Entropy-energy balance in base catalyzed keto-enol interconversion: a joint theoretical and experimental investigation.

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SUPPLEMENTARY INFORMATIONS. Contents.

1. QUANTUM-CHEMICAL CALCULATIONS

2PAT-KH

HF/6-31+G(d)

1	6	0	0.604399	1.340571	0.518315
2	8	0	0.590455	2.492578	0.192424
3	6	0	-0.503690	0.776481	1.395693
4	1	0	-0.119048	0.010135	2.058460
5	1	0	-0.854751	1.597871	2.008541
6	6	0	-1.654005	0.214676	0.572688
7	6	0	-2.019715	-1.121276	0.676839
8	6	0	-3.084720	-1.625699	-0.058621
9	6	0	-3.795894	-0.796336	-0.909782
10	6	0	-3.437238	0.540828	-1.020323
11	6	0	-2.376381	1.042678	-0.284205
12	1	0	-1.475357	-1.776204	1.334518
13	1	0	-3.353937	-2.662752	0.035866
14	1	0	-4.620580	-1.184477	-1.480606
15	1	0	-3.984784	1.192834	-1.677511
16	1	0	-2.104865	2.079189	-0.376041
17	6	0	1.698387	0.452242	0.046446
18	16	0	1.912214	-1.201344	0.533237
19	6	0	3.317377	-1.351137	-0.439068
20	6	0	3.608048	-0.208339	-1.100300
21	6	0	2.672857	0.832037	-0.816209
22	1	0	2.716681	1.820082	-1.231107
23	1	0	4.446727	-0.098223	-1.760865
24	1	0	3.854314	-2.277923	-0.471276

MP2/6-31+G(d)

1	6	0	-.811479	1.592023	-.316229
2	8	0	-1.165025	2.681654	.152080
3	6	0	.443371	1.474963	-1.161956
4	1	0	.192860	1.044219	-2.141293
5	1	0	.809897	2.495144	-1.324747
6	6	0	1.481273	.618594	-.468794
7	6	0	2.158431	-.397728	-1.156318

8	6	0	3.111547	-1.186404	-.503775
9	6	0	3.390912	-.971605	.849579
10	6	0	2.724573	.046552	1.541384
11	6	0	1.776920	.837484	.886206
12	1	0	1.937523	-.576241	-2.208359
13	1	0	3.629308	-1.972176	-1.050576
14	1	0	4.127206	-1.588522	1.360535
15	1	0	2.940731	.223237	2.593243
16	1	0	1.264150	1.630439	1.430481
17	6	0	-1.597311	.374603	-.030693
18	16	0	-1.175797	-1.211071	-.578162
19	6	0	-2.591320	-1.888095	.108562
20	6	0	-3.364589	-.934226	.750442
21	6	0	-2.800170	.355288	.669039
22	1	0	-3.228042	1.261002	1.088084
23	1	0	-4.296595	-1.168661	1.255941
24	1	0	-2.777047	-2.953238	.025955

E_{HF}= -932.6224904
E_{MP2}= -934.4709239
Thermal Correction to Free Energy 298 K, 1 bar = 0.159848

2PAT Cs

HF/6-31+G(d)

1	6	0	-1.261543	1.474089	0.000000
2	6	0	-2.566749	0.996728	0.000000
3	6	0	-3.639202	1.884573	0.000000
4	6	0	-3.430711	3.251652	0.000000
5	6	0	-2.129555	3.738379	0.000000
6	6	0	-1.063747	2.857010	0.000000
7	1	0	-0.059779	3.248531	0.000000
8	1	0	-1.946792	4.798534	0.000000
9	1	0	-4.265078	3.930461	0.000000
10	1	0	-4.641527	1.493690	0.000000
11	1	0	-2.755631	-0.055899	0.000000
12	6	0	0.000000	0.622744	0.000000
13	1	0	0.601324	0.898864	0.863529
14	1	0	0.601324	0.898864	-0.863529
15	6	0	-0.073625	-0.893139	0.000000
16	6	0	1.232119	-1.617764	0.000000
17	8	0	-1.087504	-1.525805	0.000000
18	16	0	2.798228	-0.860487	0.000000
19	6	0	3.583717	-2.387327	0.000000
20	6	0	2.707208	-3.414987	0.000000
21	6	0	1.349786	-2.967315	0.000000
22	1	0	0.495611	-3.616070	0.000000
23	1	0	2.998732	-4.447919	0.000000
24	1	0	4.654011	-2.442683	0.000000

MP2/6-31+G(d)

1	6	0	-1.261370	1.457510	.000000
2	6	0	-2.573861	.961290	.000000
3	6	0	-3.660089	1.846161	.000000
4	6	0	-3.460872	3.228173	.000000
5	6	0	-2.155028	3.730707	.000000
6	6	0	-1.070980	2.851475	.000000

7	1	0	-.057285	3.254028	.000000
8	1	0	-1.980146	4.804943	.000000
9	1	0	-4.311055	3.907244	.000000
10	1	0	-4.671190	1.443175	.000000
11	1	0	-2.747660	-.107712	.000000
12	6	0	.000000	.615935	.000000
13	1	0	.610057	.898445	.871598
14	1	0	.610057	.898445	-.871598
15	6	0	-.062341	-.900941	.000000
16	6	0	1.241109	-1.608685	.000000
17	8	0	-1.104950	-1.562462	.000000
18	16	0	2.782519	-.819057	.000000
19	6	0	3.617440	-2.313986	.000000
20	6	0	2.748137	-3.391200	.000000
21	6	0	1.394816	-2.990242	.000000
22	1	0	.538522	-3.657652	.000000
23	1	0	3.084742	-4.423492	.000000
24	1	0	4.701503	-2.329994	.000000

E_{HF}= -932.617079001
E_{MP2}= -934.45914
2 imaginary frequencies

2PAT-EH syn

HF/6-31+G(d)

1	6	0	-2.942126	0.140579	0.393412
2	6	0	-1.646319	0.277620	0.019267
3	16	0	-1.008386	-1.233434	-0.555792
4	6	0	-2.503433	-2.030268	-0.256703
5	6	0	-3.435468	-1.194875	0.244843
6	6	0	-0.910058	1.555003	0.006748
7	8	0	-1.788587	2.592541	0.018961
8	6	0	0.403209	1.766382	-0.030097
9	6	0	1.504759	0.769616	0.052801
10	6	0	2.380091	0.607068	-1.019783
11	6	0	3.441763	-0.281507	-0.943065
12	6	0	3.649700	-1.019333	0.213766
13	6	0	2.792202	-0.857541	1.291680
14	6	0	1.732231	0.033707	1.212803
15	1	0	1.074557	0.157830	2.054536
16	1	0	2.949058	-1.420566	2.194987
17	1	0	4.472987	-1.709027	0.275253
18	1	0	4.102383	-0.398755	-1.784115
19	1	0	2.220784	1.171590	-1.922107
20	1	0	0.724315	2.793956	-0.123274
21	1	0	-3.532348	0.959644	0.753528
22	1	0	-4.434184	-1.494515	0.501047
23	1	0	-2.605347	-3.076649	-0.465596
24	1	0	-1.328630	3.412391	0.142688

MP2/6-31+G(d)

1	6	0	-2.902216	.025890	.392203
2	6	0	-1.572397	.245243	.048301
3	16	0	-.835259	-1.219074	-.535640

4	6	0	-2.293071	-2.092705	-.314594
5	6	0	-3.308569	-1.310019	.195197
6	6	0	-.950665	1.564855	.015510
7	8	0	-1.926226	2.550747	.000451
8	6	0	.367847	1.868449	-.038174
9	6	0	1.445801	.867879	.060506
10	6	0	2.327633	.676383	-1.015226
11	6	0	3.353372	-.270916	-.932161
12	6	0	3.510918	-1.035270	.230738
13	6	0	2.645823	-.838633	1.312759
14	6	0	1.626763	.112349	1.230862
15	1	0	.954936	.271598	2.072813
16	1	0	2.770893	-1.421211	2.223511
17	1	0	4.307355	-1.773885	.294880
18	1	0	4.025286	-.417294	-1.773813
19	1	0	2.201140	1.253453	-1.929519
20	1	0	.656676	2.911712	-.183752
21	1	0	-3.539068	.825689	.753768
22	1	0	-4.301636	-1.692765	.411393
23	1	0	-2.323400	-3.151962	-.550069
24	1	0	-1.485671	3.412849	.131913

E_{HF}= -932.591398017
E_{MP2}= -934.4462851
Thermal Correction to Free Energy 298 K, 1 bar = 0.159478

2PAT-EH Cs

HF/6-31+G(d)

1	6	0	-0.990466	1.624391	0.000000
2	6	0	-2.378456	1.449590	0.000000
3	6	0	-3.226809	2.546131	0.000000
4	6	0	-2.721151	3.837809	0.000000
5	6	0	-1.347148	4.026624	0.000000
6	6	0	-0.497583	2.933410	0.000000
7	1	0	0.566372	3.096324	0.000000
8	1	0	-0.936765	5.021022	0.000000
9	1	0	-3.386690	4.682698	0.000000
10	1	0	-4.290902	2.387013	0.000000
11	1	0	-2.794436	0.463975	0.000000
12	6	0	0.000000	0.533629	0.000000
13	1	0	1.019213	0.871730	0.000000
14	6	0	-0.176064	-0.787095	0.000000
15	6	0	0.939483	-1.753993	0.000000
16	8	0	-1.423152	-1.316846	0.000000
17	16	0	2.606069	-1.253398	0.000000
18	6	0	3.157126	-2.886558	0.000000
19	6	0	2.135269	-3.761276	0.000000
20	6	0	0.858508	-3.108221	0.000000
21	1	0	-0.056670	-3.671483	0.000000
22	1	0	2.256566	-4.827784	0.000000
23	1	0	4.206844	-3.100328	0.000000
24	1	0	-1.411679	-2.260669	0.000000

MP2/6-31+G(d)

1	6	0	-1.019013	1.599457	.000000
2	6	0	-2.413160	1.369498	.000000
3	6	0	-3.306410	2.443397	.000000
4	6	0	-2.845725	3.764388	.000000
5	6	0	-1.467704	4.007154	.000000
6	6	0	-.570798	2.939447	.000000
7	1	0	.500592	3.139978	.000000
8	1	0	-1.091262	5.028468	.000000
9	1	0	-3.550548	4.593430	.000000
10	1	0	-4.376487	2.243148	.000000
11	1	0	-2.793737	.354936	.000000
12	6	0	.000000	.557472	.000000
13	1	0	1.026108	.922131	.000000
14	6	0	-.138110	-.795948	.000000
15	6	0	.988570	-1.725866	.000000
16	8	0	-1.400638	-1.352576	.000000
17	16	0	2.635658	-1.180785	.000000
18	6	0	3.244929	-2.786394	.000000
19	6	0	2.230093	-3.719236	.000000
20	6	0	.947183	-3.117671	.000000
21	1	0	.035064	-3.710402	.000000
22	1	0	2.402311	-4.791232	.000000
23	1	0	4.315029	-2.958495	.000000
24	1	0	-1.331618	-2.322976	.000000

E_{HF}= -932.594431111
E_{MP2}= -934.441206
1 imaginary frequency

2PAT-EH anti

MP2/6-31+G(d)

1	6	0	.626636	-3.212412	.000000
2	6	0	.812690	-1.835870	.000000
3	16	0	2.501846	-1.447434	.000000
4	6	0	2.949746	-3.107011	.000000
5	6	0	1.845627	-3.934327	.000000
6	6	0	-.239469	-.825761	.000000
7	8	0	-1.474352	-1.431969	.000000
8	6	0	.000000	.515341	.000000
9	6	0	-.888255	1.675506	.000000
10	6	0	-2.301958	1.674804	.000000
11	6	0	-3.031330	2.866669	.000000
12	6	0	-2.381157	4.103336	.000000
13	6	0	-.982849	4.132709	.000000
14	6	0	-.257879	2.942540	.000000
15	1	0	.830622	2.983885	.000000
16	1	0	-.454614	5.084176	.000000
17	1	0	-2.954961	5.027378	.000000
18	1	0	-4.118702	2.822934	.000000
19	1	0	-2.890347	.760418	.000000
20	1	0	1.056384	.778159	.000000
21	1	0	-.359534	-3.663494	.000000
22	1	0	1.915110	-5.018065	.000000
23	1	0	3.998124	-3.382208	.000000
24	1	0	-2.167615	-.751634	.000000

E_{MP2}=-934.4399739

2PAT-E$^-$

HF/6-31+G(d)

1	6	0	-0.575465	2.946747	0.000000
2	6	0	-0.993934	1.598561	0.000000
3	6	0	-2.388549	1.378883	0.000000
4	6	0	-3.279471	2.439465	0.000000
5	6	0	-2.844881	3.760555	0.000000
6	6	0	-1.474281	3.997284	0.000000
7	6	0	0.000000	0.546112	0.000000
8	6	0	-0.245030	-0.817235	0.000000
9	8	0	-1.342505	-1.404707	0.000000
10	6	0	0.961451	-1.739761	0.000000
11	6	0	0.883088	-3.090366	0.000000
12	6	0	2.159235	-3.746816	0.000000
13	6	0	3.189984	-2.876855	0.000000
14	16	0	2.635029	-1.241294	0.000000
15	1	0	0.481007	3.160416	0.000000
16	1	0	-1.103491	5.010194	0.000000
17	1	0	-3.547896	4.576594	0.000000
18	1	0	-4.337198	2.228318	0.000000
19	1	0	-2.744689	0.368601	0.000000
20	1	0	1.022673	0.881101	0.000000
21	1	0	-0.065150	-3.590481	0.000000
22	1	0	2.282535	-4.815295	0.000000
23	1	0	4.238880	-3.100521	0.000000

MP2/6-31+G(d)

1	6	0	-.646165	2.947912	.000000
2	6	0	-1.017034	1.575259	.000000
3	6	0	-2.412272	1.296956	.000000
4	6	0	-3.353040	2.330395	.000000
5	6	0	-2.962366	3.676455	.000000
6	6	0	-1.590662	3.973454	.000000
7	6	0	.000000	.559185	.000000
8	6	0	-.212133	-.825792	.000000
9	8	0	-1.333132	-1.448889	.000000
10	6	0	1.006402	-1.707913	.000000
11	6	0	.974941	-3.095943	.000000
12	6	0	2.257878	-3.698438	.000000
13	6	0	3.281387	-2.768407	.000000
14	16	0	2.658993	-1.161822	.000000
15	1	0	.416099	3.200400	.000000
16	1	0	-1.256636	5.012181	.000000
17	1	0	-3.704550	4.474421	.000000
18	1	0	-4.414310	2.076766	.000000
19	1	0	-2.719360	.254798	.000000
20	1	0	1.030093	.918989	.000000
21	1	0	.023635	-3.618477	.000000
22	1	0	2.432980	-4.772274	.000000
23	1	0	4.351612	-2.945281	.000000

E_{HF}= -932.046671514
E_{MP2}= -933.9101113

Thermal Correction to Free Energy 298 K, 1 bar = 0.145313

2PAT-E$^-$(H_2O)

HF/6-31+G(d)

1	16	0	2.605594	-1.451032	.060989
2	6	0	1.974365	.134639	-.303933
3	6	0	2.991900	1.014740	-.462047
4	6	0	4.291714	.440177	-.273963
5	6	0	4.234659	-.877683	.014576
6	6	0	.508374	.498554	-.449470
7	8	0	.300825	1.625278	-.946354
8	6	0	-.424242	-.420427	.009847
9	6	0	-1.866825	-.322057	-.097777
10	6	0	-2.649033	-1.377171	.407042
11	6	0	-4.029741	-1.367374	.337505
12	6	0	-4.698745	-.297310	-.243016
13	6	0	-3.942352	.757652	-.746642
14	6	0	-2.560224	.756896	-.680401
15	1	0	-2.153691	-2.222558	.860237
16	1	0	-4.586270	-2.199978	.737777
17	1	0	-5.773934	-.283820	-.296294
18	1	0	-4.438072	1.601740	-1.197842
19	1	0	-1.998364	1.583648	-1.066777
20	1	0	-.058873	-1.291886	.525092
21	1	0	2.809748	2.042329	-.712781
22	1	0	5.210082	.995497	-.354415
23	1	0	5.054923	-1.543909	.194992
24	1	0	-.356331	.991670	1.990479
25	8	0	-.124092	1.824196	2.399231
26	1	0	.208324	2.304181	1.650365

MP2/6-31+G(d)

1	16	0	2.600431	-1.511231	-.088425
2	6	0	1.984165	.104449	-.226912
3	6	0	3.026757	1.017833	-.168900
4	6	0	4.297053	.415329	.010374
5	6	0	4.226068	-.965323	.079121
6	6	0	.536875	.430473	-.420750
7	8	0	.288944	1.518078	-1.063643
8	6	0	-.385246	-.427811	.192288
9	6	0	-1.821463	-.375730	.049465
10	6	0	-2.629555	-1.331364	.719031
11	6	0	-4.017747	-1.350227	.585589
12	6	0	-4.663590	-.412545	-.233854
13	6	0	-3.885820	.540641	-.904193
14	6	0	-2.495165	.569249	-.768988
15	1	0	-2.142929	-2.070476	1.358271
16	1	0	-4.599786	-2.102823	1.119298
17	1	0	-5.748092	-.421542	-.339642
18	1	0	-4.369804	1.279200	-1.544708
19	1	0	-1.895962	1.312524	-1.287576
20	1	0	.012013	-1.254497	.783010
21	1	0	2.838946	2.083336	-.258853
22	1	0	5.231432	.965738	.097288
23	1	0	5.038539	-1.674139	.198919
24	1	0	-.448020	1.567351	1.648199

25	8	0	-.339806	2.536461	1.734168
26	1	0	-.150337	2.768875	.802757

E_{HF}= -1008.07802
E_{MP2}= -1010.1453287
Thermal Correction to Free Energy 298 K, 1 bar = 0.166259

TS (H_2O)

HF/6-31+G(d)

1	16	0	-2.684835	.864788	-.753672
2	6	0	-1.976753	-.427474	.161924
3	6	0	-2.922333	-1.319002	.544734
4	6	0	-4.236999	-.980384	.095566
5	6	0	-4.249141	.167512	-.619365
6	6	0	-.506231	-.568354	.475433
7	8	0	-.203716	-1.419330	1.280705
8	6	0	.409596	.370505	-.174288
9	6	0	1.879878	.027460	-.175913
10	6	0	2.811502	1.050743	.007996
11	6	0	4.176345	.797904	-.057706
12	6	0	4.644530	-.485567	-.298748
13	6	0	3.729442	-1.515479	-.472758
14	6	0	2.367006	-1.259446	-.412883
15	1	0	2.443295	2.039521	.216475
16	1	0	4.873665	1.606424	.087721
17	1	0	5.702820	-.682744	-.344716
18	1	0	4.076089	-2.519782	-.653657
19	1	0	1.673866	-2.071508	-.536738
20	1	0	.075135	.597676	-1.183623
21	1	0	-2.679427	-2.186277	1.127166
22	1	0	-5.113696	-1.566365	.303693
23	1	0	-5.099270	.651422	-1.058870
24	1	0	.255431	1.497258	.410146
25	8	0	.197230	2.778548	.896105
26	1	0	.040274	2.773511	1.832724

MP2/6-31+G(d)

1	16	0	-2.657806	.920248	-.535075
2	6	0	-1.950322	-.494603	.161729
3	6	0	-2.921933	-1.440180	.467003
4	6	0	-4.227313	-1.017641	.128271
5	6	0	-4.234318	.247496	-.439020
6	6	0	-.480012	-.666485	.358721
7	8	0	-.095929	-1.535130	1.166188
8	6	0	.383022	.263242	-.384619
9	6	0	1.857499	.013911	-.270657
10	6	0	2.689925	1.039151	.212219
11	6	0	4.072469	.838195	.307211
12	6	0	4.643955	-.380713	-.077949
13	6	0	3.819561	-1.406573	-.558132
14	6	0	2.438139	-1.207558	-.652101
15	1	0	2.213410	1.976446	.509908
16	1	0	4.708050	1.640187	.682964
17	1	0	5.720490	-.533639	-.000910
18	1	0	4.253414	-2.361736	-.855003
19	1	0	1.796656	-2.012635	-1.009942
20	1	0	.056136	.333601	-1.432362

21	1	0	-2.659306	-2.390751	.922029
22	1	0	-5.127522	-1.606890	.284858
23	1	0	-5.093707	.822871	-.766854
24	1	0	.163809	1.376035	.054553
25	8	0	.151602	2.823627	.512807
26	1	0	-.495940	2.995119	1.223955

E_{HF}= -1008.02472366
E_{MP2}= -1010.1011386
Thermal Correction to Free Energy 298 K, 1 bar = 0.161702

2PAT-E$^-$$(H_2O)_2$

HF/6-31+G(d)

1	6	0	-2.457745	0.298664	-0.840819
2	6	0	-1.768914	-0.709566	-0.136852
3	6	0	-2.560409	-1.715931	0.452219
4	6	0	-3.939242	-1.719970	0.350196
5	6	0	-4.601939	-0.716204	-0.347407
6	6	0	-3.841060	0.284775	-0.938008
7	6	0	-0.324019	-0.765043	0.017709
8	6	0	0.595261	0.124030	-0.508207
9	8	0	0.359639	1.181904	-1.133515
10	6	0	2.062036	-0.174156	-0.296819
11	16	0	2.712020	-1.672051	0.316021
12	6	0	4.331510	-1.086570	0.201046
13	6	0	4.369969	0.172540	-0.279893
14	6	0	3.063871	0.692174	-0.568757
15	8	0	0.133630	3.765631	0.146826
16	1	0	-2.072464	-2.504995	0.999888
17	1	0	-4.501579	-2.511057	0.819060
18	1	0	-5.675538	-0.715412	-0.427600
19	1	0	-4.330438	1.072526	-1.487190
20	1	0	-1.891211	1.078019	-1.308880
21	1	0	0.045847	-1.624157	0.549416
22	1	0	2.870078	1.670960	-0.960272
23	1	0	5.279109	0.726206	-0.429927
24	1	0	5.157986	-1.704820	0.491379
25	1	0	-0.214516	3.418008	0.959759
26	1	0	0.247724	2.987289	-0.400787
27	8	0	-1.152629	1.793116	2.225262
28	1	0	-1.979286	1.731293	1.763158
29	1	0	-0.629066	1.095282	1.840628

MP2/6-31+G(d)

C	6.0	-2.4803324259	0.3471364092	-0.7537401323
C	6.0	-1.7877509970	-0.6860055753	-0.0665226439
C	6.0	-2.5787183554	-1.7331759084	0.4740294807
C	6.0	-3.9656173878	-1.7599160735	0.3356543820
C	6.0	-4.6284600349	-0.7438272976	-0.3678917701
C	6.0	-3.8687502745	0.2974344196	-0.9146906806
C	6.0	-0.3552595428	-0.7062045485	0.1216940526
C	6.0	0.5682173703	0.1626700126	-0.4739723590
O	8.0	0.3034614746	1.2120613868	-1.1666837164

C	6.0	2.0257895640	-0.1069991949	-0.2529171669
S	16.0	2.6888585972	-1.6384691716	0.2275730706
C	6.0	4.3055633878	-1.0517249194	0.1644833026
C	6.0	4.3391621722	0.2775735850	-0.2170132144
C	6.0	3.0480649637	0.8083395427	-0.4579004431
O	8.0	0.0206371800	3.7209306107	0.1670507797
H	1.0	-2.0798054689	-2.5359431242	1.0191879441
H	1.0	-4.5328976545	-2.5828595968	0.7717193494
H	1.0	-5.7109891365	-0.7657542085	-0.4870853098
H	1.0	-4.3645382160	1.1009415420	-1.4603369704
H	1.0	-1.8970479567	1.1510448732	-1.1941668692
H	1.0	0.0375774806	-1.5436576408	0.7011607566
H	1.0	2.8279780257	1.8140469300	-0.8014191881
H	1.0	5.2636347507	0.8404944521	-0.3240500860
H	1.0	5.1377050699	-1.6987812700	0.4210095136
H	1.0	-0.3372100765	3.3172980697	0.9824545437
H	1.0	0.1607007796	2.9284085961	-0.4008227524
O	8.0	-1.1734735138	1.7291637111	2.1472403721
H	1.0	-2.0363770754	1.6381379865	1.7011798231
H	1.0	-0.6563199954	1.0118466960	1.7178832928

E_{HF}= -1084.1181515
E_{MP2}= -1086.38072
Thermal Correction to Free Energy 298 K, 1 bar = 0.189486

TS(H_2O)$_2$

HF/6-31+G(d)

1	6	0	-2.778811	-0.926546	0.298639
2	6	0	-1.772478	-0.077562	-0.015273
3	16	0	-2.390580	1.339426	-0.805310
4	6	0	-4.003000	0.754080	-0.705882
5	6	0	-4.068184	-0.450957	-0.097647
6	6	0	-0.318863	-0.344156	0.278743
7	8	0	-0.061061	-1.368764	0.867507
8	6	0	0.651889	0.690342	-0.095295
9	6	0	2.071919	0.261462	-0.298672
10	6	0	2.811339	-0.360894	0.713022
11	6	0	4.137413	-0.708891	0.515991
12	6	0	4.774039	-0.438561	-0.690241
13	6	0	4.059384	0.188280	-1.697978
14	6	0	2.726939	0.529429	-1.500993
15	8	0	0.172703	0.286131	3.966497
16	8	0	0.596562	2.243417	2.049074
17	1	0	2.185315	1.013204	-2.296620
18	1	0	4.533049	0.410849	-2.639872
19	1	0	5.806457	-0.707872	-0.836449
20	1	0	4.680822	-1.187775	1.313176
21	1	0	2.341602	-0.563174	1.655588
22	1	0	0.304297	1.270401	-0.942410
23	1	0	-2.598447	-1.857004	0.800153
24	1	0	-4.984262	-0.985993	0.073015
25	1	0	-4.817421	1.336206	-1.089708
26	1	0	0.315075	1.050446	3.383467

27	1	0	0.037115	-0.436272	3.367267
28	1	0	1.433098	2.678093	2.154952
29	1	0	0.618753	1.480329	0.914312

MP2/6-31+G(d)

C	6.0	2.9069325878	0.0596640419	-1.3669378962
C	6.0	1.9250241855	-0.2595694284	-0.4388144273
S	16.0	2.6121112667	-1.0806100279	0.9190093335
C	6.0	4.1892279095	-1.0117631013	0.2448945231
C	6.0	4.1948582262	-0.3650618104	-0.9798699507
C	6.0	0.4783017536	0.0509442921	-0.6090295561
O	8.0	0.1320087609	0.6716768666	-1.6277934695
C	6.0	-0.4403429014	-0.3157919101	0.4962729595
C	6.0	-1.8816085782	-0.4829642265	0.1443316918
C	6.0	-2.6352191032	0.5657681426	-0.4114493359
C	6.0	-3.9979258909	0.3969101897	-0.6794024807
C	6.0	-4.6408076617	-0.8107379677	-0.3868637771
C	6.0	-3.9040265508	-1.8558885569	0.1784777336
C	6.0	-2.5405334091	-1.6886769631	0.4350120482
O	8.0	0.0915269311	3.7580076572	0.1284926272
O	8.0	-0.2242090076	1.9286121308	2.1139583754
H	1.0	-1.9741272732	-2.5058378368	0.8799953144
H	1.0	-4.3892511754	-2.7994056832	0.4225673559
H	1.0	-5.7038668511	-0.9335996417	-0.5869719894
H	1.0	-4.5647088002	1.2213101119	-1.1084588337
H	1.0	-2.1538986312	1.5164255064	-0.6164700402
H	1.0	-0.0739595049	-1.2006220721	1.0288705626
H	1.0	2.6566601382	0.5913569513	-2.2782225733
H	1.0	5.0973129337	-0.2062856172	-1.5625673274
H	1.0	5.0396533146	-1.4221243526	0.7775290951
H	1.0	-0.0324888349	3.1377791255	0.9235992034
H	1.0	0.1654822569	3.1445046642	-0.6222836368
H	1.0	-1.0644028495	1.9931667803	2.6077734288
H	1.0	-0.3379610932	0.5617021623	1.2182266371

E_{HF}= -1084.07178668
E_{MP2}= -1086.3443515638
Thermal Correction to Free Energy 298 K, 1 bar = 0.185192

2PAT-E^{-}-$(H_2O)_3$

HF/6-31+G(d)

1	6	0	-2.477787	0.385710	-0.733161
2	6	0	-1.877128	-0.805946	-0.284320
3	6	0	-2.744225	-1.873009	0.018641
4	6	0	-4.116807	-1.763076	-0.112250
5	6	0	-4.692614	-0.577537	-0.553855
6	6	0	-3.855200	0.486873	-0.861804
7	6	0	-0.442042	-0.994495	-0.115271
8	6	0	0.547656	-0.064797	-0.338977
9	8	0	0.394320	1.146412	-0.655854
10	6	0	1.980631	-0.499445	-0.166386
11	16	0	2.512229	-2.151493	0.012907
12	6	0	4.164680	-1.668070	0.138520
13	6	0	4.298314	-0.330222	0.041492
14	6	0	3.041609	0.339295	-0.137223

15	8	0	1.602279	3.709632	-1.378157
16	1	0	-2.322646	-2.802293	0.364021
17	1	0	-4.741063	-2.606575	0.133198
18	1	0	-5.760514	-0.487634	-0.655769
19	1	0	-4.277165	1.414991	-1.210360
20	1	0	-1.852137	1.218286	-0.982484
21	1	0	-0.146214	-1.985353	0.181639
22	1	0	2.933344	1.400403	-0.242431
23	1	0	5.243101	0.179865	0.091144
24	1	0	4.938507	-2.398356	0.270121
25	1	0	1.252882	4.051461	-0.563680
26	1	0	1.276080	2.811315	-1.402817
27	8	0	-0.094793	3.225235	1.208883
28	1	0	0.024519	2.495611	0.596246
29	1	0	-0.468082	2.821799	1.983292
30	8	0	-1.429937	0.841219	2.747653
31	1	0	-2.203154	0.852943	2.196770
32	1	0	-0.830595	0.265746	2.281969

MP2/6-31+G(d)

C	6.0	-2.4317368113	-0.1953863022	-0.9514640427
C	6.0	-1.6807349566	-1.0519304620	-0.0802530134
C	6.0	-2.4081309821	-2.0655145845	0.6263922781
C	6.0	-3.7965230495	-2.2413471345	0.4545211902
C	6.0	-4.5208303266	-1.3948402092	-0.4239563849
C	6.0	-3.8179926625	-0.3984313354	-1.1441722060
C	6.0	-0.2458494610	-0.8996486894	0.1685895599
C	6.0	0.6420735256	-0.0910770198	-0.5752365051
O	8.0	0.2964401913	0.8226294431	-1.4671357527
C	6.0	2.1122449727	-0.2157827904	-0.3192988777
S	16.0	2.8802899720	-1.6447515490	0.5576298775
C	6.0	4.5274811264	-0.9157147082	0.3049413906
C	6.0	4.4461248736	0.2819810581	-0.3896227819
C	6.0	3.1010673335	0.6683603352	-0.7373809681
O	8.0	-0.1116901981	3.6337923103	-1.1813109244
H	1.0	-1.8615123438	-2.7307310084	1.3046333403
H	1.0	-4.3178501061	-3.0251998937	1.0129923305
H	1.0	-5.5954249970	-1.5366806158	-0.5709253767
H	1.0	-4.3594681324	0.2587745183	-1.8312732148
H	1.0	-1.8945163330	0.5699171300	-1.5115447096
H	1.0	0.2013891615	-1.6744872357	0.8054836839
H	1.0	2.8349510466	1.5643918112	-1.2957423629
H	1.0	5.3288928503	0.8726087090	-0.6372745508
H	1.0	5.4032893605	-1.4223660955	0.6978070138
H	1.0	-0.5854230069	3.7489187656	-0.3261734077
H	1.0	0.0653089489	2.6711430541	-1.3371374026
O	8.0	-1.7249226440	3.5326615192	1.3105109671
H	1.0	-2.6204816863	3.3148307413	0.9912556470
H	1.0	-1.3192732501	2.7438411757	1.7599478439
O	8.0	-0.6720068044	1.2280340739	2.3208880322
H	1.0	-0.5013945726	0.8563517771	3.2062443834
H	1.0	-0.4530609742	0.5623125469	1.6090048700

E_{HF}= -1160.15499302
E_{MP2}= -1161.5327949030
Thermal Correction to Free Energy 298 K, 1 bar = 0.211625

TS $(H_2O)_3$

HF/6-31+G(d)

1	6	0	2.990973	0.116988	-1.213487
2	6	0	2.027016	-0.438289	-0.443957
3	16	0	2.726324	-1.492356	0.748160
4	6	0	4.315949	-1.166487	0.178007
5	6	0	4.313196	-0.300005	-0.858030
6	6	0	0.553671	-0.167835	-0.605883
7	8	0	0.233662	0.555045	-1.523295
8	6	0	-0.348357	-0.719179	0.404424
9	6	0	-1.795828	-0.867864	0.059720
10	6	0	-2.562060	0.187800	-0.446505
11	6	0	-3.912035	0.026421	-0.711349
12	6	0	-4.547064	-1.186474	-0.471244
13	6	0	-3.804728	-2.238792	0.039835
14	6	0	-2.449616	-2.077882	0.297338
15	8	0	-0.128219	3.619124	-1.352757
16	8	0	-0.607921	3.609467	1.562602
17	8	0	-0.165485	1.078716	2.330726
18	1	0	-1.888649	-2.908277	0.692483
19	1	0	-4.275191	-3.187926	0.236899
20	1	0	-5.597649	-1.304675	-0.675979
21	1	0	-4.473684	0.857380	-1.103834
22	1	0	-2.096398	1.135334	-0.632449
23	1	0	0.040783	-1.641828	0.820631
24	1	0	2.759459	0.806228	-2.001571
25	1	0	5.202953	0.040315	-1.354821
26	1	0	5.165401	-1.627227	0.642224
27	1	0	-0.230024	3.682953	-0.403901
28	1	0	-0.003677	2.691947	-1.525971
29	1	0	-1.542605	3.666161	1.702503
30	1	0	-0.370001	2.708153	1.864539
31	1	0	0.582703	0.904945	2.887234
32	1	0	-0.237591	0.144993	1.370018

MP2/6-31+G(d)

C	3.005279	0.398252	-1.155383
C	2.016840	-0.317277	-0.487811
S	2.768478	-1.506021	0.683961
C	4.419132	-0.955317	0.176434
C	4.349683	0.041407	-0.786963
C	0.539001	-0.143563	-0.635442
O	0.131496	0.637006	-1.573279
C	-0.329001	-0.771987	0.363311
C	-1.790614	-0.868652	0.047535
C	-2.559464	0.292979	-0.245400
C	-3.943714	0.195428	-0.512840
C	-4.598167	-1.060673	-0.483306
C	-3.848979	-2.222386	-0.179309
C	-2.462285	-2.121659	0.082114
O	-0.163764	3.577128	-1.125586
O	-0.964930	3.178747	1.535507
O	-0.151278	0.879520	2.447986
H	-1.887899	-3.025960	0.309418
H	-4.339783	-3.199554	-0.148012

H	-5.669832	-1.132001	-0.687989
H	-4.512194	1.101555	-0.738935
H	-2.071955	1.267413	-0.251671
H	0.070118	-1.742986	0.704554
H	2.740201	1.170517	-1.875654
H	5.239316	0.509703	-1.208287
H	5.295052	-1.406346	0.631991
H	-0.428574	3.528773	-0.169169
H	-0.065141	2.663288	-1.470372
H	-1.860409	3.369669	1.869574
H	-0.602042	2.307194	1.952569
H	0.633092	0.776461	3.031375
H	-0.196792	-0.000461	1.413821

E_{HF}= -1160.11052809
E_{MP2}= -1161.5173659154
Thermal Correction to Free Energy 298 K, 1 bar = 0.207836

2. INTRINSIC REACTION COORDINATE CALCULATIONS (AT HF LEVEL) FOR GAS-PHASE REACTION MEDIATED BY TWO WATER MOLECULES.

Reaction coordinate value: -0.0996

1	6	0	2.919582	0.037779	-1.337845
2	6	0	1.960086	-0.275669	-0.436151
3	16	0	2.645517	-1.113382	0.921245
4	6	0	4.221272	-1.033535	0.240353
5	6	0	4.226434	-0.397275	-0.951792
6	6	0	0.498810	0.055042	-0.604519
7	8	0	0.193650	0.674978	-1.599132
8	6	0	-0.413612	-0.324308	0.475407
9	6	0	-1.860999	-0.485960	0.132141
10	6	0	-2.614881	0.555853	-0.420171
11	6	0	-3.963724	0.395445	-0.690427
12	6	0	-4.609893	-0.803353	-0.409772
13	6	0	-3.881029	-1.841076	0.148320
14	6	0	-2.526382	-1.680803	0.411513
15	8	0	0.131095	3.736066	0.139203
16	8	0	-0.215882	1.777670	2.072193
17	1	0	-1.974162	-2.499464	0.841940
18	1	0	-4.361398	-2.778099	0.377322
19	1	0	-5.659824	-0.921114	-0.618521
20	1	0	-4.517224	1.215490	-1.116396
21	1	0	-2.137149	1.492866	-0.629572
22	1	0	-0.050267	-1.189258	1.017924
23	1	0	2.694025	0.565730	-2.243476
24	1	0	5.111822	-0.232856	-1.538090
25	1	0	5.060817	-1.448783	0.762102
26	1	0	0.023062	3.138657	0.895510

27	1	0	0.208919	3.152060	-0.604169
28	1	0	-1.022563	1.888932	2.558792
29	1	0	-0.309208	0.707383	1.316265

Reaction coordinate value: -0.1995

1	6	0	2.919481	0.037661	-1.337916
2	6	0	1.960031	-0.275759	-0.436215
3	16	0	2.645538	-1.113504	0.921138
4	6	0	4.221447	-1.033624	0.240238
5	6	0	4.226467	-0.397406	-0.951838
6	6	0	0.497787	0.054565	-0.603288
7	8	0	0.193682	0.675177	-1.599590
8	6	0	-0.413239	-0.325578	0.473372
9	6	0	-1.860260	-0.485894	0.132313
10	6	0	-2.614974	0.555658	-0.420332
11	6	0	-3.963729	0.395192	-0.690528
12	6	0	-4.610019	-0.803575	-0.409913
13	6	0	-3.880919	-1.841259	0.148262
14	6	0	-2.526489	-1.681052	0.411534
15	8	0	0.131032	3.735970	0.139014
16	8	0	-0.215947	1.775415	2.070883
17	1	0	-1.974053	-2.499756	0.841599
18	1	0	-4.361308	-2.778390	0.377095
19	1	0	-5.659931	-0.921397	-0.618726
20	1	0	-4.517284	1.215222	-1.116629
21	1	0	-2.137188	1.492546	-0.630337
22	1	0	-0.049663	-1.187317	1.020436
23	1	0	2.693757	0.565535	-2.243537
24	1	0	5.111869	-0.233019	-1.538210
25	1	0	5.061016	-1.448919	0.761922
26	1	0	0.023415	3.139694	0.893875
27	1	0	0.208958	3.151885	-0.604571
28	1	0	-1.023153	1.885647	2.556780
29	1	0	-0.308683	0.748248	1.345491

Reaction coordinate value: -0.3995

1	6	0	2.919282	0.037420	-1.338069
2	6	0	1.959895	-0.275957	-0.436352
3	16	0	2.645557	-1.113761	0.920923
4	6	0	4.221775	-1.033820	0.240003
5	6	0	4.226516	-0.397686	-0.951932
6	6	0	0.495743	0.053559	-0.600828
7	8	0	0.193722	0.675607	-1.600561
8	6	0	-0.412582	-0.328785	0.468810
9	6	0	-1.858873	-0.485762	0.132629
10	6	0	-2.615177	0.555301	-0.420658
11	6	0	-3.963749	0.394714	-0.690733
12	6	0	-4.610282	-0.803989	-0.410197
13	6	0	-3.880720	-1.841616	0.148142
14	6	0	-2.526750	-1.681559	0.411571
15	8	0	0.130893	3.735771	0.138643
16	8	0	-0.216183	1.771476	2.068655
17	1	0	-1.973870	-2.500325	0.840926
18	1	0	-4.361165	-2.778949	0.376645
19	1	0	-5.660159	-0.921929	-0.619134
20	1	0	-4.517416	1.214721	-1.117081
21	1	0	-2.137250	1.491921	-0.631840
22	1	0	-0.048617	-1.183874	1.025244
23	1	0	2.693213	0.565130	-2.243666
24	1	0	5.111954	-0.233368	-1.538446
25	1	0	5.061382	-1.449214	0.761568

26	1	0	0.024625	3.141621	0.890672
27	1	0	0.208994	3.151399	-0.605359
28	1	0	-1.024390	1.879652	2.552936
29	1	0	-0.304139	0.829627	1.404547

Reaction coordinate value: -0.5994

1	6	0	2.918903	0.036796	-1.338503
2	6	0	1.959615	-0.276269	-0.436561
3	16	0	2.645672	-1.113746	0.920782
4	6	0	4.222228	-1.033944	0.239662
5	6	0	4.226477	-0.398263	-0.952287
6	6	0	0.493189	0.052209	-0.597811
7	8	0	0.193609	0.675798	-1.601957
8	6	0	-0.411713	-0.333244	0.462776
9	6	0	-1.857179	-0.485459	0.133403
10	6	0	-2.615436	0.554858	-0.420910
11	6	0	-3.963844	0.394029	-0.690663
12	6	0	-4.610656	-0.804493	-0.409811
13	6	0	-3.880464	-1.841907	0.148971
14	6	0	-2.527046	-1.681957	0.412436
15	8	0	0.130765	3.735682	0.137055
16	8	0	-0.216175	1.769079	2.066764
17	1	0	-1.973610	-2.500722	0.841068
18	1	0	-4.360934	-2.779404	0.377370
19	1	0	-5.660504	-0.922647	-0.618772
20	1	0	-4.517643	1.213877	-1.117502
21	1	0	-2.137365	1.491053	-0.633976
22	1	0	-0.047261	-1.179271	1.031748
23	1	0	2.692301	0.564025	-2.244201
24	1	0	5.111899	-0.234220	-1.539106
25	1	0	5.061926	-1.449318	0.761113
26	1	0	0.026379	3.143884	0.886502
27	1	0	0.209001	3.150708	-0.607204
28	1	0	-1.025776	1.873952	2.548304
29	1	0	-0.299192	0.909410	1.463044

Reaction coordinate value: -0.7953

1	6	0	2.918158	0.035991	-1.338745
2	6	0	1.958734	-0.276486	-0.436340
3	16	0	2.645856	-1.113492	0.920955
4	6	0	4.223228	-1.033956	0.239626
5	6	0	4.226457	-0.399052	-0.952333
6	6	0	0.488503	0.050396	-0.592442
7	8	0	0.193620	0.676731	-1.604010
8	6	0	-0.410111	-0.343227	0.450090
9	6	0	-1.854191	-0.484564	0.134896
10	6	0	-2.615593	0.554469	-0.421281
11	6	0	-3.964002	0.393161	-0.690588
12	6	0	-4.611362	-0.804913	-0.409283
13	6	0	-3.880045	-1.841952	0.150381
14	6	0	-2.527522	-1.682094	0.414206
15	8	0	0.130659	3.736096	0.134071
16	8	0	-0.215852	1.771356	2.068623
17	1	0	-1.973419	-2.501371	0.841081
18	1	0	-4.360322	-2.779785	0.378320
19	1	0	-5.661106	-0.923521	-0.618516
20	1	0	-4.517662	1.212704	-1.118489
21	1	0	-2.137491	1.489714	-0.638700
22	1	0	-0.044423	-1.168798	1.045810
23	1	0	2.690622	0.562324	-2.244660
24	1	0	5.111793	-0.235566	-1.539677

25	1	0	5.063069	-1.449373	0.760820
26	1	0	0.029927	3.146757	0.881896
27	1	0	0.209237	3.150090	-0.610097
28	1	0	-1.030212	1.866303	2.542148
29	1	0	-0.294646	0.966300	1.506191

Reaction coordinate value: -0.9948

1	6	0	2.914769	0.033816	-1.337888
2	6	0	1.954985	-0.276163	-0.433966
3	16	0	2.646697	-1.112832	0.922143
4	6	0	4.226082	-1.034005	0.240233
5	6	0	4.225426	-0.401088	-0.952131
6	6	0	0.481368	0.047776	-0.588213
7	8	0	0.193704	0.680841	-1.606395
8	6	0	-0.407446	-0.376508	0.416065
9	6	0	-1.850713	-0.484254	0.137224
10	6	0	-2.614175	0.553654	-0.421682
11	6	0	-3.964239	0.391377	-0.689532
12	6	0	-4.613019	-0.805026	-0.407086
13	6	0	-3.879689	-1.840683	0.155233
14	6	0	-2.528643	-1.680321	0.420772
15	8	0	0.130974	3.738715	0.124070
16	8	0	-0.215038	1.788211	2.084965
17	1	0	-1.973841	-2.502536	0.841051
18	1	0	-4.358186	-2.779909	0.381152
19	1	0	-5.662185	-0.925102	-0.618347
20	1	0	-4.516010	1.209974	-1.121686
21	1	0	-2.135923	1.485215	-0.654009
22	1	0	-0.036637	-1.144259	1.078124
23	1	0	2.685484	0.557776	-2.244715
24	1	0	5.109715	-0.239088	-1.541714
25	1	0	5.066464	-1.449582	0.760471
26	1	0	0.039826	3.155374	0.876059
27	1	0	0.210641	3.148661	-0.617341
28	1	0	-1.047261	1.858849	2.531162
29	1	0	-0.274601	0.996347	1.520205

Reaction coordinate value: 0.02963

1	6	0	2.919769	0.037921	-1.337781
2	6	0	1.960218	-0.275570	-0.436112
3	16	0	2.645496	-1.113225	0.921378
4	6	0	4.221013	-1.033435	0.240495
5	6	0	4.226400	-0.397108	-0.951753
6	6	0	0.500479	0.055707	-0.606318
7	8	0	0.193577	0.674650	-1.598540
8	6	0	-0.414230	-0.323194	0.477809
9	6	0	-1.862067	-0.486156	0.131798
10	6	0	-2.614741	0.556121	-0.419954
11	6	0	-3.963697	0.395800	-0.690301
12	6	0	-4.609693	-0.803051	-0.409591
13	6	0	-3.881180	-1.840842	0.148381
14	6	0	-2.526244	-1.680498	0.411440
15	8	0	0.131213	3.736162	0.139498
16	8	0	-0.215639	1.781190	2.074205
17	1	0	-1.974307	-2.499061	0.842411
18	1	0	-4.361548	-2.777700	0.377643
19	1	0	-5.659649	-0.920716	-0.618240
20	1	0	-4.517134	1.215872	-1.116062
21	1	0	-2.137056	1.493324	-0.628419
22	1	0	-0.051183	-1.192477	1.013996
23	1	0	2.694458	0.566004	-2.243415

24	1	0	5.111782	-0.232636	-1.537930
25	1	0	5.060519	-1.448606	0.762350
26	1	0	0.021889	3.137259	0.897708
27	1	0	0.208974	3.152331	-0.603646
28	1	0	-1.021084	1.894626	2.562492
29	1	0	-0.312972	0.653199	1.279070

Reaction coordinate value: 0.08945

1	6	0	2.919929	0.037584	-1.337737
2	6	0	1.960347	-0.275673	-0.436018
3	16	0	2.645469	-1.112912	0.921794
4	6	0	4.220869	-1.033355	0.240919
5	6	0	4.226416	-0.397322	-0.951560
6	6	0	0.501492	0.055918	-0.607201
7	8	0	0.193555	0.673985	-1.598468
8	6	0	-0.414708	-0.322918	0.478784
9	6	0	-1.862601	-0.486353	0.131582
10	6	0	-2.614653	0.556125	-0.420062
11	6	0	-3.963648	0.395789	-0.690437
12	6	0	-4.609574	-0.803015	-0.409385
13	6	0	-3.881266	-1.840690	0.148835
14	6	0	-2.526203	-1.680276	0.411783
15	8	0	0.131307	3.736224	0.138631
16	8	0	-0.215379	1.783669	2.074751
17	1	0	-1.974398	-2.498647	0.843272
18	1	0	-4.361664	-2.777392	0.378490
19	1	0	-5.659539	-0.920678	-0.617973
20	1	0	-4.517054	1.215765	-1.116321
21	1	0	-2.136961	1.493368	-0.628266
22	1	0	-0.051698	-1.193950	1.012296
23	1	0	2.694767	0.565502	-2.243512
24	1	0	5.111820	-0.232984	-1.537690
25	1	0	5.060342	-1.448338	0.762970
26	1	0	0.020574	3.136868	0.897762
27	1	0	0.209182	3.152335	-0.604296
28	1	0	-1.019554	1.899187	2.564734
29	1	0	-0.317581	0.629645	1.263495

Reaction coordinate value: 0.1494

1	6	0	2.920100	0.037158	-1.337734
2	6	0	1.960493	-0.275819	-0.435948
3	16	0	2.645426	-1.112556	0.922250
4	6	0	4.220677	-1.033282	0.241367
5	6	0	4.226413	-0.397613	-0.951387
6	6	0	0.502593	0.056039	-0.608242
7	8	0	0.193502	0.673199	-1.598455
8	6	0	-0.415263	-0.323106	0.479569
9	6	0	-1.863311	-0.486574	0.131334
10	6	0	-2.614586	0.556127	-0.420190
11	6	0	-3.963611	0.395775	-0.690571
12	6	0	-4.609449	-0.802978	-0.409097
13	6	0	-3.881393	-1.840529	0.149417
14	6	0	-2.526207	-1.680051	0.412204
15	8	0	0.131391	3.736255	0.137580
16	8	0	-0.215167	1.786803	2.075478
17	1	0	-1.974518	-2.498153	0.844324
18	1	0	-4.361854	-2.777031	0.379565
19	1	0	-5.659431	-0.920632	-0.617589
20	1	0	-4.517006	1.215640	-1.116579
21	1	0	-2.136836	1.493400	-0.628033
22	1	0	-0.052472	-1.196265	1.009871

23	1	0	2.695098	0.564864	-2.243680
24	1	0	5.111844	-0.233444	-1.537469
25	1	0	5.060109	-1.448044	0.763652
26	1	0	0.019693	3.136440	0.897714
27	1	0	0.209339	3.152224	-0.605079
28	1	0	-1.017992	1.904603	2.567197
29	1	0	-0.319330	0.606339	1.248955

Reaction coordinate value: 0.2093

1	6	0	2.920335	0.036411	-1.337777
2	6	0	1.960720	-0.276092	-0.435874
3	16	0	2.645360	-1.112013	0.922946
4	6	0	4.220430	-1.033190	0.242038
5	6	0	4.226420	-0.398149	-0.951137
6	6	0	0.503888	0.055932	-0.609457
7	8	0	0.193423	0.672007	-1.598658
8	6	0	-0.415910	-0.324055	0.479980
9	6	0	-1.864186	-0.486868	0.131044
10	6	0	-2.614536	0.556062	-0.420457
11	6	0	-3.963568	0.395650	-0.690812
12	6	0	-4.609300	-0.803007	-0.408653
13	6	0	-3.881570	-1.840355	0.150378
14	6	0	-2.526288	-1.679797	0.412921
15	8	0	0.131485	3.736245	0.135769
16	8	0	-0.214905	1.791195	2.076204
17	1	0	-1.974671	-2.497454	0.845925
18	1	0	-4.362160	-2.776561	0.381281
19	1	0	-5.659305	-0.920668	-0.617001
20	1	0	-4.516986	1.215320	-1.117070
21	1	0	-2.136648	1.493321	-0.627939
22	1	0	-0.053540	-1.199741	1.006492
23	1	0	2.695513	0.563721	-2.244004
24	1	0	5.111902	-0.234280	-1.537174
25	1	0	5.059802	-1.447608	0.764681
26	1	0	0.018796	3.136219	0.896986
27	1	0	0.209509	3.151912	-0.606519
28	1	0	-1.016008	1.911945	2.570067
29	1	0	-0.320584	0.585258	1.237470

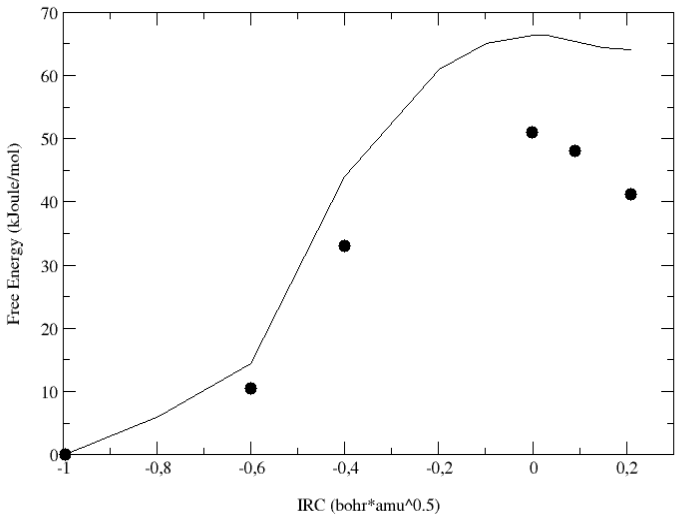

Figure S1: Summary of IRC calculation in Gas-phase (continuous line) and in water (PMM calculations, full-circles)

3. MOLECULAR DYNAMICS SIMULATIONS

Structures (pdb format), atom type (Gromos force-field) and MP2 atomic charges (see text) and atomic mass utilized in the simulations.

2PAT-KH

```
ATOM      1  C   FNT     1      15.400  16.500  15.510  1.00  0.00
ATOM      2  O   FNT     1      15.010  16.950  16.600  1.00  0.00
ATOM      3  C   FNT     1      16.880  16.450  15.170  1.00  0.00
ATOM      4  H   FNT     1      17.070  17.000  14.240  1.00  0.00
ATOM      5  H   FNT     1      17.410  16.970  15.980  1.00  0.00
ATOM      6  C   FNT     1      17.360  15.020  15.040  1.00  0.00
ATOM      7  C   FNT     1      18.140  14.610  13.950  1.00  0.00
ATOM      8  C   FNT     1      18.570  13.290  13.840  1.00  0.00
ATOM      9  C   FNT     1      18.210  12.350  14.810  1.00  0.00
ATOM     10  C   FNT     1      17.430  12.750  15.910  1.00  0.00
ATOM     11  C   FNT     1      17.010  14.070  16.020  1.00  0.00
ATOM     12  H   FNT     1      18.420  15.340  13.190  1.00  0.00
ATOM     13  H   FNT     1      19.180  12.980  12.990  1.00  0.00
ATOM     14  H   FNT     1      18.540  11.310  14.720  1.00  0.00
ATOM     15  H   FNT     1      17.150  12.020  16.670  1.00  0.00
ATOM     16  H   FNT     1      16.410  14.380  16.880  1.00  0.00
ATOM     17  C   FNT     1      14.430  15.970  14.540  1.00  0.00
ATOM     18  S   FNT     1      14.850  15.260  13.020  1.00  0.00
ATOM     19  C   FNT     1      13.210  15.040  12.600  1.00  0.00
ATOM     20  C   FNT     1      12.350  15.480  13.590  1.00  0.00
ATOM     21  C   FNT     1      13.050  16.020  14.700  1.00  0.00
ATOM     22  H   FNT     1      12.590  16.430  15.590  1.00  0.00
ATOM     23  H   FNT     1      11.270  15.420  13.510  1.00  0.00
ATOM     24  H   FNT     1      12.950  14.580  11.650  1.00  0.00
```

```
 Nr. Atom-Type  Res.  Res.Name Atom-Name   Charge Atomic-Mass
  1       C     1    FNT      C     1    -1.1433      12.011   ; qtot 0
  2       O     1    FNT      O     1     -0.0783     15.9994  ; qtot 0
  3       C     1    FNT      C     1    0.9070       12.011   ; qtot 0
  4       HC    1    FNT      H     1    -0.5039       1.008   ; qtot 0
  5       HC    1    FNT      H     1    0.3971        1.008   ; qtot 0
  6       C     1    FNT      C     1    -1.7279       12.011   ; qtot 0
  7       C     1    FNT      C     1    0.7017        12.011   ; qtot 0
  8       C     1    FNT      C     1    -0.9976      12.011   ; qtot 0
  9       C     1    FNT      C     1    0.7066        12.011   ; qtot 0
 10       C     1    FNT      C     1     -0.9207      12.011   ; qtot 0
 11       C     1    FNT      C     1     0.9910       12.011   ; qtot 0
 12       HC    1    FNT      H     1      0.2035      1.008   ; qtot 0
 13       HC    1    FNT      H     1      0.2563      1.008   ; qtot 0
 14       HC    1    FNT      H     1      0.0209      1.008   ; qtot 0
 15       HC    1    FNT      H     1      0.2986      1.008   ; qtot 0
 16       HC    1    FNT      H     1      -0.1828      1.008   ; qtot 0
 17       C     1    FNT      C     1     1.5542       12.011   ; qtot 0
 18       S     1    FNT      S     1     0.4676     32.065    ; qtot -0.83
 19       C     1    FNT      C     1    -1.6000       12.011   ; qtot 0
 20       C     1    FNT      C     1     0.9603       12.011   ; qtot 0
 21       C     1    FNT      C     1     -1.1735      12.011   ; qtot 0
 22       HC    1    FNT      H     1      0.3911      1.008   ; qtot 0
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23	HC	1	FNT	H	1	-0.1498	1.008 ; qtot 0
24	HC	1	FNT	H	1	0.6220	1.008 ; qtot 0

2PAT-EH

ATOM	1	S	FNT	1	10.910	9.990	17.640	1.00	0.00
ATOM	2	C	FNT	1	10.660	10.000	19.350	1.00	0.00
ATOM	3	C	FNT	1	11.810	10.040	20.100	1.00	0.00
ATOM	4	C	FNT	1	12.920	10.070	19.220	1.00	0.00
ATOM	5	C	FNT	1	12.620	10.010	17.860	1.00	0.00
ATOM	6	H	FNT	1	9.590	9.950	19.550	1.00	0.00
ATOM	7	H	FNT	1	11.790	10.000	21.190	1.00	0.00
ATOM	8	H	FNT	1	13.970	10.090	19.520	1.00	0.00
ATOM	9	C	FNT	1	13.510	10.080	16.700	1.00	0.00
ATOM	10	O	FNT	1	14.620	9.320	16.910	1.00	0.00
ATOM	11	H	FNT	1	15.100	9.520	16.050	1.00	0.00
ATOM	12	C	FNT	1	13.210	10.480	15.430	1.00	0.00
ATOM	13	H	FNT	1	12.290	11.070	15.410	1.00	0.00
ATOM	14	C	FNT	1	13.570	10.240	14.040	1.00	0.00
ATOM	15	C	FNT	1	13.600	8.960	13.490	1.00	0.00
ATOM	16	C	FNT	1	13.630	8.710	12.120	1.00	0.00
ATOM	17	C	FNT	1	13.600	9.820	11.290	1.00	0.00
ATOM	18	C	FNT	1	13.560	11.100	11.820	1.00	0.00
ATOM	19	C	FNT	1	13.540	11.340	13.190	1.00	0.00
ATOM	20	H	FNT	1	13.710	8.160	14.210	1.00	0.00
ATOM	21	H	FNT	1	13.450	7.700	11.730	1.00	0.00
ATOM	22	H	FNT	1	13.780	9.720	10.220	1.00	0.00
ATOM	23	H	FNT	1	13.600	12.040	11.250	1.00	0.00
ATOM	24	H	FNT	1	13.420	12.350	13.570	1.00	0.00

Nr.	Atom-Type	Res.	Res.Name	Atom-Name	Charge	Atomic-Mass	
1	S	1	FNT	S	1	0.0	32.065 ; qtot -0.83
2	CR1	1	FNT	C	1	-0.2	12.011 ; qtot -0.415
3	CR1	1	FNT	C	1	-0.3	12.011 ; qtot -0.415
4	CR1	1	FNT	C	1	0.00	12.011 ; qtot -0.415
5	CR1	1	FNT	C	1	-0.1	12.011 ; qtot -0.415
6	HC	1	FNT	H	1	0.1	1.008 ; qtot 0
7	HC	1	FNT	H	1	0.1	1.008 ; qtot -0.28
8	HC	1	FNT	H	1	0.1	1.008 ; qtot 0
9	C	1	FNT	C	1	0.6	12.011 ; qtot 0
10	O	1	FNT	O	1	-0.7	15.9994 ; qtot 0.38
11	H	1	FNT	H	1	0.5	1.008 ; qtot 0
12	C	1	FNT	C	1	-0.7	12.011 ; qtot -0.28
13	H	1	FNT	H	1	0.3	1.008 ; qtot 0
14	CR1	1	FNT	C	1	0.6	12.011 ; qtot 0
15	CR1	1	FNT	C	1	-0.3	12.011 ; qtot 0
16	CR1	1	FNT	C	1	0.00	12.011 ; qtot 0
17	CR1	1	FNT	C	1	-0.2	12.011 ; qtot 0
18	CR1	1	FNT	C	1	0.00	12.011 ; qtot 0
19	CR1	1	FNT	C	1	-0.3	12.011 ; qtot -0.83
20	HC	1	FNT	H	1	0.1	1.008 ; qtot -0.415
21	HC	1	FNT	H	1	0.1	1.008 ; qtot 0
22	HC	1	FNT	H	1	0.1	1.008 ; qtot 0.38
23	HC	1	FNT	H	1	0.1	1.008
24	HC	1	FNT	H	1	0.1	1.008

2PAT-E$^-$

```
ATOM      1  S   FNT     1      11.170   9.180  17.880  1.00  0.00
ATOM      2  C   FNT     1      10.670   9.870  19.380  1.00  0.00
ATOM      3  C   FNT     1      11.650  10.750  19.820  1.00  0.00
ATOM      4  C   FNT     1      12.750  10.920  18.940  1.00  0.00
ATOM      5  C   FNT     1      12.620  10.120  17.810  1.00  0.00
ATOM      6  H   FNT     1       9.790   9.470  19.870  1.00  0.00
ATOM      7  H   FNT     1      11.540  11.350  20.720  1.00  0.00
ATOM      8  H   FNT     1      13.700  11.370  19.230  1.00  0.00
ATOM      9  C   FNT     1      13.430  10.080  16.600  1.00  0.00
ATOM     10  O   FNT     1      14.670  10.660  16.640  1.00  0.00
ATOM     11  C   FNT     1      12.940   9.590  15.430  1.00  0.00
ATOM     12  H   FNT     1      11.880   9.340  15.520  1.00  0.00
ATOM     13  C   FNT     1      13.320   9.500  14.030  1.00  0.00
ATOM     14  C   FNT     1      12.340   9.340  13.050  1.00  0.00
ATOM     15  C   FNT     1      12.630   9.840  11.780  1.00  0.00
ATOM     16  C   FNT     1      13.820  10.450  11.430  1.00  0.00
ATOM     17  C   FNT     1      14.800  10.580  12.400  1.00  0.00
ATOM     18  C   FNT     1      14.520  10.110  13.680  1.00  0.00
ATOM     19  H   FNT     1      11.380   8.850  13.200  1.00  0.00
ATOM     20  H   FNT     1      11.850   9.710  11.030  1.00  0.00
ATOM     21  H   FNT     1      13.990  10.660  10.370  1.00  0.00
ATOM     22  H   FNT     1      15.830  10.670  12.040  1.00  0.00
ATOM     23  H   FNT     1      15.350  10.260  14.370  1.00  0.00
```

```
Nr. Atom-Type  Res.  Res.Name Atom-Name    Charge Atomic-Mass
 1        S     1    FNT      S     1     -0.1     32.065    ; qtot -0.83
 2      CR1     1    FNT      C     1     -0.2      12.011   ; qtot -0.415
 3      CR1     1    FNT      C     1     -0.2      12.011   ; qtot -0.415
 4      CR1     1    FNT      C     1     -0.1      12.011   ; qtot -0.415
 5      CR1     1    FNT      C     1     -0.1      12.011   ; qtot -0.415
 6       HC     1    FNT      H     1      0.2      1.008    ; qtot 0
 7       HC     1    FNT      H     1      0.1      1.008    ; qtot -0.28
 8       HC     1    FNT      H     1      0.1      1.008    ; qtot 0
 9        C     1    FNT      C     1      0.7      12.011   ; qtot 0
10        O     1    FNT      O     1     -0.8      15.9994  ; qtot 0.38
11        C     1    FNT      C     1     -1.0      12.011   ; qtot -0.28
12        H     1    FNT      H     1      0.2      1.008    ; qtot 0
13      CR1     1    FNT      C     1      0.8      12.011   ; qtot 0
14      CR1     1    FNT      C     1     -0.3      12.011   ; qtot 0
15      CR1     1    FNT      C     1      0.00     12.011   ; qtot 0
16      CR1     1    FNT      C     1     -0.3      12.011   ; qtot 0
17      CR1     1    FNT      C     1     -0.1      12.011   ; qtot 0
18      CR1     1    FNT      C     1     -0.4      12.011   ; qtot -0.83
19       HC     1    FNT      H     1      0.1      1.008    ; qtot -0.415
20       HC     1    FNT      H     1      0.1      1.008    ; qtot 0
21       HC     1    FNT      H     1      0.1      1.008    ; qtot 0.38
22       HC     1    FNT      H     1      0.1      1.008
23       HC     1    FNT      H     1      0.1      1.008
```

2PAT-E$^-$(H_2O)

```
ATOM      1  C   KOS     1      -2.468   0.413  -0.737
ATOM      2  C   KOS     1      -1.758  -0.573   0.027
ATOM      3  C   KOS     1      -2.540  -1.592   0.666
ATOM      4  C   KOS     1      -3.948  -1.604   0.588
ATOM      5  C   KOS     1      -4.637  -0.612  -0.155
ATOM      6  C   KOS     1      -3.880   0.393  -0.808
ATOM      7  C   KOS     1      -0.303  -0.620   0.131
```

ATOM 8 C KOS 1 0.592 0.394 -0.246
ATOM 9 O KOS 1 0.266 1.612 -0.689
ATOM 10 C KOS 1 2.056 0.143 -0.107
ATOM 11 S KOS 1 2.796 -1.541 -0.168
ATOM 12 C KOS 1 4.448 -0.828 0.094
ATOM 13 C KOS 1 4.390 0.556 0.177
ATOM 14 C KOS 1 3.057 1.094 0.063
ATOM 15 O KOS 1 -1.173 3.260 0.976
ATOM 16 H KOS 1 -2.026 -2.369 1.241
ATOM 17 H KOS 1 -4.511 -2.400 1.087
ATOM 18 H KOS 1 -5.729 -0.615 -0.211
ATOM 19 H KOS 1 -4.394 1.170 -1.383
ATOM 20 H KOS 1 -1.892 1.183 -1.249
ATOM 21 H KOS 1 0.119 -1.518 0.598
ATOM 22 H KOS 1 2.808 2.153 0.099
ATOM 23 H KOS 1 5.281 1.166 0.334
ATOM 24 H KOS 1 5.312 -1.483 0.145
ATOM 25 H KOS 1 -1.923 2.686 1.217
ATOM 26 H KOS 1 -0.582 2.739 0.350

Nr.	Atom-Type	Res.	Res.Name	Atom-Name	Charge	Atomic-Mass	
1	C	1	KOS	C	1	-0.213921	12.011 ; qtot 0.129
2	C	1	KOS	C	1	0.442430	12.011 ; qtot 0.129
3	C	1	KOS	C	1	-0.310291	12.011 ; qtot 0.129
4	C	1	KOS	C	1	-0.137327	12.011 ; qtot 0.129
5	C	1	KOS	C	1	-0.221977	12.011 ; qtot 0.129
6	C	1	KOS	C	1	-0.141429	12.011 ; qtot 0.129
7	C	1	KOS	C	1	-0.689984	12.011 ; qtot 0.129
8	C	1	KOS	C	1	0.465256	12.011 ; qtot 0.129
9	O	1	KOS	O	1	-0.693002	15.9994 ; qtot 1
10	C	1	KOS	C	1	0.039896	12.011 ; qtot 0.129
11	S	1	KOS	S	1	-0.067124	32.06 ; qtot 0.129
12	C	1	KOS	C	1	-0.307258	12.011 ; qtot 0.129
13	C	1	KOS	C	1	-0.110329	12.011 ; qtot 0.129
14	C	1	KOS	C	1	-0.221246	12.011 ; qtot 0.129
15	O	1	KOS	O	1	-0.956732	15.9994 ; qtot 1
16	H	1	KOS	H	1	0.133165	1.008 ; qtot 1
17	H	1	KOS	H	1	0.104031	1.008 ; qtot 1
18	H	1	KOS	H	1	0.107999	1.008 ; qtot 1
19	H	1	KOS	H	1	0.100533	1.008 ; qtot 1
20	H	1	KOS	H	1	0.147879	1.008 ; qtot 1
21	H	1	KOS	H	1	0.162550	1.008 ; qtot 1
22	H	1	KOS	H	1	0.171121	1.008 ; qtot 1
23	H	1	KOS	H	1	0.115276	1.008 ; qtot 1
24	H	1	KOS	H	1	0.187285	1.008 ; qtot 1
25	H	1	KOS	H	1	0.404491	1.008 ; qtot 1
26	H	1	KOS	H	1	0.488709	1.008 ; qtot 1

2PAT-E$^-$$(H_2O)_2$

ATOM 1 C NNT 1 -2.505 0.337 -0.772
ATOM 2 C NNT 1 -1.801 -0.699 -0.071
ATOM 3 C NNT 1 -2.594 -1.737 0.523
ATOM 4 C NNT 1 -3.996 -1.778 0.378
ATOM 5 C NNT 1 -4.672 -0.756 -0.338
ATOM 6 C NNT 1 -3.909 0.280 -0.929
ATOM 7 C NNT 1 -0.354 -0.708 0.127
ATOM 8 C NNT 1 0.575 0.155 -0.485
ATOM 9 O NNT 1 0.282 1.232 -1.208
ATOM 10 C NNT 1 2.035 -0.098 -0.278

ATOM	11	S	NNT	1	2.721	-1.710	0.294	
ATOM	12	C	NNT	1	4.405	-1.037	0.181	
ATOM	13	C	NNT	1	4.393	0.274	-0.270	
ATOM	14	C	NNT	1	3.073	0.794	-0.525	
ATOM	15	O	NNT	1	0.004	3.733	0.082	
ATOM	16	H	NNT	1	-2.087	-2.543	1.065	
ATOM	17	H	NNT	1	-4.566	-2.590	0.840	
ATOM	18	H	NNT	1	-5.758	-0.787	-0.458	
ATOM	19	H	NNT	1	-4.412	1.069	-1.495	
ATOM	20	H	NNT	1	-1.919	1.128	-1.242	
ATOM	21	H	NNT	1	0.041	-1.556	0.699	
ATOM	22	H	NNT	1	2.860	1.799	-0.887	
ATOM	23	H	NNT	1	5.308	0.857	-0.391	
ATOM	24	H	NNT	1	5.251	-1.658	0.461	
ATOM	25	H	NNT	1	-0.334	3.416	0.947	
ATOM	26	H	NNT	1	0.141	2.932	-0.490	
ATOM	27	O	NNT	1	-1.194	1.787	2.096	
ATOM	28	H	NNT	1	-2.076	1.706	1.678	
ATOM	29	H	NNT	1	-0.636	1.056	1.736	

Nr.	Atom-Type	Res.	Res.Name	Atom-Name	Charge	Atomic-Mass	
1	C	1	KOS	C	1	-0.260957	12.011 ; qtot 0.129
2	C	1	KOS	C	1	0.434001	12.011 ; qtot 0.129
3	C	1	KOS	C	1	-0.424645	12.011 ; qtot 0.129
4	C	1	KOS	C	1	-0.036938	12.011 ; qtot 0.129
5	C	1	KOS	C	1	-0.300801	12.011 ; qtot 0.129
6	C	1	KOS	C	1	-0.047830	12.011 ; qtot 0.129
7	C	1	KOS	C	1	-0.525785	12.011 ; qtot 0.129
8	C	1	KOS	C	1	0.348563	12.011 ; qtot 0.129
9	O	1	KOS	O	1	-0.672904	15.9994 ; qtot 1
10	C	1	KOS	C	1	0.088404	12.011 ; qtot 0.129
11	S	1	KOS	S	1	-0.109046	32.06 ; qtot 0.129
12	C	1	KOS	C	1	-0.254866	12.011 ; qtot 0.129
13	C	1	KOS	C	1	-0.156812	12.011 ; qtot 0.129
14	C	1	KOS	C	1	-0.146846	12.011 ; qtot 0.129
15	O	1	KOS	O	1	-1.018330	15.9994 ; qtot 1
16	H	1	KOS	H	1	0.162413	1.008 ; qtot 1
17	H	1	KOS	H	1	0.090918	1.008 ; qtot 1
18	H	1	KOS	H	1	0.121807	1.008 ; qtot 1
19	H	1	KOS	H	1	0.087069	1.008 ; qtot 1
20	H	1	KOS	H	1	0.139910	1.008 ; qtot 1
21	H	1	KOS	H	1	0.129536	1.008 ; qtot 1
22	H	1	KOS	H	1	0.133553	1.008 ; qtot 1
23	H	1	KOS	H	1	0.124425	1.008 ; qtot 1
24	H	1	KOS	H	1	0.178601	1.008 ; qtot 1
25	H	1	KOS	H	1	0.475884	1.008 ; qtot 1
26	H	1	KOS	H	1	0.524603	1.008 ; qtot 1
27	O	1	KOS	O	1	-0.819932	15.9994 ; qtot 1
28	H	1	KOS	H	1	0.393469	1.008 ; qtot 1
29	H	1	KOS	H	1	0.342539	1.008 ; qtot 1

2PAT-E$^-$(H_2O)$_3$

ATOM	1	C	KOS	1	15.440	14.900	13.470	1.00	0.000
ATOM	2	C	KOS	1	16.180	14.080	14.340	1.00	0.000
ATOM	3	C	KOS	1	15.450	13.110	15.060	1.00	0.000
ATOM	4	C	KOS	1	14.080	12.970	14.930	1.00	0.000
ATOM	5	C	KOS	1	13.370	13.790	14.060	1.00	0.000
ATOM	6	C	KOS	1	14.070	14.750	13.340	1.00	0.000
ATOM	7	C	KOS	1	17.620	14.180	14.540	1.00	0.000

ATOM	8	C	KOS	1	18.480	15.030	13.870	1.00	0.000
ATOM	9	O	KOS	1	18.180	15.940	13.060	1.00	0.000
ATOM	10	C	KOS	1	19.960	14.890	14.130	1.00	0.000
ATOM	11	S	KOS	1	20.720	13.590	15.010	1.00	0.000
ATOM	12	C	KOS	1	22.290	14.270	14.800	1.00	0.000
ATOM	13	C	KOS	1	22.240	15.420	14.090	1.00	0.000
ATOM	14	C	KOS	1	20.900	15.770	13.710	1.00	0.000
ATOM	15	O	KOS	1	17.660	18.820	13.290	1.00	0.000
ATOM	16	H	KOS	1	15.980	12.460	15.740	1.00	0.000
ATOM	17	H	KOS	1	13.570	12.220	15.500	1.00	0.000
ATOM	18	H	KOS	1	12.300	13.680	13.950	1.00	0.000
ATOM	19	H	KOS	1	13.540	15.390	12.650	1.00	0.000
ATOM	20	H	KOS	1	15.960	15.640	12.890	1.00	0.000
ATOM	21	H	KOS	1	18.050	13.440	15.190	1.00	0.000
ATOM	22	H	KOS	1	20.630	16.650	13.150	1.00	0.000
ATOM	23	H	KOS	1	23.100	16.000	13.840	1.00	0.000
ATOM	24	H	KOS	1	23.150	13.780	15.200	1.00	0.000
ATOM	25	H	KOS	1	17.280	18.920	14.150	1.00	0.000
ATOM	26	H	KOS	1	17.820	17.880	13.200	1.00	0.000
ATOM	27	O	KOS	1	16.000	18.850	15.910	1.00	0.000
ATOM	28	H	KOS	1	15.220	18.540	15.480	1.00	0.000
ATOM	29	H	KOS	1	16.440	18.070	16.250	1.00	0.000
ATOM	30	O	KOS	1	17.280	16.460	16.950	1.00	0.000
ATOM	31	H	KOS	1	17.250	15.970	17.760	1.00	0.000
ATOM	32	H	KOS	1	17.380	15.800	16.250	1.00	0.000

Nr.	Atom-Type	Res.	Res.Name	Atom-Name	Charge	Atomic-Mass	
1	C	1	KOS	C	1	-0.238697	12.011 ; qtot 0.129
2	C	1	KOS	C	1	0.439186	12.011 ; qtot 0.129
3	C	1	KOS	C	1	-0.370371	12.011 ; qtot 0.129
4	C	1	KOS	C	1	-0.087716	12.011 ; qtot 0.129
5	C	1	KOS	C	1	-0.272005	12.011 ; qtot 0.129
6	C	1	KOS	C	1	-0.086497	12.011 ; qtot 0.129
7	C	1	KOS	C	1	-0.677566	12.011 ; qtot 0.129
8	C	1	KOS	C	1	0.627647	12.011 ; qtot 0.129
9	O	1	KOS	O	1	-0.671982	15.9994 ; qtot 1
10	C	1	KOS	C	1	-0.116895	12.011 ; qtot 0.129
11	S	1	KOS	S	1	-0.087999	32.06 ; qtot 0.129
12	C	1	KOS	C	1	-0.181151	12.011 ; qtot 0.129
13	C	1	KOS	C	1	-0.206576	12.011 ; qtot 0.129
14	C	1	KOS	C	1	-0.072092	12.011 ; qtot 0.129
15	O	1	KOS	O	1	-0.991806	15.9994 ; qtot 1
16	H	1	KOS	H	1	0.143302	1.008 ; qtot 1
17	H	1	KOS	H	1	0.098402	1.008 ; qtot 1
18	H	1	KOS	H	1	0.115826	1.008 ; qtot 1
19	H	1	KOS	H	1	0.099003	1.008 ; qtot 1
20	H	1	KOS	H	1	0.114118	1.008 ; qtot 1
21	H	1	KOS	H	1	0.144534	1.008 ; qtot 1
22	H	1	KOS	H	1	0.120882	1.008 ; qtot 1
23	H	1	KOS	H	1	0.129750	1.008 ; qtot 1
24	H	1	KOS	H	1	0.151944	1.008 ; qtot 1
25	H	1	KOS	H	1	0.480146	1.008 ; qtot 1
26	H	1	KOS	H	1	0.498283	1.008 ; qtot 1
27	O	1	KOS	O	1	-0.841328	15.9994 ; qtot 1
28	H	1	KOS	H	1	0.382236	1.008 ; qtot 1
29	H	1	KOS	H	1	0.428961	1.008 ; qtot 1
30	O	1	KOS	O	1	-0.830252	15.9994 ; qtot 1
31	H	1	KOS	H	1	0.415680	1.008 ; qtot 1
32	H	1	KOS	H	1	0.343031	1.008 ; qtot 1

4. CALCULATION OF DIFFUSION CONSTANT

Mean square displacement along the IRC represented by the mass-weighted Hessian eigenvector characterizing the first order saddle point.

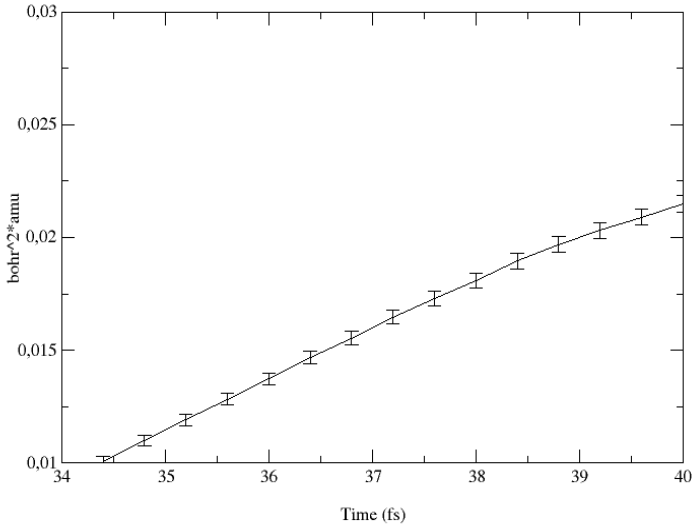

Figure S2: Mean Square Displacements

5. MOLECULAR DYNAMICS. ALGORITHM FOR THE CLUSTER ANALYSIS

The analysis was carried out on the simulation of the enolate in water.
The analysis was performed at each step of the simulation by fitting the QM geometry of the enolate within the adduct (with one, two or three molecules) to the enolate structure of MD simulation. In this way the water molecules to be fitted are included in the simulation box in the correct 'reacting configuration'. Such water molecules are hereafter called as 'dummy-water'.

Then, considering all the water molecules of the box, we extracted the ones (one, two or three) closer to the 'dummy-water', i.e. the ones showing the lowest Root Mean Square Deviation. For example in the figure S3 these water are depicted in yellow.

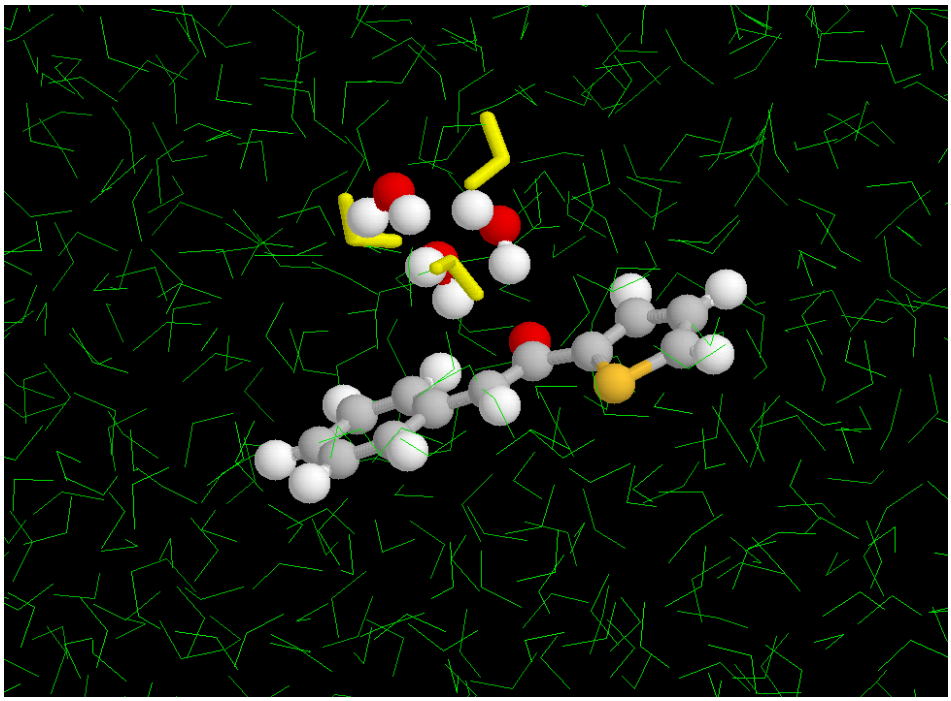

Figure S3: schematic picture representing the reactive cluster representing the reference and the lowest-RMSD-valued water molecules at a given MD frame

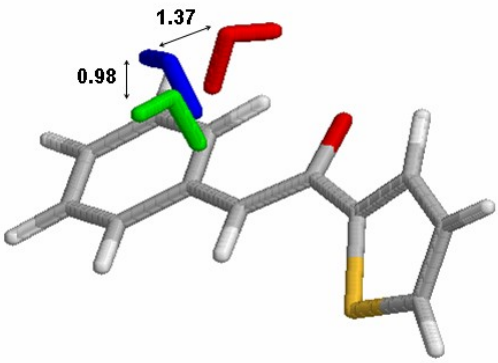

Figure S4: RMSD (Angstrom) between reactive clusters with one, two and three assisting water molecules. Only the reacting water molecule in the three cases (green: three assisting molecule, blue: two assisting molecules, red: one assisting molecule) is shown for the sake of clarity