

# **Role of Hydrogen Bonding in Bulk Aqueous Phase Decomposition, Complexation, and Covalent Hydration of Pyruvic Acid**

## **Supplementary Material-C (Coordinates)**

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## XYZ COORDINATES (MONOMERS IN AQUEOUS PHASE)

## PA CONFORMERS

## Tc

C	0.778695	-0.056568	0.001664
C	-0.762306	0.019117	0.001036
C	1.383516	-1.411051	0.000111
H	1.032861	-1.955983	-0.876845
H	1.032699	-1.959610	0.874683
H	2.465776	-1.340808	0.000241
O	-1.237842	1.255727	-0.003320
H	-0.482024	1.873499	-0.004030
O	-1.472986	-0.959833	0.003480
O	1.384457	0.998111	0.002980

## Tt

C	-0.776918	0.171882	-0.001965
C	0.725310	-0.182249	-0.004087
C	-1.710511	-0.987473	0.002774
H	-1.517187	-1.612858	-0.868727
H	-1.520567	-1.601154	0.883515
H	-2.736186	-0.634767	-0.001145
O	1.496886	0.896297	0.008217
H	2.427935	0.616921	0.006429
O	1.123594	-1.326773	-0.015609
O	-1.113541	1.337686	-0.004593

## Ct

C	-0.791255	-0.044376	-0.002508
C	0.753446	-0.142605	-0.001777
C	-1.415044	1.307125	0.000169
H	-1.070818	1.864878	0.870975
H	-1.087868	1.857078	-0.882517
H	-2.496071	1.213603	0.010465
O	1.336465	1.049626	0.002748
H	2.301932	0.932630	0.010188
O	1.336274	-1.201718	-0.002742
O	-1.406052	-1.089300	-0.005002

## Cc

C	-0.755750	-0.237598	0.068706
C	0.761424	0.057714	-0.067799
C	-1.712636	0.898223	-0.063268
H	-1.574637	1.594734	0.767072
H	-1.518991	1.440983	-0.989296
H	-2.731671	0.526700	-0.049903
O	1.158751	1.317882	0.096469
H	0.420501	1.916403	0.280901
O	1.556123	-0.817772	-0.310183
O	-1.072124	-1.390075	0.267300

## PA HT TAUTOMERS

PAHT<sub>a</sub>

C	0.886585	-0.130036	0.095267
C	-0.569521	0.176261	-0.189901
O	1.681409	0.712431	-0.362407
H	-2.396697	1.087282	0.367181
O	1.065276	-1.172827	0.752308
O	-1.129142	-0.264885	-1.245046
C	-1.377655	0.981709	0.722181
H	-1.346401	0.512378	1.707074
H	-0.893563	1.954870	0.827126
H	-0.531817	-0.791334	-1.809863

PAHT<sub>b</sub>

C	0.909975	-0.126525	0.085650
C	-0.573188	0.082855	-0.130545
O	1.638282	0.599741	-0.615058
H	-2.396646	1.028684	0.407426
O	1.175812	-0.984902	0.947120
O	-1.087128	-0.594869	-1.074734
C	-1.350271	1.002829	0.696617
H	-1.237890	0.696887	1.738293
H	-0.896336	1.992348	0.611100
H	-2.044404	-0.430726	-1.178047

PAHT<sub>c</sub>

C	0.790928	-0.173380	-0.074224
C	-0.732487	0.002351	0.158065
C	1.594815	-1.275797	0.422970
H	1.471926	-1.317555	1.507215
H	1.161699	-2.202189	0.038763
H	2.636959	-1.178940	0.142574
O	-1.313606	-0.866039	0.820917
H	0.513386	1.362612	-0.957794
O	-1.148847	1.051801	-0.393655
O	1.295532	0.754831	-0.758820

## XYZ COORDINATES (MONOMERS IN AQUEOUS PHASE)

## ENOL ISOMERS

enol<sub>a</sub>

C	0.102748	-0.783279	-0.000176
C	-0.112007	0.687724	0.000701
C	-0.879649	-1.685868	0.000469
H	-1.907135	-1.365838	0.001777
H	-0.653622	-2.741672	-0.000485
O	0.832022	1.460891	0.002583
O	-1.387307	1.062724	-0.001690
O	1.415461	-1.134877	-0.001606
H	1.940740	-0.318601	-0.000080
H	-1.427841	2.033039	-0.001494

enol<sub>e</sub>

C	0.730145	0.002623	-0.047029
C	-0.753886	-0.108309	0.039234
O	1.332004	-1.185113	-0.138126
H	2.290403	-1.036552	-0.194206
O	1.332884	1.058422	-0.031437
O	-1.212440	-1.381448	-0.107817
C	-1.506558	0.972479	0.251387
H	-2.581246	0.896440	0.328954
H	-1.037054	1.935336	0.362071
H	-2.176687	-1.379963	-0.038721

enol<sub>b</sub>

C	0.780411	0.484544	-0.052368
C	1.598017	1.707251	-0.299971
C	-0.548066	0.462930	0.066297
H	-1.066194	-0.469636	0.230616
H	-1.140626	1.360130	-0.004535
H	2.453493	-0.395757	-0.134542
O	1.011575	2.900693	-0.304320
H	0.071002	2.840886	-0.084862
O	2.795925	1.613014	-0.498926
O	1.528729	-0.645872	0.025388

enol<sub>f</sub>

C	0.725711	0.108281	0.029709
C	-0.761079	0.122182	0.168477
C	1.452139	1.220127	0.128290
H	0.959632	2.158831	0.319196
H	2.526394	1.198239	0.020415
H	2.158193	-1.131508	-0.323005
O	-1.365581	-1.056634	-0.002500
H	-0.704594	-1.743347	-0.193404
O	-1.412076	1.117380	0.414974
O	1.198451	-1.148729	-0.208564

enol<sub>c</sub>

C	0.731074	-0.034320	-0.052462
C	-0.759306	-0.076717	0.029014
O	1.324527	1.163212	-0.088076
H	0.680394	1.883948	-0.117924
O	1.406970	-1.041606	-0.079686
O	-1.211122	-1.347794	-0.133049
C	-1.530992	0.987979	0.259537
H	-2.604044	0.884660	0.329037
H	-1.117498	1.971461	0.413783
H	-2.173260	-1.358279	-0.039466

enol<sub>d</sub>

C	0.728080	-0.056192	-0.136196
C	-0.750149	-0.096968	0.034277
O	1.237926	1.175708	-0.050777
H	2.200173	1.112239	-0.163031
O	1.404158	-1.047764	-0.332583
O	-1.216606	-1.371525	-0.062617
C	-1.496627	0.987699	0.252237
H	-2.567697	0.907326	0.369848
H	-1.037568	1.959160	0.313899
H	-2.175865	-1.366567	0.054793

XYZ COORDINATES (CO AND CO<sub>2</sub> COMPLEXES IN AQUEOUS PHASE)

MHC-CO<sub>2</sub> complex

C	-0.960259	-0.258606	0.056766
C	2.033832	0.065855	-0.495188
C	-2.303467	-0.891404	0.114258
H	-2.198340	-1.840767	0.645208
H	-3.080516	-0.278044	0.575527
H	-2.584388	-1.161526	-0.906780
O	1.817155	1.103577	-0.007166
O	2.306398	-0.951216	-0.987618
O	-1.024219	0.935496	0.590541
H	-0.145185	1.348189	0.552338

acetic acid-CO complex

C	0.458965	-0.102180	0.082406
C	-1.513894	-2.681752	0.897744
C	1.279648	-0.362948	1.301524
H	1.535786	-1.418329	1.355505
H	2.207156	0.203026	1.224593
H	0.733946	-0.058088	2.186808
O	-0.600463	0.496243	0.059043
O	-2.624676	-2.831996	0.749667
O	1.023781	-0.597414	-1.030000
H	0.457107	-0.379916	-1.788217

vinyl alcohol-CO<sub>2</sub> complex

C	-1.659841	-0.224569	0.126272
C	1.445101	0.383107	-0.473328
O	-1.724630	0.322740	-0.898121
H	1.426803	0.867332	-1.438849
O	-1.599074	-0.771921	1.151638
O	1.266083	-0.965158	-0.599086
C	1.605722	1.045182	0.669746
H	1.736328	2.115471	0.646201
H	1.618749	0.537283	1.624689
H	1.340656	-1.384900	0.269068

acetaldehyde-CO complex

C	-0.192400	1.368300	-0.187319
C	-0.714105	-0.912532	2.705486
C	-0.293085	2.473196	0.803504
H	0.657202	2.546934	1.336143
H	-0.534430	3.417581	0.324295
H	-1.050272	2.216026	1.546313
O	0.069732	-1.147427	3.485412
O	-0.334893	1.501939	-1.391435
H	0.031054	0.372310	0.222471

acetaldehyde-CO<sub>2</sub> complex

C	1.403682	0.395225	0.608091
C	-1.777008	0.677127	-0.897541
C	1.472150	-1.045573	0.247744
H	1.721258	-1.130239	-0.811448
H	2.294901	-1.501423	0.801879
H	0.538122	-1.556031	0.464111
O	-2.579438	0.933480	-0.095170
H	2.309919	0.985810	0.407883
O	-0.981586	0.420201	-1.707090
O	0.426176	0.936846	1.097961

## XYZ COORDINATES (DHPA MONOMER AND HYDRATE)

## GAS PHASE

## DHPA

C	0.956062	0.063125	-0.180706
C	-0.555306	0.263963	-0.421454
C	1.247677	-1.339410	0.323817
H	0.884867	-2.073681	-0.390870
H	0.778141	-1.514025	1.289758
H	2.325443	-1.439271	0.428903
O	-1.272196	0.548404	0.672556
H	-0.648203	0.729314	1.393407
O	-1.049288	0.165914	-1.516436
O	1.383578	0.964612	0.828221
O	1.629294	0.332266	-1.376248
H	0.960773	0.336420	-2.077503
H	1.584974	1.802441	0.394422

DHPA-H<sub>2</sub>O

C	0.999746	0.073794	-0.340057
C	-0.513712	0.346566	-0.560715
C	1.235502	-1.195167	0.455653
H	0.744052	-2.030712	-0.037515
H	0.855799	-1.104046	1.470318
H	2.306643	-1.378996	0.487910
O	-1.265614	0.606999	0.496501
H	-0.747879	0.729442	1.327707
O	-0.973055	0.297452	-1.680883
O	1.589688	1.157438	0.390762
O	1.599505	0.008837	-1.593270
H	0.874114	0.087015	-2.237547
H	1.885065	1.795237	-0.269349
O	0.187718	1.110085	2.732210
H	-0.073613	1.862383	3.269583
H	0.937865	1.399062	2.187794

## AQUEOUS PHASE

## DHPA

C	0.969397	0.067145	-0.179888
C	-0.541991	0.266572	-0.410146
C	1.240566	-1.326840	0.357070
H	0.865284	-2.071190	-0.340542
H	0.765842	-1.467458	1.325518
H	2.317367	-1.441437	0.464429
O	-1.273566	0.486600	0.678687
H	-0.693866	0.603237	1.449560
O	-1.048393	0.210153	-1.509424
O	1.420663	0.981623	0.796234
O	1.640591	0.280182	-1.394861
H	0.976386	0.380543	-2.093082
H	1.364228	1.876343	0.432376

DHPA-H<sub>2</sub>O

C	1.034487	0.045533	-0.375554
C	-0.470112	0.363701	-0.553123
C	1.235026	-1.212801	0.446834
H	0.722197	-2.045357	-0.028509
H	0.858195	-1.087248	1.458002
H	2.301997	-1.423086	0.485373
O	-1.158620	0.698985	0.517485
H	-0.612629	0.812963	1.352413
O	-0.997758	0.292238	-1.649243
O	1.673411	1.105260	0.314739
O	1.599786	-0.119229	-1.648774
H	0.914406	0.093429	-2.301860
H	1.616329	1.907180	-0.222591
O	0.159697	1.080378	2.758042
H	-0.234211	1.829264	3.222386
H	0.995035	1.413695	2.401602

## XYZ COORDINATES (ANIONIC MONOMERS)

## GAS PHASE

Pyruvate<sup>-</sup>

C	0.775259	-0.198718	-0.297703
C	-0.700823	-0.055127	0.086343
C	1.578427	-1.095127	0.628219
H	1.519218	-0.700939	1.642942
H	1.129698	-2.088775	0.636377
H	2.615482	-1.149529	0.301166
O	-1.454869	-0.920595	-0.416321
O	-0.936668	0.874330	0.893417
O	1.299819	0.345832	-1.259130

DHP<sup>-</sup>

C	0.954409	-0.033255	-0.222540
C	-0.569057	0.289541	-0.373922
C	1.275541	-1.324131	0.483988
H	0.834002	-2.153946	-0.062650
H	0.854121	-1.306155	1.484679
H	2.356851	-1.455932	0.535958
O	-1.385576	-0.320552	0.337721
O	-0.769236	1.198991	-1.236988
O	1.547610	1.029474	0.540949
O	1.517288	-0.053616	-1.521096
H	0.909960	0.538670	-2.002686
H	1.170462	1.833147	0.162957

## AQUEOUS PHASE

Pyruvate<sup>-</sup>

C	0.783901	-0.226061	-0.267933
C	-0.692893	-0.056247	0.084475
C	1.597033	-1.101196	0.632510
H	1.545322	-0.713077	1.650292
H	1.160101	-2.100492	0.647765
H	2.629547	-1.146838	0.297881
O	-1.481900	-0.875605	-0.447599
O	-0.963340	0.887420	0.867835
O	1.247772	0.343447	-1.249917

DHP<sup>-</sup>

C	0.953150	0.010643	-0.196823
C	-0.573335	0.274284	-0.389540
C	1.257075	-1.330627	0.428343
H	0.846828	-2.124438	-0.192003
H	0.824796	-1.395587	1.422331
H	2.337234	-1.454291	0.494191
O	-1.329036	0.055340	0.584433
O	-0.911033	0.716189	-1.523525
O	1.485825	1.006358	0.680842
O	1.584160	0.093337	-1.454432
H	0.917572	0.515790	-2.027735
H	1.303138	1.875238	0.300289

## XYZ COORDINATES (MONOHYDRATES)

## GAS PHASE

Tc-H<sub>2</sub>O<sub>a</sub>

C	0.866122	-0.108939	0.015013
C	-0.672490	0.065957	0.025706
C	1.349453	-1.522652	0.013459
H	0.945319	-2.045341	-0.852720
H	0.959624	-2.041979	0.887943
H	2.433973	-1.539708	0.004028
O	-1.140578	1.301562	-0.038135
H	-0.446403	2.000325	-0.100269
O	-1.383469	-0.907523	0.098869
O	1.604787	0.856315	0.017900
O	0.576086	3.407372	-0.254091
H	0.568399	4.115307	0.395325
H	1.358997	2.870901	-0.072441

Tc-H<sub>2</sub>O<sub>b</sub>'

C	0.513901	-0.220616	0.906021
C	-0.533759	0.468393	-0.002258
C	1.621943	-0.959592	0.246407
H	2.181857	-0.291679	-0.409096
H	1.208424	-1.729774	-0.405308
H	2.268475	-1.400673	0.997129
O	-1.494472	1.068257	0.691845
H	-1.281912	0.922736	1.634005
O	-0.488088	0.461548	-1.208172
O	0.350712	-0.110378	2.105925
O	1.944484	0.243330	-2.729835
H	1.036075	0.335231	-2.409917
H	1.976033	0.732581	-3.555039

## AQUEOUS PHASE

Tc-H<sub>2</sub>O<sub>a</sub>

C	0.892124	-0.172839	-0.003594
C	-0.634027	0.073688	0.025347
C	1.328748	-1.594684	0.031042
H	0.887609	-2.130291	-0.809318
H	0.953581	-2.064727	0.940215
H	2.411495	-1.649535	-0.006818
O	-1.033719	1.325248	-0.030263
H	-0.301171	2.005278	-0.086076
O	-1.417013	-0.853366	0.096769
O	1.638876	0.784211	-0.048961
O	0.509862	3.452888	-0.240715
H	0.153148	4.147194	0.326310
H	1.400132	3.289922	0.092413

Tc-H<sub>2</sub>O<sub>b</sub>

C	0.826981	-0.070584	0.119984
C	-0.700620	0.028916	-0.067321
C	1.419873	-1.430802	0.133863
H	1.102330	-1.981374	-0.749230
H	1.035910	-1.966660	1.003633
H	2.501644	-1.366090	0.182125
O	-1.156836	1.274979	-0.073020
H	-0.396752	1.874101	0.054327
O	-1.425977	-0.933050	-0.175837
O	1.435919	0.971002	0.280329
O	0.516065	0.041161	-2.700180
H	-0.210085	-0.430512	-3.124104
H	0.393133	0.957089	-2.974849

Tc-H<sub>2</sub>O<sub>b</sub>'

C	0.483154	-0.259725	0.969589
C	-0.441363	0.570435	0.052046
C	1.715127	-0.821661	0.364786
H	2.318048	-0.011063	-0.044854
H	1.441661	-1.470432	-0.467806
H	2.276609	-1.375457	1.109163
O	-1.524754	1.027963	0.653618
H	-1.506279	0.728835	1.583339
O	-0.203160	0.789967	-1.116365
O	0.131464	-0.394283	2.125790
O	1.808372	0.031671	-3.036459
H	1.139030	0.295441	-2.386590
H	1.586651	0.534165	-3.828013

## XYZ COORDINATES (MONOHYDRATES)

## GAS PHASE

Ct-H<sub>2</sub>O<sub>a</sub>

C	1.209285	-0.075298	0.013419
C	-0.257228	0.421235	0.065474
C	1.437359	-1.556340	-0.070607
H	0.932440	-1.962961	-0.946322
H	1.000024	-2.049965	0.796481
H	2.503229	-1.752615	-0.121359
O	-0.550504	1.595299	0.029593
O	-1.127627	-0.584982	0.154522
O	2.090666	0.747704	0.041813
H	-2.038657	-0.198553	0.189763
O	-3.274219	1.032599	0.116978
H	-3.877807	1.281914	0.821573
H	-2.561742	1.693350	0.113318

Ct-H<sub>2</sub>O<sub>b</sub>

C	-0.844756	0.011255	0.029382
C	0.697830	-0.117236	-0.004576
C	-1.431607	1.386099	0.111462
H	-1.114558	1.958945	-0.759344
H	-1.057925	1.906598	0.992082
H	-2.513723	1.313638	0.139961
O	1.302282	1.074157	0.195015
H	2.257535	0.916117	0.161419
O	1.284079	-1.151110	-0.174639
O	-1.492075	-1.006917	-0.022050
O	-0.476111	-0.264198	-2.782397
H	0.178176	-0.447062	-3.461767
H	-0.671891	-1.121900	-2.389609

Ct-H<sub>2</sub>O<sub>c</sub>

C	1.417173	0.105002	-0.006424
C	-0.104100	0.377499	0.112155
C	1.869591	-1.316919	-0.132747
H	1.413765	-1.775550	-1.009811
H	1.532734	-1.891739	0.729513
H	2.951305	-1.344908	-0.208487
O	-0.585966	1.473248	0.207781
O	-0.814905	-0.767840	0.094321
O	2.162259	1.055191	0.008947
H	-1.751264	-0.529017	0.171938
O	1.294010	3.958710	0.288954
H	1.756894	3.118420	0.193323
H	0.373800	3.681377	0.316198

## AQUEOUS PHASE

Ct-H<sub>2</sub>O<sub>a</sub>

C	1.271958	-0.117293	0.005343
C	-0.119504	0.563133	0.037664
C	1.329159	-1.605875	-0.012202
H	0.781348	-1.981397	-0.876339
H	0.831084	-1.997502	0.874775
H	2.362312	-1.935834	-0.044148
O	-0.236224	1.772469	0.030489
O	-1.109332	-0.303208	0.073878
O	2.246304	0.606776	-0.002877
H	-1.998898	0.168455	0.108188
O	-3.489986	0.790505	0.139999
H	-3.941099	0.525943	0.951225
H	-3.480940	1.755169	0.166054

Ct-H<sub>2</sub>O<sub>b</sub>

C	-0.871937	-0.016594	0.096277
C	0.662927	-0.163338	-0.019036
C	-1.455262	1.353616	0.065679
H	-1.139252	1.872557	-0.837008
H	-1.071682	1.919726	0.915531
H	-2.537679	1.293908	0.114139
O	1.277255	1.009172	-0.136781
H	2.236602	0.861828	-0.193320
O	1.218787	-1.237119	0.021302
O	-1.514069	-1.035912	0.239948
O	-0.400299	-0.128484	-2.732596
H	0.405268	0.200759	-3.147373
H	-0.374257	-1.078652	-2.893148

Ct-H<sub>2</sub>O<sub>c</sub>

C	1.394742	0.115935	-0.013486
C	-0.129986	0.343503	0.113882
C	1.899657	-1.276511	-0.138627
H	1.450289	-1.747087	-1.013142
H	1.584617	-1.854085	0.730758
H	2.981247	-1.272018	-0.221551
O	-0.606910	1.446996	0.244608
O	-0.815086	-0.791655	0.058737
O	2.099538	1.105687	-0.002909
H	-1.765009	-0.597492	0.135273
O	1.417521	3.890766	0.102690
H	1.474772	2.921068	0.088643
H	0.472810	4.075096	0.134186



## XYZ COORDINATES (MONOHYDRATES)

## GAS PHASE

Tt-H<sub>2</sub>O<sub>a</sub>

C	-0.925414	0.173120	0.018839
C	0.545358	-0.252455	-0.180007
C	-1.928692	-0.932161	-0.124821
H	-1.714379	-1.723098	0.592920
H	-1.845057	-1.382645	-1.113343
H	-2.926150	-0.535275	0.030344
O	1.393983	0.755270	-0.110434
H	2.305629	0.396109	-0.245610
O	0.844796	-1.418434	-0.376133
O	-1.198404	1.320768	0.274836
O	3.554301	-0.782030	-0.609695
H	4.257216	-1.062837	-0.018068
H	2.866684	-1.466421	-0.571150

Tt-H<sub>2</sub>O<sub>d</sub>

C	-0.442775	0.374015	-0.048680
C	0.856821	-0.450605	-0.145994
C	-1.704226	-0.407233	-0.226371
H	-1.747529	-1.199462	0.520922
H	-1.687731	-0.905215	-1.195682
H	-2.564577	0.247972	-0.143915
O	1.950240	0.297745	0.039406
H	2.714307	-0.292915	-0.038224
O	0.861768	-1.637070	-0.366453
O	-0.381076	1.566468	0.157107
O	-3.057716	2.622904	0.243265
H	-3.206607	3.559523	0.390422
H	-2.096866	2.505266	0.256752

Tt-H<sub>2</sub>O<sub>b</sub>

C	-0.803621	0.135541	-0.025987
C	0.689513	-0.221374	-0.158859
C	-1.737293	-1.027426	-0.135524
H	-1.533945	-1.716768	0.683365
H	-1.555851	-1.571253	-1.061131
H	-2.761742	-0.674523	-0.086250
O	1.488117	0.837851	0.035584
H	2.397327	0.522083	-0.071337
O	1.080194	-1.330393	-0.430402
O	-1.142659	1.282714	0.151311
O	-0.246509	0.047716	2.734781
H	-0.341246	0.983666	2.529741
H	0.266532	0.014064	3.546108

Tt-H<sub>2</sub>O<sub>c</sub>

C	-0.765786	-0.114596	-0.071527
C	0.712786	-0.524148	-0.223980
C	-1.750993	-1.233217	-0.186191
H	-1.535160	-1.990973	0.566477
H	-1.640618	-1.722289	-1.153655
H	-2.756931	-0.846784	-0.064435
O	1.526194	0.529139	-0.117810
H	2.438077	0.218302	-0.217247
O	1.061704	-1.663502	-0.414343
O	-1.057137	1.043407	0.126682
O	0.735783	3.467961	0.533918
H	0.281208	2.634775	0.355563
H	0.028966	4.103160	0.670405

## XYZ COORDINATES (MONOHYDRATES)

## AQUEOUS PHASE

Tt-H<sub>2</sub>O<sub>a</sub>

C	-0.960774	0.168757	0.020037
C	0.443424	-0.424494	-0.230150
C	-2.094469	-0.794802	-0.050546
H	-1.937907	-1.593730	0.674128
H	-2.113836	-1.259351	-1.036463
H	-3.029201	-0.280569	0.145757
O	1.400659	0.471764	-0.143174
H	2.298625	0.044364	-0.297331
O	0.598470	-1.606230	-0.478215
O	-1.075570	1.354748	0.254681
O	3.803391	-0.504695	-0.541934
H	4.293407	-0.516024	0.289515
H	3.804503	-1.422392	-0.840487

Tt-H<sub>2</sub>O<sub>d</sub>

C	-0.489393	0.265872	-0.041414
C	0.873307	-0.453444	-0.096843
C	-1.685474	-0.603993	-0.189447
H	-1.686286	-1.350278	0.605340
H	-1.623797	-1.144914	-1.133671
H	-2.590393	-0.007595	-0.150643
O	1.890751	0.386600	0.027590
H	2.721823	-0.115825	-0.018328
O	0.966367	-1.652874	-0.239981
O	-0.515913	1.471104	0.116673
O	-3.011587	2.885273	0.261075
H	-2.819807	3.825658	0.345420
H	-2.139264	2.460635	0.213813

Tt-H<sub>2</sub>O<sub>b</sub>

C	-0.833542	0.164032	-0.102040
C	0.671040	-0.167145	-0.067126
C	-1.751061	-1.008799	-0.077479
H	-1.516363	-1.648166	0.771017
H	-1.590659	-1.598618	-0.981048
H	-2.780413	-0.669313	-0.031135
O	1.426789	0.922634	-0.012977
H	2.360905	0.654813	-0.002555
O	1.091437	-1.303144	-0.112823
O	-1.188687	1.321570	-0.187733
O	-0.239354	0.014589	2.698212
H	0.328083	0.757505	2.933522
H	0.238508	-0.757946	3.020876

Tt-H<sub>2</sub>O<sub>c</sub>

C	-0.736901	-0.102883	-0.042401
C	0.732404	-0.534193	-0.223163
C	-1.751574	-1.178185	-0.192766
H	-1.547031	-1.971121	0.526784
H	-1.663224	-1.619747	-1.185633
H	-2.746004	-0.772465	-0.042437
O	1.572166	0.476911	-0.054719
H	2.482389	0.157822	-0.175976
O	1.046637	-1.673819	-0.487939
O	-0.990508	1.059910	0.204994
O	0.640335	3.446493	0.464892
H	0.188641	2.593388	0.366694
H	-0.072959	4.081546	0.591865

## XYZ COORDINATES (MONOHYDRATES)

## AQUEOUS PHASE

PAHT-H<sub>2</sub>O<sub>a</sub>

C	0.959226	-0.098760	0.123055
C	-0.493863	0.117302	-0.265201
O	1.738622	0.786242	-0.284674
H	-2.385489	0.961068	0.189310
O	1.167456	-1.124720	0.801593
O	-0.938932	-0.350781	-1.346867
C	-1.392664	0.872064	0.616704
H	-1.427801	0.360594	1.580460
H	-0.952725	1.853418	0.799480
H	-0.217879	-0.883962	-1.913356
O	0.712276	-1.610818	-2.698528
H	1.487351	-1.096122	-2.958588
H	1.055261	-2.399525	-2.258646

PYRUVATE<sup>-</sup>-H<sub>3</sub>O<sup>+</sup> COMPLEX

C	1.138862	-0.332509	-0.155367
C	-0.340421	0.018983	-0.180427
O	1.851595	0.309917	-0.958368
H	-1.898128	1.230581	0.657672
O	1.460097	-1.214370	0.672211
O	-1.073026	-0.604216	-0.968280
C	-0.826103	1.082165	0.730904
H	-0.546878	0.816237	1.750784
H	-0.298658	2.005757	0.487767
H	-2.327061	-0.312831	-1.023161
O	-3.430931	-0.067884	-1.086475
H	-3.608973	0.416702	-1.907314
H	-3.948354	-0.887413	-1.122038

PAHT-H<sub>2</sub>O<sub>b</sub>

C	0.866689	-0.134430	0.055538
C	-0.615005	0.125006	-0.134553
O	1.614773	0.566368	-0.656634
H	-2.355737	1.197920	0.489212
O	1.133318	-1.003965	0.910655
O	-1.196978	-0.560716	-1.012709
C	-1.292249	1.138657	0.690386
H	-1.107538	0.901721	1.738861
H	-0.810956	2.099081	0.496232
H	-2.244807	-0.367562	-1.137555
O	-3.610785	-0.149785	-1.326256
H	-3.763529	0.321605	-2.156147
H	-4.072339	-0.994031	-1.418402

PAHT-H<sub>2</sub>O<sub>c</sub>

C	0.694342	0.004879	-0.211047
C	-0.633018	0.330331	0.488974
C	1.514952	-1.125038	0.249875
H	0.960074	-2.044021	0.053893
H	2.474586	-1.143896	-0.255007
H	1.635141	-1.057993	1.331387
O	-1.377554	-0.656727	0.647166
H	0.430388	1.545511	-1.455631
O	-0.805322	1.529894	0.803033
O	1.072882	0.682364	-1.193850
O	-0.349202	2.590643	-1.738289
H	0.185225	3.350507	-2.006496
H	-0.718444	2.809074	-0.866181

## XYZ COORDINATES (DIHYDRATES)

## GAS PHASE

Tc-2H<sub>2</sub>O

C	0.585250	-0.321207	0.957250
C	-0.487749	0.413017	0.110954
C	1.686691	-0.976481	0.196959
H	2.219318	-0.241948	-0.407291
H	1.269959	-1.690625	-0.513004
H	2.360656	-1.470764	0.888243
O	-1.479628	0.983928	0.761789
H	-1.432370	0.899155	1.746418
O	-0.403367	0.441409	-1.097841
O	0.488762	-0.340537	2.168710
O	1.905207	0.263579	-2.779291
H	1.036212	0.342065	-2.359585
H	1.851004	0.793802	-3.577459
O	-1.575003	0.955924	3.468022
H	-0.831096	0.350292	3.581204
H	-2.320099	0.572845	3.938263

Tc-2H<sub>2</sub>O'

C	0.899362	-0.128188	-0.032838
C	-0.639631	0.030026	-0.002041
C	1.401113	-1.534298	-0.042876
H	0.995343	-2.060729	-0.906171
H	1.028194	-2.061064	0.834727
H	2.485479	-1.536360	-0.063943
O	-1.127593	1.253792	-0.036842
H	-0.447730	1.971895	-0.095261
O	-1.340967	-0.955964	0.060796
O	1.617089	0.851314	-0.038845
O	0.514059	3.379761	-0.257378
H	0.474761	4.110032	0.365895
H	1.340821	2.910399	-0.088700
O	-4.224557	-0.511153	0.508555
H	-4.303788	0.429851	0.335455
H	-3.290675	-0.703230	0.345119

## AQUEOUS PHASE

Tc-2H<sub>2</sub>O

C	0.737714	-0.285548	1.023927
C	-0.230642	0.623020	0.230922
C	1.793237	-0.974382	0.234160
H	2.421534	-0.229646	-0.254767
H	1.330148	-1.570355	-0.551981
H	2.390544	-1.602339	0.886432
O	-1.216280	1.169447	0.899388
H	-1.265465	0.924659	1.871625
O	-0.074345	0.824116	-0.960912
O	0.592425	-0.381288	2.225718
O	1.632566	0.039956	-3.117897
H	1.072101	0.304728	-2.371269
H	1.350989	0.608441	-3.842989
O	-1.744530	0.837883	3.448459
H	-1.245750	0.106421	3.831341
H	-2.670499	0.579343	3.531185

## XYZ COORDINATES (DIHYDRATES)

## GAS PHASE

Ct-2H<sub>2</sub>O

C	1.210452	-0.156419	-0.085517
C	-0.242410	0.370894	0.009582
C	1.416153	-1.640412	-0.061682
H	0.877854	-2.103078	-0.888338
H	0.998414	-2.059163	0.853358
H	2.476732	-1.858124	-0.129727
O	-0.501067	1.556874	0.014011
O	-1.139424	-0.602888	0.083267
O	2.099183	0.655812	-0.173931
H	-2.040133	-0.188225	0.144970
O	-3.258427	1.016580	0.135564
H	-3.885963	1.220525	0.834061
H	-2.595775	1.724133	0.140695
O	1.450117	3.781394	0.269844
H	2.315085	3.394598	0.112351
H	0.852702	3.028168	0.175795

Tt-2H<sub>2</sub>O

C	-1.005154	0.114785	-0.233555
C	0.362559	-0.560163	-0.345364
C	-2.211905	-0.763897	-0.219313
H	-2.085578	-1.527972	0.546990
H	-2.291466	-1.282528	-1.176109
H	-3.105076	-0.175601	-0.036256
O	1.098656	-0.044947	-1.313847
H	2.063476	-0.180294	-1.098716
O	0.702006	-1.395553	0.464110
O	-1.027150	1.321139	-0.070521
O	3.477039	0.272058	-0.261304
H	3.037791	1.047176	0.137176
H	3.613367	-0.345582	0.463343
O	1.688263	2.285372	0.540115
H	1.617169	2.967306	1.211535
H	0.780659	2.109049	0.241704

## AQUEOUS PHASE

Ct-2H<sub>2</sub>O

C	1.268385	-0.118475	-0.026843
C	-0.130611	0.542833	0.031317
C	1.342358	-1.605842	-0.049385
H	0.793103	-1.983903	-0.911594
H	0.854656	-2.006793	0.839209
H	2.378877	-1.923790	-0.089919
O	-0.258754	1.754132	0.065929
O	-1.112565	-0.325700	0.038603
O	2.229990	0.621699	-0.049827
H	-2.009278	0.138143	0.085276
O	-3.488239	0.745729	0.127943
H	-3.933218	0.478428	0.941730
H	-3.485555	1.710561	0.152646
O	1.756611	3.752161	0.115128
H	2.648856	3.391604	0.080627
H	1.178878	2.969881	0.083463

Tt-2H<sub>2</sub>O

C	-1.057524	0.113749	-0.258076
C	0.319344	-0.553259	-0.266750
C	-2.254186	-0.764024	-0.249092
H	-2.197435	-1.431533	0.611299
H	-2.234669	-1.391515	-1.141760
H	-3.162602	-0.171702	-0.214658
O	1.078823	-0.126959	-1.255045
H	2.046596	-0.243958	-1.025262
O	0.654536	-1.311435	0.622896
O	-1.070762	1.332329	-0.190389
O	3.483664	0.348880	-0.375444
H	3.029865	1.090474	0.072383
H	3.849005	-0.194697	0.332209
O	1.731197	2.377865	0.501079
H	1.678877	2.604866	1.436636
H	0.819927	2.161265	0.249962

## XYZ COORDINATES (TRANSITION STATES OF PA, PAHT and ENOL SWITCHING IN AQUEOUS PHASE)

## TSa1

C	-0.910389	0.160345	-0.100187
C	0.497617	0.012347	-0.715347
C	-1.284486	1.528197	0.352537
H	-0.569552	1.871224	1.099936
H	-2.289724	1.523154	0.759960
H	-1.218217	2.214088	-0.492774
O	0.665644	-1.076470	-1.500523
H	1.013430	-1.833150	-1.004812
O	1.352254	0.839828	-0.533446
O	-1.606506	-0.828500	0.002916

## TSa2

C	0.782689	0.022637	0.045047
C	-0.730156	0.228754	0.011164
C	1.259492	-1.382872	-0.028746
H	0.901889	-1.827414	-0.958954
H	0.821932	-1.957537	0.787929
H	2.342885	-1.412594	0.016946
O	-1.297371	1.339887	-0.230219
H	-2.231042	0.437729	-0.007885
O	-1.583782	-0.686481	0.233903
O	1.480399	1.010191	0.130831

## TSa3

C	-0.812587	-0.055787	-0.001962
C	0.737911	-0.140668	0.026755
C	-1.431315	1.296639	0.001906
H	-1.086314	1.852568	-0.870236
H	-1.094279	1.846115	0.881306
H	-2.512762	1.210551	-0.002473
O	1.379948	1.054631	0.014877
H	1.560729	1.377107	0.910934
O	1.310361	-1.195092	-0.012600
O	-1.425321	-1.101557	-0.021971

## TSb

C	0.910424	-0.217949	0.198714
C	-0.474953	0.102565	-0.080110
O	0.812664	0.698060	-0.760438
H	-1.823186	1.723315	0.004200
O	1.794907	-0.803620	0.755707
O	-1.187869	-0.731509	-0.899233
C	-1.272502	1.087653	0.696001
H	-1.984683	0.537125	1.309150
H	-0.635886	1.689093	1.337589
H	-1.018619	-0.513867	-1.827052

## TSc1

C	0.753604	0.427886	-0.072602
C	1.479796	1.682343	-0.379573
C	-0.575893	0.358101	0.036014
H	-1.063543	-0.580520	0.251781
H	-1.170504	1.245278	-0.094662
H	2.470185	-0.382536	-0.081488
O	0.726042	2.799586	-0.552511
H	0.625333	3.280920	0.281974
O	2.683221	1.686362	-0.532116
O	1.556025	-0.659238	0.085958

## TSc2

C	0.762988	-0.017046	-0.062812
C	-0.725208	-0.087624	0.051300
O	1.337643	1.190522	-0.131605
H	0.681805	1.900004	-0.163974
O	1.459025	-1.011519	-0.085061
O	-1.227652	-1.354504	-0.138410
C	-1.508943	0.962064	0.290223
H	-2.577234	0.831993	0.376809
H	-1.116419	1.957317	0.433094
H	-1.394270	-1.772111	0.716168

## TSc5

C	0.769497	-0.044815	-0.112488
C	0.333866	0.530531	-1.388878
O	1.517379	-1.074734	-0.000301
H	1.229162	-0.649726	1.203448
O	0.460834	0.400798	1.045968
O	0.845886	-0.140719	-2.454319
C	-0.475195	1.591411	-1.427672
H	-0.801681	2.007037	-2.369399
H	-0.812119	2.039799	-0.508341
H	0.523596	0.260548	-3.272442

## TSc6

C	0.703599	-0.029762	-0.062111
C	0.300349	0.535057	-1.381505
O	1.448173	-1.170618	-0.127758
H	2.396581	-0.974585	-0.099464
O	0.346926	0.433937	0.995299
O	0.801835	-0.151704	-2.444521
C	-0.472776	1.621654	-1.454337
H	-0.765685	2.033664	-2.408723
H	-0.812132	2.096229	-0.549308
H	0.489820	0.258463	-3.262105

## XYZ COORDINATES (TRANSITION STATES OF PA THERMAL DEGRADATION IN AQUEOUS PHASE)

## TS1

C	0.367206	-0.593863	-0.312091
C	-0.437119	0.489968	0.389857
C	1.459326	-1.183091	0.528215
H	1.877542	-0.453444	1.216288
H	1.046210	-2.020162	1.088075
H	2.234044	-1.543634	-0.145453
O	-0.232867	-1.201015	-1.216148
H	0.539393	1.154239	-1.594944
O	-1.188559	1.237310	0.801854
O	1.015381	0.940320	-0.774084

## TS2

C	0.219211	-0.118341	0.113329
C	-1.169917	-0.622408	0.332112
C	1.156434	-0.271585	1.282726
H	1.531659	-1.289814	1.344732
H	1.984199	0.415231	1.109303
H	0.652372	-0.002682	2.206307
O	-0.446855	1.064389	-0.036982
O	-2.278057	-0.882090	0.430721
O	0.825072	-0.634898	-1.027923
H	0.318325	-0.341464	-1.799355

## TS3

C	0.817356	-0.185094	-0.074362
C	-0.711738	0.004817	0.136713
C	1.618892	-1.292065	0.424002
H	1.532907	-1.299325	1.513207
H	1.167204	-2.223656	0.078793
H	2.654397	-1.213176	0.114434
O	-1.373077	-0.816340	0.765422
H	0.301077	1.311137	-0.857338
O	-1.045154	1.090588	-0.439009
O	1.263668	0.772964	-0.741613

## TS4

C	0.837453	-0.029299	0.036364
C	-0.690760	-0.136468	0.079671
O	1.130356	1.166475	-0.345788
H	-0.196811	1.529720	-0.380214
O	1.586560	-0.961478	0.310666
O	-1.200477	-1.270443	-0.280347
C	-1.312691	1.087048	0.255025
H	-2.357145	1.196111	0.001284
H	-0.950539	1.698184	1.078436
H	-2.171547	-1.262551	-0.220596

## TS5

C	0.856676	0.443978	-0.114470
C	1.655367	1.722453	-0.381847
C	-0.506930	0.657241	-0.066351
H	-1.146385	-0.070848	0.409146
H	-0.934411	1.194520	-0.910404
H	2.431450	-0.488298	0.295374
O	0.921412	2.727347	-0.054161
H	-0.117125	1.911233	0.303435
O	2.811966	1.691767	-0.794996
O	1.469712	-0.639198	0.243546

## TS5a

C	0.686711	0.055801	0.032257
C	-0.806145	0.091141	0.195752
C	1.575974	1.126244	-0.002780
H	1.356519	2.095269	0.418927
H	2.229939	1.113344	-0.873771
H	2.245974	-0.169141	0.211534
O	-1.445304	-1.014030	-0.173922
H	-0.807431	-1.708707	-0.413427
O	-1.386693	1.060283	0.629322
O	1.291730	-1.088760	-0.023893

## TS6

C	0.827278	0.330461	-0.186278
C	-0.744995	0.040576	0.239380
C	1.398418	1.546052	0.121683
H	0.752414	2.410575	0.160758
H	2.468305	1.667660	0.234817
O	-0.913446	-1.171472	0.402851
O	-1.461994	1.034400	0.319063
O	1.609746	-0.779937	-0.248577
H	0.997349	-1.534476	-0.190647
H	0.562650	0.803572	-1.210253

## TS7

C	-0.746123	-0.145709	0.061687
C	1.717898	-0.001278	-0.435036
C	-1.995912	-0.939178	0.033089
H	-1.819786	-1.834292	0.635565
H	-2.878942	-0.406871	0.391077
H	-2.146633	-1.299681	-0.986181
O	1.749224	1.066887	0.055357
O	1.972423	-1.012715	-0.965117
O	-0.964487	1.032700	0.567055
H	-0.121337	1.523828	0.583635

## XYZ COORDINATES (TRANSITION STATES OF PA THERMAL DEGRADATION IN AQUEOUS PHASE)

## TS8

C	-0.796219	0.136937	0.211232
C	2.094455	1.117707	-0.088753
C	-1.739181	-0.873077	0.254598
H	-0.826506	-0.682278	-0.755235
H	-1.398461	-1.874943	0.474312
H	-2.810902	-0.705745	0.147471
O	1.558464	2.138343	-0.262588
O	2.672912	0.122355	0.077338
O	-1.352260	1.365250	-0.038624
H	-0.630726	1.997434	-0.136945

## TS8a

C	-0.781837	0.125704	0.139144
C	-1.731865	-0.873265	0.240826
H	-0.885907	-0.684918	-0.828564
H	-1.389385	-1.880636	0.430046
H	-2.806374	-0.692175	0.209390
O	-1.343026	1.362042	-0.064566
H	-0.629965	1.993534	-0.205277

## TS9

C	-0.959055	0.568839	-0.049176
C	2.222472	0.831690	0.172615
C	-1.254415	-0.876975	-0.038846
H	-0.905581	-1.315386	-0.975622
H	-0.673045	-1.344474	0.758467
H	-2.322311	-1.058481	0.104658
O	2.296128	1.961480	-0.098558
O	2.178130	-0.298651	0.447369
O	-1.965005	1.396802	0.137091
H	-0.895116	1.843241	-0.037786

## TS9a

C	-0.740925	0.036568	-0.026350
C	-1.743982	-1.045803	-0.003887
H	-1.580714	-1.702783	-0.859883
H	-1.574503	-1.650636	0.889850
H	-2.757832	-0.638266	-0.008643
O	-1.181318	1.275365	0.005003
H	-0.021316	1.090503	0.002294

## TS10

C	1.492451	0.418047	0.602271
C	-1.742691	0.771561	-1.057905
C	1.665701	-0.955440	0.386805
H	0.953010	-1.355287	-0.333693
H	2.641256	-1.422702	0.368273
H	0.438251	-0.648606	1.173701
O	-2.523526	1.240660	-0.333528
H	2.188638	1.241003	0.467530
O	-0.970107	0.301181	-1.790755
O	0.317477	0.657483	1.088860

## TS10a

C	1.911888	0.778526	-0.191038
C	3.138036	1.331889	0.197897
H	3.980787	0.874155	-0.319220
H	3.257964	2.381666	0.429143
O	1.873335	-0.484745	0.087226
H	2.943951	-0.047373	0.716189
H	1.032841	1.254194	-0.616191

## TS11

C	0.540986	0.467974	-0.165324
C	-1.387000	0.406719	-0.239707
C	1.133012	-0.857351	0.151770
H	1.099257	-0.989970	1.234217
H	0.527093	-1.645131	-0.292467
H	2.157119	-0.911047	-0.207433
O	-1.859924	1.193095	0.629246
H	-0.563636	1.008009	0.678556
O	-1.707211	-0.331829	-1.111469
O	1.078533	1.418774	-0.677388



XYZ COORDINATES (TRANSITION STATES OF DHPA AND DHPA-H<sub>2</sub>O PES IN AQUEOUS PHASE)

TS-DHPA

C	0.857003	0.002032	0.057311
C	-0.637782	0.130185	-0.311380
C	1.315644	-1.419007	0.211167
H	1.057835	-2.009615	-0.663373
H	0.821739	-1.840386	1.085780
H	2.391500	-1.428741	0.368099
O	-1.272849	1.007458	0.449776
H	-0.581064	1.393043	1.036894
O	-1.181794	-0.501799	-1.190464
O	1.234543	0.902915	0.998453
O	1.675238	0.668694	-1.088784
H	1.120319	1.087163	-1.769415
H	1.809660	1.341465	-0.138663

TS-DHPA-H<sub>2</sub>O

C	0.875805	0.360992	-0.017562
C	-0.575385	0.524189	-0.503767
C	1.100411	-0.919298	0.745149
H	0.753531	-1.776982	0.172484
H	0.552229	-0.877372	1.684076
H	2.162680	-1.017386	0.956160
O	-1.471879	0.828759	0.411567
H	-1.071603	1.079125	1.299524
O	-0.875222	0.373129	-1.674876
O	1.411778	1.508867	0.506408
O	1.742557	0.362208	-1.267501
H	1.171056	0.511942	-2.047418
H	2.007562	1.347460	-0.700787
O	-0.321336	1.720505	2.586169
H	0.535945	1.795443	2.121288
H	-0.166904	1.148421	3.346873