Supplementary Material for PCCP

"Mechanistic Aspects of Proton Chain Transfer in the Green Fluorescent Protein. II: A Comparison of Minimal Quantum Chemical Models"

Supplementary Material

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1. The results for the three-step chain model with His-148 attached to the phenolic oxygen.

The differences between the model in Figure S1 (named model 1s) and the model 1b in Figure 1 is the His-148 function group added to the phenolic oxygen. With His-148 interacted with the phenolic oxygen, it can reduce the reaction barrier, and obviously, stabilize the anionic for the proton transfer process.

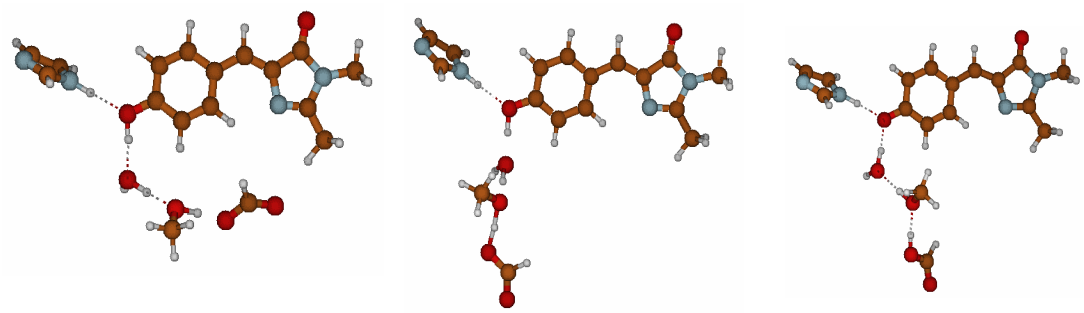

Figure S1: Stationary structures for the proton transfer in model 1s

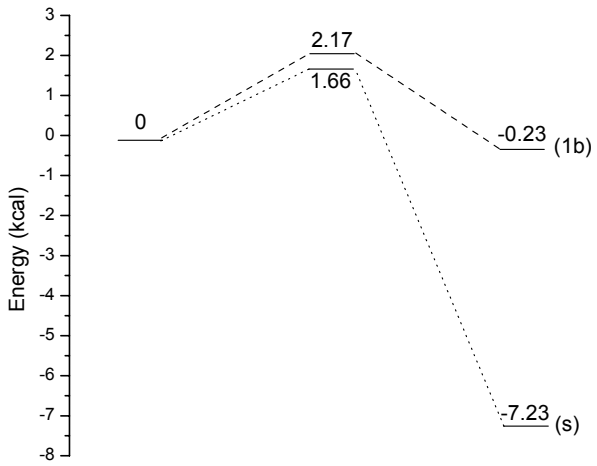

Figure S2: Potential energy profiles associated with the optimized stationary points for proton chain transfer in clusters 1b of Figure 1 and 1s of Figure S1. Energies in kcal.

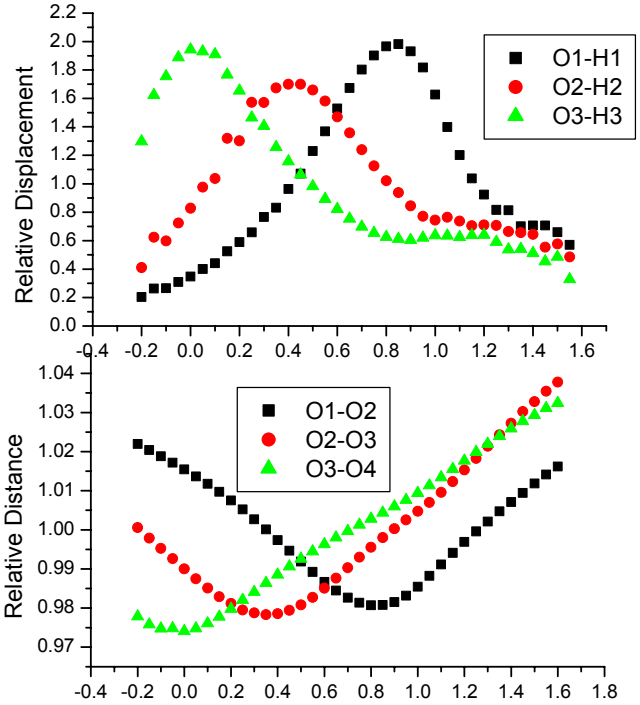

Figure S3: Plot of the relative displacement (D_{OH}) parameter for each of the three protons in the proton wire and the corresponding relative separation (D_{OO}) parameters as a function of reaction coordinate for model 1s of Figure S1. Squares represent the phenolic proton on the chromophore, circles the bridging water proton and triangles the bridging methanol proton.

2. Absolute energies for the stationary points, namely neutral forms (N), the transition states (TS) and Anionic forms (A). (in a.u.)

System	N	TS	A
cluster 1b*	−1105. 9854131	−1105. 9819493	−1105. 9887506
cluster 1c	–1145.307871	–1145.306441	–1145.314235
cluster 1d	–1299.171544	–1299.162845	–1299.1617131
cluster 1e	–1525.423283	–1525.418196	–1525.4311639
cluster 1s	–1332.237762	–1332.235122	–1332.249288

* Further details for cluster 1b are to be found in reference 29.

3. The atomic coordinates for the stationary geometries, namely neutral forms (N) the transition states (TS) and Anionic forms (A).

1. the proton transfer reaction for cluster 1b

N-form

C	1.752441	1.349924	-0.592642
C	2.167923	2.658690	-0.906876
C	1.200580	3.673213	-1.038686
C	-0.142933	3.381849	-0.837670

C	-0.577693	2.079764	-0.493202
C	0.411587	1.071443	-0.383889
O	3.465535	2.981012	-1.091125
H	4.060100	2.214074	-0.867285
C	-1.985034	1.837388	-0.260504
C	-2.599658	0.687646	0.141564
C	-4.059843	0.563257	0.373408
N	-1.983282	-0.538510	0.425083
N	-4.194172	-0.767547	0.793963
C	-2.920318	-1.355160	0.801763
O	-4.985323	1.367551	0.254681
C	-5.456692	-1.373663	1.157285
H	-6.230890	-0.618144	1.003391
H	-5.464018	-1.684475	2.208167
C	-2.697633	-2.771914	1.208478
H	-3.075057	-2.951838	2.223335
H	-5.675298	-2.245309	0.530563
H	-1.625704	-3.001125	1.182860
O	5.115773	0.964030	-0.376669
H	2.482443	0.551014	-0.516759
H	4.736208	0.029476	-0.430044
H	5.447793	1.057898	0.523815
H	1.527043	4.677815	-1.290218
H	1.076268	-2.307245	-0.152194
H	-0.879900	4.176382	-0.936491
H	-3.229285	-3.460457	0.538313
H	0.109294	0.064381	-0.126372
H	-2.654409	2.683746	-0.410043
O	2.698346	-2.816422	0.947228
C	1.443901	-2.917688	0.711556
O	0.605218	-3.604267	1.320787
O	4.087105	-1.419862	-0.591761
C	4.621074	-2.274463	-1.582503
H	3.482545	-1.978923	0.071739
H	5.259385	-1.684926	-2.252009
H	3.826659	-2.738951	-2.185313
H	5.229565	-3.079019	-1.142363

TS

C	1.202658	-1.467747	-0.004688
C	1.502708	-2.844167	-0.220517
C	0.414922	-3.732612	-0.443319
C	-0.885712	-3.269435	-0.445183
C	-1.197262	-1.900530	-0.229348

C	-0.104307	-1.016893	-0.010062
O	2.727190	-3.324755	-0.220456
H	3.547022	-2.583326	-0.043699
C	-2.571878	-1.499489	-0.246558
C	-3.159066	-0.273235	-0.073024
C	-4.617691	-0.072434	-0.132079
N	-2.529193	0.957664	0.176988
N	-4.754346	1.310685	0.093298
C	-3.476723	1.843749	0.265918
O	-5.559751	-0.846748	-0.322816
C	-6.027241	1.996717	0.128762
H	-6.797799	1.242227	-0.047339
H	-6.093713	2.763239	-0.651949
C	-3.259263	3.297659	0.525079
H	-3.645446	3.917029	-0.295384
H	-6.204550	2.466662	1.103083
H	-2.187757	3.476496	0.625764
O	4.555846	-1.745449	0.194006
H	2.020605	-0.770956	0.161979
H	4.340899	-0.465530	0.557513
H	5.239349	-1.806222	-0.483422
H	0.641365	-4.781590	-0.608798
H	3.528819	2.709895	-1.043742
H	-1.701504	-3.969224	-0.616635
H	-3.761564	3.624560	1.444829
H	-0.311799	0.033981	0.155427
H	-3.291699	-2.297391	-0.428726
O	5.385709	2.358446	-0.290211
C	4.576272	3.071188	-1.046644
O	4.914468	4.039900	-1.703428
O	4.140043	0.536961	0.859096
C	4.127726	0.664545	2.267183
H	4.879942	1.581675	0.175263
H	5.043832	0.259635	2.722026
H	3.266517	0.135836	2.701901
H	4.048283	1.725285	2.532488

A-form

C	0.844014	1.145842	0.179801
C	1.507627	2.241400	-0.485216
C	0.655349	3.135595	-1.224773
C	-0.706544	2.945926	-1.282368
C	-1.355954	1.861393	-0.619587
C	-0.520453	0.967312	0.114998

O	2.775912	2.426353	-0.433909
H	3.743094	1.542107	0.327830
C	-2.769607	1.737796	-0.728278
C	-3.653183	0.815759	-0.208065
C	-5.096886	0.876275	-0.456578
N	-3.363110	-0.292975	0.605936
N	-5.585285	-0.243584	0.251256
C	-4.499779	-0.878947	0.849733
O	-5.809175	1.656006	-1.100962
C	-6.982163	-0.610037	0.300163
H	-7.521550	0.127072	-0.300205
H	-7.371782	-0.588301	1.325175
C	-4.664846	-2.108464	1.681288
H	-5.317909	-1.930481	2.545611
H	-7.153937	-1.607745	-0.121529
H	-3.682114	-2.417547	2.041625
O	4.434377	0.958820	0.825013
H	1.459282	0.449230	0.744207
H	4.647750	-0.544856	0.258901
H	4.264816	1.076275	1.766309
H	1.130724	3.967919	-1.736512
H	5.701307	-3.664721	1.530457
H	-1.320030	3.643297	-1.851602
H	-5.104372	-2.933133	1.105114
H	-0.986979	0.132930	0.627612
H	-3.262885	2.501867	-1.329634
O	6.921296	-2.834759	0.122086
C	6.704361	-3.738346	1.068791
O	7.514486	-4.575905	1.411471
O	4.741433	-1.458349	-0.146948
C	4.070835	-1.477544	-1.405902
H	6.103934	-2.248398	0.002909
H	4.542815	-0.794071	-2.123243
H	3.018087	-1.196260	-1.290242
H	4.124868	-2.497062	-1.798802

2. the proton transfer reaction for cluster 1c

N-form

C	2.087584	1.224616	1.053461
C	2.478270	2.577910	1.049207
C	1.492918	3.575689	1.179276
C	0.156474	3.219319	1.308461
C	-0.255277	1.865116	1.312898

C	0.753246	0.878060	1.184652
O	3.765962	2.960108	0.926168
C	-1.660719	1.548878	1.444808
C	-2.266513	0.326373	1.431794
C	-3.725170	0.118855	1.602438
N	-1.640872	-0.917134	1.270993
N	-3.849149	-1.276636	1.535482
C	-2.571399	-1.820597	1.336703
O	-4.657133	0.907222	1.768957
C	-5.107870	-1.979458	1.656339
C	-2.336750	-3.287866	1.218209
H	2.832417	0.444459	0.947409
H	1.800078	4.617177	1.175999
H	-0.594910	4.000285	1.407179
H	0.471953	-0.167114	1.188622
H	4.372801	2.170827	0.879420
H	-2.338274	2.392138	1.573551
H	-5.884124	-1.223489	1.797287
H	-5.106264	-2.656737	2.517771
H	-5.331000	-2.558595	0.753219
H	-2.655905	-3.809431	2.130037
H	-1.269799	-3.477305	1.053553
H	-2.911452	-3.711448	0.384176
O	5.449680	0.853545	0.898730
H	5.133620	0.009210	0.437949
H	5.693880	0.580923	1.791232
C	1.414231	-2.520466	-1.124230
O	2.909684	-2.801743	0.754654
C	1.787348	-3.150311	0.233406
O	0.968944	-3.945790	0.738062
H	1.126510	-3.311751	-1.825229
H	2.225230	-1.924016	-1.551599
H	0.539067	-1.876391	-0.982734
O	4.617833	-1.313316	-0.285133
C	5.565588	-2.115643	-0.957039
H	3.862453	-1.926111	0.131867
H	6.344488	-1.467638	-1.377867
H	5.102419	-2.675273	-1.783609
H	6.044744	-2.842548	-0.282734

TS

C	-0.911279	0.996315	1.319920
C	-1.271482	2.317032	1.697522
C	-0.443049	3.388838	1.283996

C	0.692420	3.147517	0.532746
C	1.068267	1.834769	0.146498
C	0.227473	0.769033	0.565588
O	-2.346231	2.600062	2.420806
C	2.260654	1.667931	-0.636559
C	2.849985	0.545023	-1.152724
C	4.092520	0.590813	-1.948250
N	2.416138	-0.786929	-1.043201
N	4.311337	-0.762990	-2.264792
C	3.279165	-1.508859	-1.694827
O	4.822428	1.520073	-2.298997
C	5.430715	-1.232227	-3.051949
C	3.206488	-2.992324	-1.842991
H	-1.538778	0.162637	1.624247
H	-0.723839	4.396377	1.575401
H	1.317733	3.983700	0.225896
H	0.491003	-0.243407	0.282554
H	-2.911087	1.761836	2.708105
H	2.801115	2.584674	-0.871893
H	6.025021	-0.353047	-3.312316
H	5.097327	-1.722828	-3.973735
H	6.056766	-1.930649	-2.484843
H	3.141982	-3.288820	-2.897369
H	2.317960	-3.350953	-1.321370
H	4.090461	-3.483988	-1.417658
O	-3.724048	0.651570	3.175068
H	-4.672207	0.760076	3.039141
H	-3.434202	-0.432632	2.896398
C	-3.904986	-2.343699	-0.465046
O	-4.858928	-3.046554	1.646746
C	-4.892217	-3.189277	0.333709
O	-5.688673	-3.937483	-0.224472
H	-3.814814	-2.745879	-1.475531
H	-2.929532	-2.291127	0.024930
H	-4.283213	-1.316494	-0.527918
H	-4.085228	-2.403699	2.018483
O	-3.071795	-1.602070	2.578769
C	-2.400692	-2.246224	3.635459
H	-2.986813	-2.239361	4.571061
H	-1.433136	-1.762643	3.847165
H	-2.197727	-3.297600	3.379386

A-form

C	-0.066136	-0.356128	-1.411188

C	0.489007	-0.254290	-2.738612
C	1.907078	-0.019025	-2.812316
C	2.673896	0.103071	-1.675799
C	2.118199	0.002992	-0.365201
C	0.712399	-0.232848	-0.281718
O	-0.220318	-0.361616	-3.802723
C	2.981408	0.140504	0.757637
C	2.738249	0.089220	2.114295
C	3.794877	0.261666	3.115875
N	1.508680	-0.124259	2.761081
N	3.095558	0.134594	4.335776
C	1.753475	-0.091789	4.039120
O	5.011879	0.469234	3.031010
C	3.726417	0.233186	5.631907
C	0.728268	-0.275017	5.109644
H	-1.133983	-0.539370	-1.322071
H	2.349210	0.061269	-3.801692
H	3.744393	0.282230	-1.769443
H	0.263470	-0.315151	0.702249
H	4.031131	0.319649	0.523411
H	4.787466	0.424008	5.451534
H	3.624209	-0.696632	6.204614
H	3.311098	1.058636	6.222689
H	0.954829	-1.140403	5.746139
H	-0.242564	-0.432753	4.636680
H	0.662975	0.603282	5.765042
O	-2.714794	-0.807130	-3.918051
H	-1.702643	-0.616054	-3.817108
H	-2.793374	-1.535794	-4.543091
O	-4.456577	-0.479332	-1.990702
C	-4.646192	0.926053	-1.865852
H	-3.786106	-0.653883	-2.715705
H	-5.003827	1.370604	-2.804086
H	-3.712832	1.421786	-1.572334
H	-5.395274	1.096051	-1.086736
C	-5.126473	-3.450238	-0.751959
O	-6.654090	-1.922352	-1.861805
C	-6.530803	-3.081245	-1.202083
O	-7.498217	-3.794193	-1.001554
H	-5.175985	-4.312080	-0.085938
H	-4.631727	-2.610141	-0.256789
H	-4.516038	-3.706844	-1.625235
H	-5.790735	-1.413082	-1.930512

3. the proton transfer reaction for cluster 1d

N-form

C	-2.513669	1.491767	0.198566
C	-3.298954	2.645935	0.013298
C	-2.664176	3.896906	-0.101203
C	-1.277536	3.977162	-0.069610
C	-0.469411	2.825790	0.085207
C	-1.131640	1.581915	0.229753
O	-4.646279	2.598539	-0.061987
C	0.971137	2.954166	0.030104
C	1.921616	1.981826	0.143704
C	3.367410	2.205513	-0.091939
N	1.710986	0.624856	0.405979
N	3.909109	0.912155	0.007432
C	2.866062	0.027776	0.316539
O	4.012164	3.223858	-0.341167
C	5.317739	0.648122	-0.217209
C	2.976304	-1.463433	0.469608
C	2.998207	-2.186383	-0.912114
C	4.092261	-1.970617	1.396658
O	2.691123	-3.553227	-0.777104
H	-2.991241	0.523425	0.303041
H	-3.276255	4.783482	-0.236278
H	-0.798476	4.947644	-0.181535
H	-0.538510	0.685032	0.350482
H	-4.962349	1.659904	-0.151497
H	1.361451	3.950887	-0.171590
H	5.742682	1.554654	-0.654770
H	5.845060	0.428782	0.717328
H	5.453293	-0.187135	-0.909067
H	2.015830	-1.737521	0.915603
H	4.001292	-2.105965	-1.357825
H	2.284614	-1.688832	-1.582141
H	5.092086	-1.792990	0.987354
H	4.037945	-1.503474	2.386569
H	3.974141	-3.051202	1.515294
H	1.701068	-3.640127	-0.853944
O	-5.516623	0.077401	-0.537594
H	-5.592265	-0.042787	-1.491908
H	-4.967623	-0.701135	-0.215523
C	-0.740442	-2.997796	1.059218
O	0.031636	-3.526653	-1.153337
C	-0.951280	-3.163410	-0.456796
O	-2.109774	-2.899539	-0.914421

H	-0.492673	-1.950846	1.271852
H	-1.649908	-3.238800	1.617405
H	0.085828	-3.622872	1.408703
O	-4.096230	-1.954263	0.350486
C	-4.832360	-3.034313	0.892480
H	-3.261590	-2.319250	-0.139749
H	-5.742397	-2.637359	1.356519
H	-4.256318	-3.564938	1.664824
H	-5.122102	-3.762144	0.120398

TS

C	2.932342	-0.023419	0.329670
N	1.768073	0.557273	0.411557
C	1.959677	1.918488	0.143373
C	3.396363	2.161001	-0.090135
N	3.960519	0.872538	0.021204
C	0.994074	2.881984	0.018068
C	-0.438455	2.751899	0.070667
C	-1.258226	3.886791	-0.154837
C	-2.639726	3.790280	-0.202955
C	-3.278335	2.537124	-0.035951
C	-2.472997	1.402228	0.230557
C	-1.097143	1.511677	0.277657
O	-4.600506	2.462562	-0.136000
O	4.034039	3.184336	-0.345657
C	5.373770	0.635148	-0.197441
C	3.055748	-1.517306	0.481978
C	4.205591	-2.025924	1.365502
H	1.381345	3.877468	-0.197496
H	-0.785541	4.855060	-0.310438
H	-3.258300	4.663145	-0.393612
H	-2.948287	0.439507	0.377619
H	-0.494202	0.632508	0.458633
H	-4.934840	1.472221	-0.184487
H	5.787095	1.559881	-0.606260
H	5.897838	0.399108	0.735001
H	5.532255	-0.178716	-0.912100
H	2.114566	-1.793702	0.967488
H	4.192215	-1.551726	2.353173
H	5.188156	-1.852569	0.915459
H	4.090764	-3.105549	1.498098
C	3.024712	-2.232109	-0.898844
O	2.705750	-3.603877	-0.768143
H	2.302589	-1.723512	-1.548965

H	4.013965	-2.171532	-1.375487
H	1.727414	-3.683091	-0.772402
O	-0.126848	-3.563161	-0.964740
C	-1.098805	-3.026414	-0.424360
O	-2.260416	-2.944944	-1.035135
C	-0.985467	-2.437887	0.974160
H	-0.273818	-1.607844	0.946573
H	-1.943144	-2.074752	1.353025
H	-0.576775	-3.200359	1.643751
O	-4.129926	-1.843780	0.237959
C	-4.949091	-2.727930	0.966988
H	-3.033636	-2.465512	-0.491157
H	-5.621045	-2.172869	1.638844
H	-4.338152	-3.403995	1.585929
H	-5.576215	-3.357956	0.311363
O	-5.411129	0.112546	-0.342154
H	-5.820783	-0.003844	-1.207772
H	-4.762910	-0.865217	-0.090796

A-form

C	-2.723086	-1.094050	-1.086361
C	-3.795165	-1.881013	-0.531214
C	-3.395065	-3.076671	0.164834
C	-2.064525	-3.382597	0.362352
C	-1.012232	-2.543861	-0.110067
C	-1.400319	-1.404725	-0.873876
O	-5.027401	-1.534126	-0.639214
C	0.338945	-2.834415	0.239861
C	1.481421	-2.079190	0.079173
C	2.800172	-2.493772	0.564470
N	1.578667	-0.793912	-0.474249
N	3.617180	-1.377315	0.271006
C	2.820627	-0.411481	-0.346863
O	3.205266	-3.525608	1.112546
C	5.025311	-1.352658	0.610549
C	3.261533	0.968633	-0.762077
C	3.416711	1.917695	0.456460
C	4.487972	1.026943	-1.688784
O	3.434991	3.281220	0.064880
H	-2.992363	-0.216010	-1.667056
H	-4.181938	-3.712621	0.561621
H	-1.799805	-4.276935	0.925458
H	-0.619832	-0.774097	-1.280857
H	0.509721	-3.776972	0.760184

H	5.662262	-1.449250	-0.276211
H	5.202934	-2.211784	1.262412
H	5.291630	-0.434403	1.141761
H	2.401669	1.347198	-1.324454
H	4.365733	1.720996	0.972464
H	2.602655	1.728124	1.168224
H	5.404097	0.699120	-1.187037
H	4.639967	2.061185	-2.010986
H	4.342900	0.402363	-2.576878
H	2.511023	3.597482	0.042869
O	-5.412983	1.008762	-0.795663
H	-5.285003	-0.009755	-0.775706
H	-5.611963	1.241996	-1.708920
C	-0.611651	2.296332	-0.901366
O	0.646238	3.965888	0.283338
C	-0.427948	3.397478	0.121919
O	-1.480198	3.741619	0.860494
H	-0.045493	1.413293	-0.585076
H	-0.190808	2.631151	-1.853501
H	-1.655308	2.008442	-1.034080
H	-2.293222	3.176648	0.701124
O	-3.658944	2.263959	0.811615
C	-3.691729	1.427679	1.969874
H	-4.271110	1.875062	0.132131
H	-3.348924	0.412587	1.738689
H	-3.025192	1.870004	2.715366
H	-4.706132	1.379092	2.383906

4. the proton transfer reaction for cluster 1e

N-form

C	1.485529	0.107749	0.199546
C	2.724227	-0.529525	0.020458
C	2.777038	-1.929116	-0.077623
C	1.599677	-2.668922	-0.036256
C	0.338424	-2.047691	0.109396
C	0.317703	-0.638258	0.238950
O	3.884277	0.179297	-0.065158
C	-0.865115	-2.855542	0.058335
C	-2.162745	-2.453178	0.165312
C	-3.328990	-3.341066	-0.069644
N	-2.625273	-1.159229	0.418364
N	-4.420716	-2.460623	0.018403
C	-3.925315	-1.185401	0.323187
O	-3.407770	-4.543946	-0.310577

C	-5.785581	-2.900948	-0.203684
C	-4.729882	0.075949	0.464156
C	-5.066559	0.700894	-0.925350
C	-5.968275	-0.001364	1.370560
O	-5.434354	2.053185	-0.798827
H	1.436220	1.187014	0.294682
H	3.737487	-2.419112	-0.205996
H	1.649867	-3.751025	-0.134045
H	-0.634099	-0.137055	0.354494
H	3.704933	1.157355	-0.211421
H	-0.728943	-3.918411	-0.135759
H	-5.727525	-3.904349	-0.631916
H	-6.353481	-2.949686	0.731265
H	-6.301292	-2.237139	-0.902153
H	-4.019615	0.771217	0.920975
H	-5.909358	0.159291	-1.380742
H	-4.193888	0.592637	-1.582688
H	-6.761577	-0.625331	0.946659
H	-5.718294	-0.389944	2.364282
H	-6.371649	1.008528	1.484353
H	-4.599823	2.591110	-0.881445
O	3.465962	2.730743	-0.600956
H	3.464747	2.890170	-1.552602
H	2.619832	3.162569	-0.252062
C	-2.167880	3.205507	1.043549
O	-3.059397	3.251321	-1.186657
C	-2.033437	3.404804	-0.476462
O	-0.876020	3.694297	-0.924521
H	-1.863213	2.183241	1.297660
H	-1.513833	3.888375	1.593980
H	-3.203151	3.345676	1.365418
O	1.298212	3.811655	0.351879
C	1.432859	5.101416	0.921279
H	0.386605	3.742961	-0.143312
H	2.425547	5.179306	1.378596
H	0.679538	5.272469	1.703639
H	1.331285	5.894440	0.166267
C	8.599390	-1.531686	-0.604974
N	8.676170	-1.229085	0.737507
C	7.346737	-1.236085	-1.095042
C	7.481080	-0.756787	1.049124
N	6.639663	-0.739987	-0.022669
H	9.444785	-1.942257	-1.139626
H	6.907899	-1.329014	-2.076790

H	7.174723	-0.415039	2.027869
H	5.666785	-0.422446	-0.031177

TS

C	1.439974	0.112033	0.336932
C	2.675846	-0.536312	0.125517
C	2.693270	-1.941007	-0.005719
C	1.505411	-2.660343	0.025780
C	0.253695	-2.021556	0.195684
C	0.263497	-0.614815	0.367517
O	3.824208	0.155077	0.043156
C	-0.961515	-2.798765	0.121575
C	-2.259145	-2.377234	0.199460
C	-3.425226	-3.249648	-0.059348
N	-2.712768	-1.073947	0.433424
N	-4.512491	-2.355226	-0.000789
C	-4.010227	-1.086362	0.306852
O	-3.518034	-4.453255	-0.297561
C	-5.874335	-2.784313	-0.256839
C	-4.800486	0.190556	0.413587
C	-5.046688	0.822007	-0.987926
C	-6.086918	0.136891	1.252081
O	-5.376665	2.192487	-0.885688
H	1.415475	1.189196	0.459279
H	3.643500	-2.445572	-0.153367
H	1.535076	-3.740568	-0.100917
H	-0.679428	-0.104678	0.508125
H	3.666070	1.210486	-0.086380
H	-0.843785	-3.864234	-0.072125
H	-5.812872	-3.800754	-0.652875
H	-6.475426	-2.799138	0.658315
H	-6.358871	-2.137730	-0.993646
H	-4.103339	0.870468	0.912755
H	-5.887418	0.317576	-1.484267
H	-4.150708	0.681243	-1.605780
H	-6.870017	-0.464931	0.780522
H	-5.898277	-0.267106	2.252925
H	-6.474216	1.154117	1.357178
H	-4.533982	2.696818	-0.880031
O	3.498606	2.583349	-0.317874
H	3.752385	2.826829	-1.215960
H	2.490200	3.136689	-0.057227
C	-1.645336	2.906875	0.990581
O	-2.823798	3.354983	-1.051087

C	-1.738838	3.363305	-0.459997
O	-0.639780	3.761709	-1.051501
H	-1.921517	1.848992	1.043209
H	-0.644149	3.034034	1.405340
H	-2.375067	3.466668	1.583623
O	1.445634	3.709851	0.278572
C	1.715952	4.906872	0.972056
H	0.260355	3.724939	-0.458899
H	2.657168	4.823185	1.534610
H	0.914029	5.132145	1.692842
H	1.804550	5.772296	0.293218
C	8.401063	-1.666337	-0.796681
N	8.585754	-1.367327	0.535953
C	7.124768	-1.331539	-1.193089
C	7.430350	-0.858481	0.932532
N	6.513592	-0.814811	-0.073488
H	9.191829	-2.102205	-1.391766
H	6.612227	-1.409548	-2.139880
H	7.207452	-0.507155	1.930277
H	5.548119	-0.467445	-0.012254

A-form

C	-1.576623	-0.083569	-1.039352
C	-2.823725	-0.512801	-0.482642
C	-2.803420	-1.740194	0.252330
C	-1.620578	-2.424008	0.467467
C	-0.372981	-1.950948	-0.022926
C	-0.402165	-0.767591	-0.810757
O	-3.907823	0.191325	-0.635736
C	0.833570	-2.636562	0.331774
C	2.144878	-2.272267	0.146688
C	3.280240	-3.065900	0.639296
N	2.630877	-1.097633	-0.446805
N	4.397787	-2.268902	0.308002
C	3.931501	-1.120871	-0.336339
O	3.346481	-4.154927	1.215071
C	5.750000	-2.677375	0.634251
C	4.778146	0.036024	-0.799642
C	5.258055	0.914203	0.387783
C	5.934787	-0.323982	-1.747910
O	5.694052	2.191155	-0.046289
H	-1.576797	0.821166	-1.640452
H	-3.738517	-2.109947	0.663966
H	-1.635462	-3.339897	1.056079

H	0.529465	-0.404816	-1.226110
H	0.711964	-3.574769	0.872812
H	6.309624	-2.983315	-0.256457
H	5.662127	-3.536478	1.303803
H	6.296380	-1.878148	1.142600
H	4.070965	0.656412	-1.359683
H	6.110623	0.439480	0.890477
H	4.445859	1.008070	1.120659
H	6.712346	-0.913658	-1.251970
H	6.398879	0.599609	-2.105453
H	5.575516	-0.890832	-2.613497
H	4.914305	2.778923	-0.071328
O	-3.461342	2.765706	-0.729416
H	-3.659470	1.771664	-0.739966
H	-3.741663	3.116458	-1.581438
C	1.492619	2.510927	-0.946766
O	3.255764	3.695002	0.177682
C	2.051825	3.509476	0.045643
O	1.187193	4.201300	0.784975
H	1.824743	1.504758	-0.670492
H	1.906903	2.734616	-1.934376
H	0.402886	2.519150	-0.991814
H	0.233820	3.929174	0.651257
O	-1.362204	3.505566	0.804975
C	-1.664898	2.824992	2.024280
H	-2.072678	3.294415	0.148420
H	-1.700325	1.739203	1.876682
H	-0.872953	3.062406	2.739523
H	-2.624882	3.165279	2.430880
C	-8.545571	-0.770375	0.599103
N	-8.520301	-1.467990	-0.588879
C	-7.312094	-0.207934	0.852158
C	-7.281657	-1.320768	-1.037359
N	-6.511490	-0.569276	-0.205380
H	-9.442904	-0.712550	1.200409
H	-6.943770	0.401140	1.663943
H	-6.895669	-1.739492	-1.956550
H	-5.507827	-0.315297	-0.343085

5. the proton transfer reaction for cluster 1s

N-form

C	0.014922	0.319012	0.139026
C	-1.235137	0.951490	0.034971
C	-1.303827	2.354049	0.005673

C	-0.132846	3.103407	0.057719
C	1.137846	2.488676	0.131948
C	1.176478	1.074467	0.179478
O	-2.391874	0.237294	-0.036600
C	2.330429	3.313341	0.142816
C	3.634666	2.919262	0.131720
C	4.786927	3.857905	0.112444
N	4.114928	1.603561	0.105767
N	5.889261	2.993435	0.067634
C	5.411341	1.674780	0.063871
O	4.846023	5.086731	0.127322
C	7.264347	3.443281	0.024682
C	6.321794	0.496064	0.012191
H	0.078757	-0.762362	0.194544
H	-2.272435	2.840295	-0.061898
H	-0.196466	4.188932	0.028610
H	2.135235	0.576019	0.241165
H	-2.214744	-0.749954	-0.124842
H	2.176972	4.391605	0.142910
H	7.245025	4.535042	0.059555
H	7.760708	3.122914	-0.898095
H	7.833602	3.066231	0.881302
H	6.978415	0.547711	-0.865551
H	5.729942	-0.425353	-0.039820
H	6.968287	0.461808	0.899096
O	-1.997946	-2.349757	-0.333441
H	-1.110669	-2.719398	0.002318
H	-2.097051	-2.674239	-1.236145
O	2.508477	-3.315400	-0.423015
C	3.393415	-2.493823	0.007451
O	4.587759	-2.418116	-0.324236
H	3.024999	-1.766074	0.774427
O	0.244275	-3.209064	0.590489
C	0.205532	-4.103798	1.684676
H	1.212732	-3.227292	0.139904
H	-0.805800	-4.103108	2.109361
H	0.910274	-3.803282	2.473815
H	0.452896	-5.131279	1.378690
C	-6.907620	1.970270	-1.428470
N	-7.235559	1.690706	-0.119178
C	-5.589491	1.654912	-1.673312
C	-6.124539	1.212361	0.415250
N	-5.099419	1.170059	-0.481498
H	-7.634139	2.380121	-2.116465

H	-4.974485	1.728728	-2.557253
H	-6.008915	0.883855	1.438637
H	-4.145447	0.841329	-0.306314

TS

C	0.134509	1.586361	-0.354038
C	-1.023674	2.092756	0.277175
C	-1.223320	3.487098	0.328200
C	-0.291156	4.342290	-0.238316
C	0.874563	3.856197	-0.878299
C	1.059933	2.450910	-0.917637
O	-1.944944	1.288010	0.831958
C	1.794823	4.811069	-1.444608
C	2.973884	4.628197	-2.107834
C	3.785342	5.757589	-2.616320
N	3.616238	3.418118	-2.420060
N	4.883801	5.110754	-3.209511
C	4.708220	3.736138	-3.051041
O	3.622025	6.975811	-2.577057
C	5.975613	5.809492	-3.854576
C	5.704031	2.754260	-3.571537
H	0.283739	0.511871	-0.387935
H	-2.110539	3.876127	0.818113
H	-0.457676	5.416099	-0.191225
H	1.946120	2.054378	-1.398936
H	1.516933	5.858564	-1.332182
H	5.760276	6.877379	-3.773084
H	6.053671	5.541412	-4.914153
H	6.931905	5.599751	-3.362632
H	5.823755	2.842657	-4.658357
H	5.358919	1.747038	-3.334322
H	6.691665	2.906881	-3.119308
O	-1.421455	-1.137361	0.578232
H	-1.722899	0.266294	0.734823
H	-2.093930	-1.686604	0.159201
O	-0.301533	-2.521828	2.253809
C	-0.656808	-2.259747	3.592877
H	-0.920184	-1.751476	1.341746
H	-1.750188	-2.224379	3.736887
H	-0.241342	-1.295077	3.919813
H	-0.259105	-3.040683	4.256894
O	-0.348226	-4.883835	1.764857
C	0.808596	-5.387852	1.455883
O	1.043371	-6.560964	1.172271

H	-0.313996	-3.710735	2.003063
H	1.642094	-4.648057	1.460936
C	-6.582137	2.874679	1.937274
N	-6.203622	2.608214	3.235380
C	-5.563093	2.564138	1.064448
C	-4.969511	2.142249	3.141497
N	-4.534485	2.095390	1.850865
H	-7.561041	3.271255	1.705599
H	-5.478235	2.629530	-0.009606
H	-4.351864	1.824819	3.969958
H	-3.615209	1.783445	1.522713

A-frorm

C	0.341352	0.490533	-0.241308
C	-0.997806	1.001765	-0.229050
C	-1.140067	2.419845	-0.102229
C	-0.035345	3.240853	0.001221
C	1.292693	2.731600	-0.012633
C	1.438970	1.320604	-0.138025
O	-2.032164	0.221150	-0.327710
C	2.382549	3.650518	0.096361
C	3.741433	3.449442	0.110414
C	4.706478	4.553162	0.233496
N	4.435141	2.230307	0.016574
N	5.949262	3.888130	0.203482
C	5.701796	2.522921	0.073630
O	4.571145	5.775383	0.340853
C	7.222693	4.566901	0.296386
C	6.810472	1.524807	0.010402
H	0.476325	-0.582929	-0.343093
H	-2.143214	2.836588	-0.083150
H	-0.178382	4.315880	0.097967
H	2.440173	0.904411	-0.152771
H	-1.920055	-1.342731	-0.328565
H	2.105329	4.701003	0.184724
H	7.005015	5.632972	0.398202
H	7.830194	4.411886	-0.603105
H	7.794055	4.234620	1.171027
H	7.475501	1.712345	-0.842233
H	6.376842	0.529015	-0.094265
H	7.427916	1.548008	0.917441
O	-1.911569	-2.360787	-0.320604
H	-0.631584	-3.176485	0.310791
H	-2.289495	-2.647271	-1.159403

O	0.631319	-6.145292	0.267271
C	1.711715	-6.204479	-0.504192
O	2.222004	-7.239564	-0.879282
H	2.114638	-5.211871	-0.780699
O	0.126958	-3.638190	0.768182
C	0.204706	-3.183214	2.117540
H	0.389418	-5.184955	0.460898
H	0.380467	-2.101882	2.153886
H	1.046868	-3.693220	2.593672
H	-0.712389	-3.416340	2.673675
C	-6.584732	1.708310	-1.387900
N	-6.866979	1.086395	-0.191212
C	-5.234773	1.636408	-1.659871
C	-5.694181	0.648870	0.244435
N	-4.676181	0.954286	-0.604521
H	-7.362588	2.169148	-1.981738
H	-4.639645	1.998590	-2.484767
H	-5.531302	0.105352	1.164781
H	-3.667191	0.720144	-0.480804