	3.647696	-2.872925	-0.246490
C	2.055939	-1.632419	1.087227
C	4.688115	-2.311305	0.483818

H	3.848288	-3.573496	-1.051948
C	3.108154	-1.076043	1.808165
H	1.028549	-1.370700	1.324099
C	4.433531	-1.407614	1.519090
H	5.715294	-2.572818	0.242373
H	2.894549	-0.375260	2.610374
C	-6.492626	-1.731137	-0.662698
H	-6.870227	-1.886441	-1.679227
H	-7.010414	-2.444415	-0.012985
C	5.581511	-0.764749	2.268323
H	6.317891	-1.527716	2.538102
H	5.203495	-0.321139	3.194435
C	-6.818582	-0.319025	-0.229618
C	-7.297392	0.625546	-1.139759
C	-6.613678	0.075268	1.096605
C	-7.572562	1.930769	-0.744023
H	-7.460293	0.337213	-2.174595
C	-6.886946	1.372554	1.509577
H	-6.231979	-0.646278	1.814596
C	-7.367547	2.300321	0.584912
H	-7.945903	2.661893	-1.454768
H	-6.732570	1.676841	2.539233
C	6.254001	0.301075	1.429391
C	7.489561	0.068056	0.821635
C	5.620134	1.527545	1.209079
C	8.085163	1.031303	0.014156
H	7.995547	-0.879756	0.983598
C	6.202107	2.501257	0.407632
H	4.655245	1.720719	1.671273
C	7.436294	2.249227	-0.191453
H	9.046657	0.847352	-0.455775
H	5.712339	3.454351	0.239521
N	-7.637673	3.605033	1.027852
N	8.001818	3.248797	-0.998573
C	-8.042243	4.644291	0.573552
C	8.986543	3.423128	-1.668733
O	-8.421500	5.712487	0.261263
O	9.894837	3.722588	-2.352842

TS5p-6-I

Geometry with 61 atoms:

Total energy: -1638.819358850

N	1.017672	0.441194	0.043954
C	0.119590	0.198810	0.979721

O	0.069871	-0.598811	1.915132
N	-1.074188	1.112473	0.796982
H	-0.759709	1.876171	-0.163976
H	-1.199447	1.612191	1.681107
O	-0.109747	2.263714	-1.147180
H	0.615129	1.469631	-0.768520
H	0.267477	3.131641	-0.940901
C	2.231262	-0.256504	-0.076332
C	2.679428	-1.274621	0.775545
C	3.046469	0.116942	-1.158194
C	3.906389	-1.893082	0.535605
H	2.076161	-1.583453	1.617444
C	4.264618	-0.505032	-1.382103
H	2.701619	0.903804	-1.823612
C	4.715089	-1.526904	-0.538681
H	4.237369	-2.684382	1.203942
H	4.878544	-0.196700	-2.225384
C	-2.269055	0.346393	0.505314
C	-3.250706	0.167254	1.475151
C	-2.402195	-0.217088	-0.758911
C	-4.382927	-0.577447	1.165796
H	-3.124992	0.611401	2.458438
C	-3.537116	-0.968859	-1.051729
H	-1.626721	-0.064871	-1.504137
C	-4.537189	-1.159641	-0.096487
H	-5.158062	-0.712970	1.915813
H	-3.647395	-1.412008	-2.037385
C	6.063805	-2.175517	-0.768599
H	6.121027	-3.099490	-0.184564
H	6.171902	-2.442557	-1.824683
C	-5.783729	-1.957088	-0.418485
H	-5.903974	-2.761428	0.314296
H	-5.664427	-2.422177	-1.401945
C	7.198091	-1.254231	-0.372779
C	7.967195	-0.599615	-1.337325
C	7.466915	-1.006504	0.976958
C	8.981809	0.279278	-0.972867
H	7.772396	-0.781401	-2.390773
C	8.477947	-0.133981	1.358474
H	6.873910	-1.504276	1.740175
C	9.234942	0.509866	0.379489
H	9.577843	0.785156	-1.726530
H	8.688798	0.055138	2.405538
C	-7.025501	-1.091977	-0.409082

C	-7.992165	-1.228071	0.589237
C	-7.210162	-0.112476	-1.390228
C	-9.120258	-0.414044	0.613202
H	-7.863333	-1.983556	1.359208
C	-8.331364	0.707032	-1.382291
H	-6.462785	0.010777	-2.170071
C	-9.286899	0.553913	-0.377206
H	-9.870581	-0.525097	1.390168
H	-8.476279	1.464178	-2.145211
N	10.250974	1.386605	0.791521
N	-10.410906	1.394336	-0.393736
C	11.089643	2.096837	0.300282
C	-11.412367	1.573380	0.250599
O	-12.421167	1.851954	0.786241
O	11.946207	2.824379	-0.045936

TS5p-6-II

Geometry with 64 atoms:

Total energy: -1715.222395330

N	0.886785	-2.579973	0.102926
C	0.123776	-2.913748	-0.918668
O	0.397457	-3.188081	-2.098096
N	-1.320155	-3.004363	-0.569301
H	-1.551236	-3.795368	0.547221
H	-1.754659	-3.439299	-1.384422
O	-1.721924	-4.329554	1.532120
H	-0.902702	-3.977748	2.103963
H	-1.605651	-5.282573	1.392608
O	0.290610	-3.340791	2.548647
H	0.531455	-2.938995	1.628992
H	0.097613	-2.597264	3.136326
C	2.259694	-2.354643	-0.111724
C	2.793884	-1.773937	-1.276058
C	3.144765	-2.655115	0.933359
C	4.156807	-1.526669	-1.381985
H	2.133665	-1.514631	-2.094812
C	4.509218	-2.407337	0.814715
H	2.750005	-3.093908	1.844962
C	5.040518	-1.844463	-0.345853
H	4.545881	-1.071868	-2.290911
H	5.171912	-2.659920	1.639064
C	-1.937303	-1.709014	-0.360294
C	-1.902452	-1.116558	0.897314
C	-2.562418	-1.062106	-1.426017

C	-2.492865	0.131350	1.084879
H	-1.416407	-1.628689	1.721127
C	-3.157964	0.177283	-1.224100
H	-2.579713	-1.534613	-2.404377
C	-3.126560	0.791788	0.031255
H	-2.462258	0.595641	2.066770
H	-3.653484	0.677545	-2.052488
C	6.518199	-1.538665	-0.472316
H	7.060270	-2.058518	0.324252
H	6.896108	-1.914294	-1.428555
C	-3.814261	2.124256	0.243309
H	-3.483276	2.551076	1.194902
H	-3.526144	2.817497	-0.552876
C	6.793209	-0.052865	-0.383499
C	7.144099	0.688351	-1.512176
C	6.658763	0.614949	0.839622
C	7.360964	2.061783	-1.431110
H	7.254044	0.186693	-2.469609
C	6.873986	1.981793	0.938870
H	6.380450	0.052129	1.727301
C	7.225417	2.705561	-0.204924
H	7.635240	2.636675	-2.309041
H	6.773145	2.495700	1.890196
C	-5.319970	1.970058	0.248059
C	-5.964478	1.388619	1.344023
C	-6.089073	2.357700	-0.851476
C	-7.340480	1.199069	1.348639
H	-5.378671	1.079211	2.205933
C	-7.467763	2.173499	-0.864000
H	-5.604283	2.813327	-1.710509
C	-8.090906	1.591155	0.240010
H	-7.840767	0.749363	2.199479
H	-8.062582	2.476334	-1.720337
N	7.450555	4.090241	-0.146804
N	-9.479051	1.385085	0.268207
C	7.436215	4.971123	0.674111
C	-10.436312	1.562755	-0.439811
O	7.458356	5.919342	1.369044
O	-11.448893	1.679552	-1.026124