

A Theoretical Study of the Duff Reaction: Insights into its Selectivity

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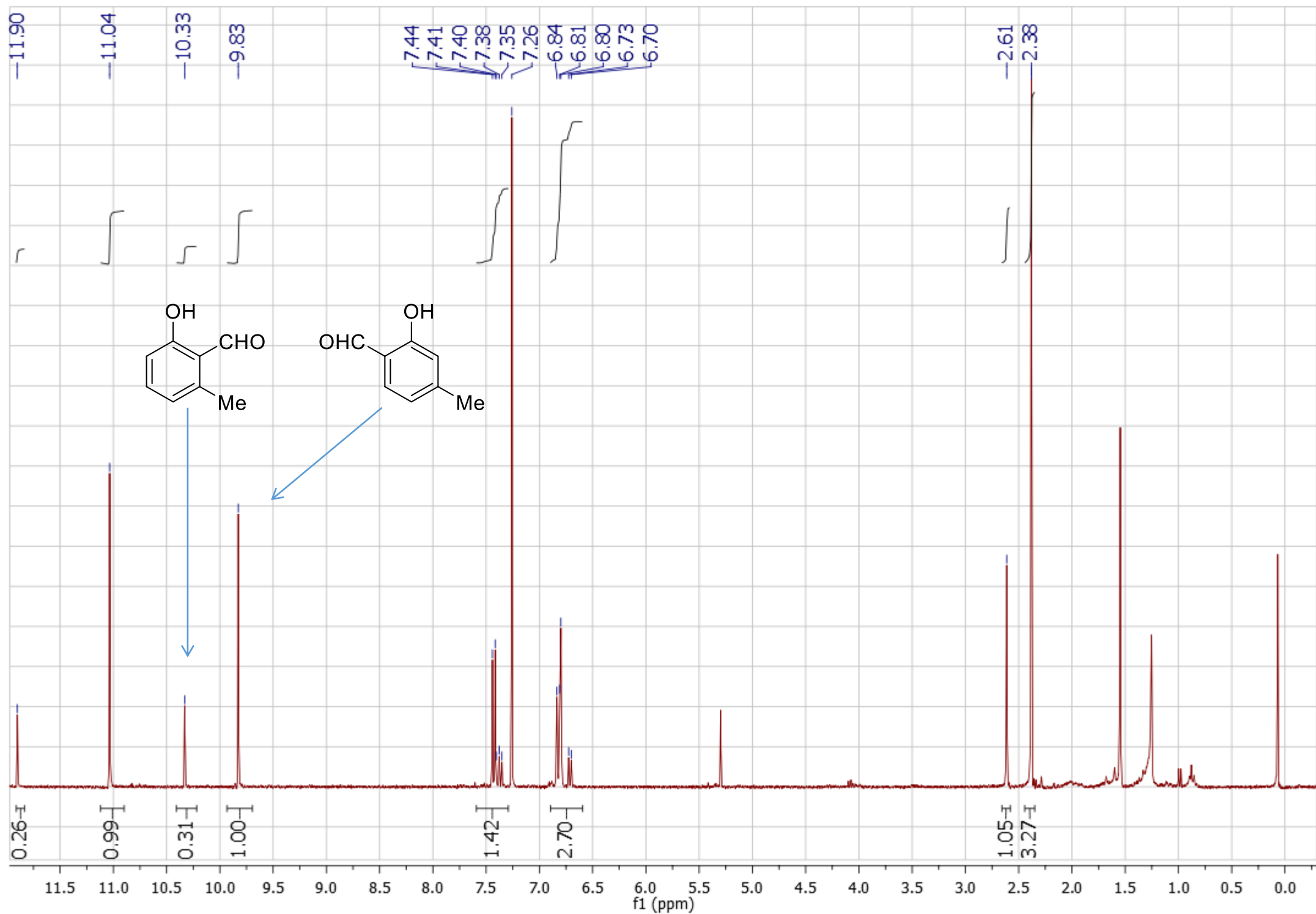
Supporting Information

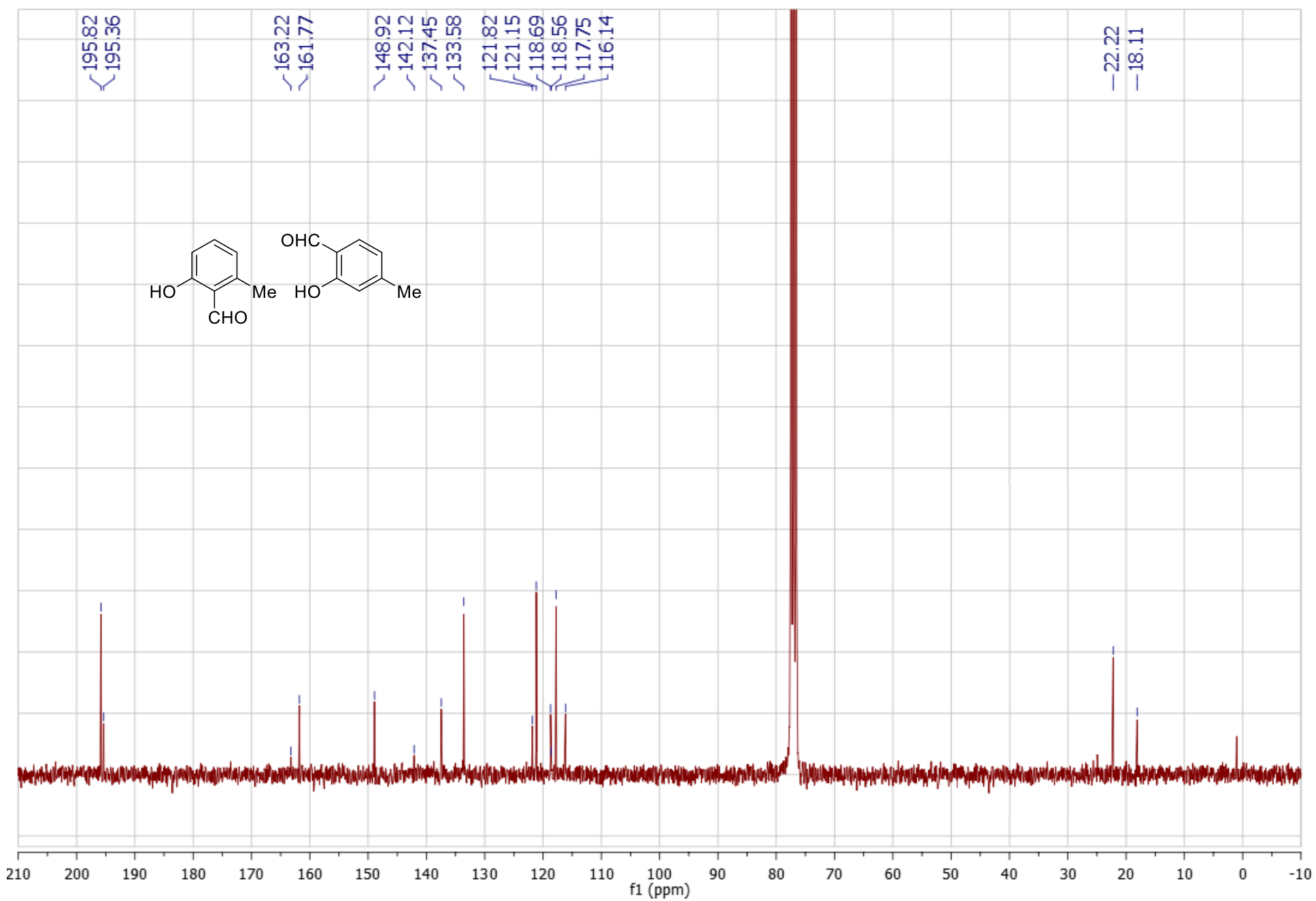
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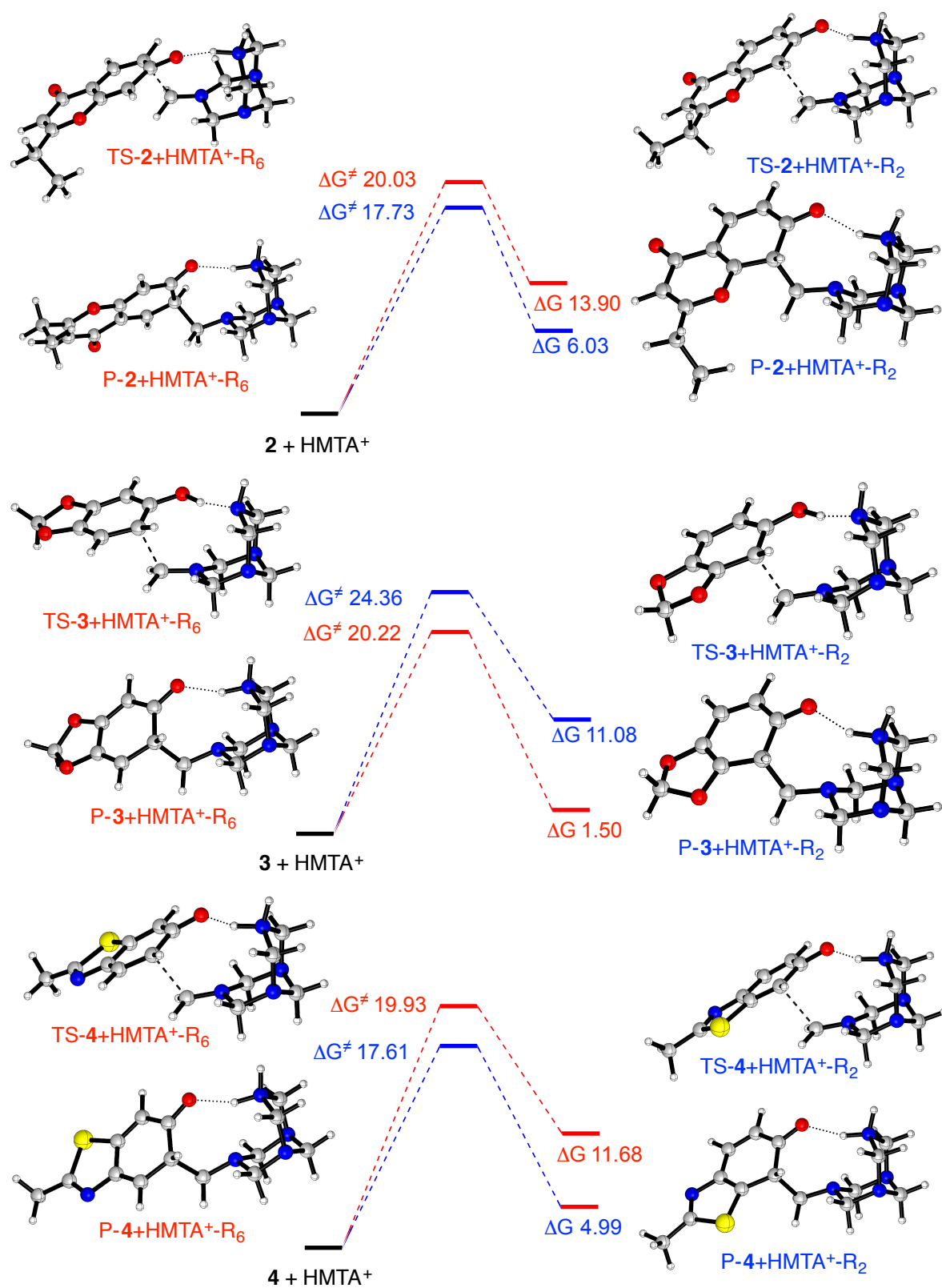
Computational methods

Conformational searches for the reactants, the transition structures (TSs) and the products were run to locate the global minima employing the M06-2X functional¹ coupled with the 6-311+G(d,p) level of theory. Initially, a large number of geometries were generated using the conformational search module of Hyperchem² with the MM+ method for the TSs and Spartan's conformer distribution module employing MMFF was employed for both reactants and products.³ Selected structures were then optimized at the M06-2X/6-311+G** level of theory using Gaussian 09.⁴ Geometries for all structures were fully optimized including Acetic Acid ($\epsilon=6.2528$) as solvent using SMD.⁵ Reported thermochemical properties include zero-point energies (ZPEs) without scaling and were calculated at 1 atm and the corresponding temperature for each reaction.⁶ Normal mode analysis was used to confirm the nature of the stationary points and to evaluate the thermochemical properties. All transition structures were confirmed to have only one imaginary frequency corresponding to the formation of the expected bonds. Intrinsic reaction coordinate (IRCs) calculations were run to verify the connectivity between reactants, TSs and products.





Reaction coordinates for phenols not included in the paper



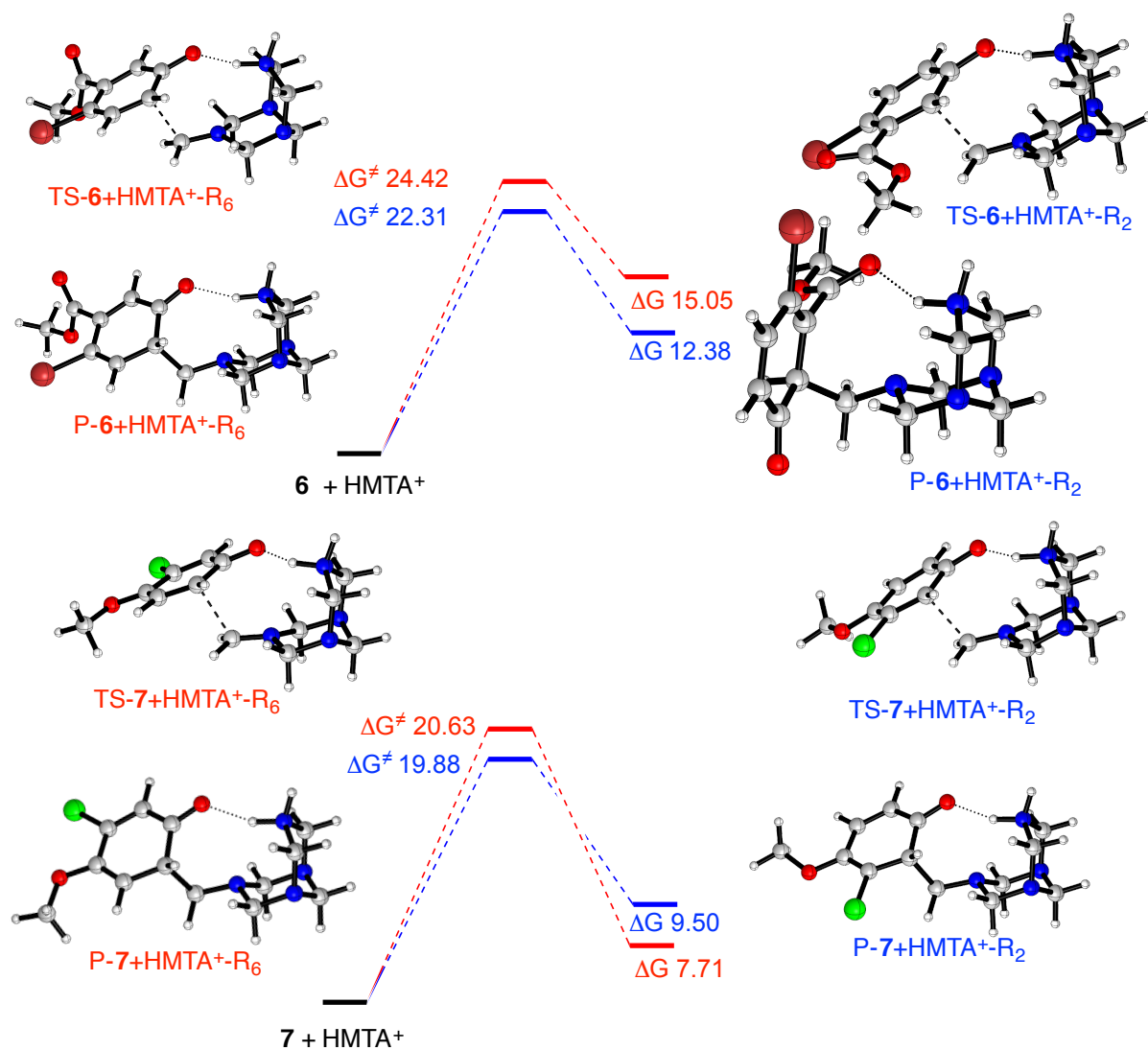


Figure S3. Reaction coordinates for the phenol derivatives not included in the manuscript

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CARTESIAN COORDINATES, ABSOLUTE ENERGIES INCLUDING ZERO-POINT ENERGY CORRECTIONS, FREE ENERGIES IN SOLUTION AND NUMBER OF IMAGINARY FREQUENCIES OF ALL THE STATIONARY POINTS REPORTED IN THE PAPER; VALUES OF IMAGINARY FREQUENCIES OF ALL TRANSITION STRUCTURES.

REACTANTS

1

RM062X/6-311+G(d,p) (AceticAcid)

O 1

O	2.390859	-1.046563	0.001086
C	1.218378	-0.341811	0.000580
C	-1.105045	1.177018	-0.004251
C	1.310504	1.048902	0.003680
C	-0.021670	-0.970179	-0.005124
C	-1.197514	-0.214483	-0.006074
C	0.142779	1.798698	0.001137
C	-2.533433	-0.909539	0.004667
H	2.208159	-1.993661	-0.001791
H	-2.009585	1.775475	-0.007677
H	2.288376	1.516487	0.006200
H	-0.070806	-2.055972	-0.008889
H	0.205478	2.881363	0.001638
H	-2.703983	-1.403569	0.965555
H	-3.346543	-0.201349	-0.160670
H	-2.581960	-1.677898	-0.770746

NUMBER OF IMAGINARY FREQUENCIES = 0

ZPE ENERGY = -346.608227

FREE ENERGY = -346.652187

2

RM062X/6-311+G(d,p) (AceticAcid)

O 1

O	0.689141	2.885990	-0.007059
C	0.687222	1.654131	-0.008509
C	1.871679	-0.482420	-0.020358
C	-0.484132	-0.524793	-0.011824
O	0.710430	-1.180838	-0.022962
C	-0.551590	0.869006	-0.005508
C	1.904185	0.866038	-0.011741
C	-1.819440	1.468159	0.006677
C	-2.963949	0.703303	0.013742
C	-2.859412	-0.698609	0.008233
C	-1.622787	-1.322241	-0.005054
O	-3.956646	-1.494193	0.015599
C	3.042223	-1.410109	-0.033227
C	4.397690	-0.726462	0.062426
H	2.852604	1.386279	-0.009089
H	-1.880872	2.550281	0.011094

H	-3.945486	1.164459	0.024070
H	-1.539809	-2.402079	-0.008796
H	-4.761394	-0.960721	0.025340
H	2.904758	-2.114268	0.793905
H	2.972950	-2.003310	-0.951742
H	4.486507	-0.148350	0.984932
H	5.187418	-1.479288	0.059304
H	4.569783	-0.056687	-0.782791

NUMBER OF IMAGINARY FREQUENCIES = 0

ZPE ENERGY = -650.611154

FREE ENERGY = -650.660445

3

RM062X/6-311+G(d,p) (AceticAcid)

O 1

O	3.119063	-0.709565	0.036503
C	1.847329	-0.202301	0.009826
C	-0.729015	0.729951	-0.034685
C	0.807702	-1.143758	-0.026935
C	1.597710	1.165020	0.022731
C	0.282992	1.655858	-0.003189
C	-0.467900	-0.634612	-0.045855
O	-1.653577	-1.319115	-0.122102
C	-2.651504	-0.344876	0.197832
O	-2.092368	0.925855	-0.120876
H	3.760878	0.010299	0.059077
H	1.013921	-2.206443	-0.040782
H	2.432167	1.856759	0.055492
H	0.079492	2.719308	-0.002805
H	-3.536011	-0.517873	-0.409400
H	-2.859273	-0.391143	1.271868

Number of imaginary frequencies = 0

ZPE Energy = -495.832896

Free Energy = -495.876902

4

RM062X/6-311+G(d,p) (AceticAcid)

O 1

N	-1.456566	1.254126	-0.000008
C	-0.122928	0.862013	-0.000007
C	2.446489	-0.197136	0.000005
C	0.975395	1.723566	-0.000008
C	0.093875	-0.526530	-0.000005

C	1.372662	-1.075963	0.000003
C	2.252957	1.192846	-0.000002
S	-1.445520	-1.339320	-0.000014
C	-2.246601	0.239421	-0.000012
C	-3.735096	0.311026	0.000027
O	3.698083	-0.745427	0.000015
H	0.818615	2.795947	-0.000014
H	1.547288	-2.145095	0.000007
H	3.118560	1.846868	-0.000003
H	-4.145962	-0.182693	-0.883613
H	-4.041375	1.356731	-0.000034
H	-4.145883	-0.182557	0.883781
H	4.367875	-0.051003	0.000019

NUMBER OF IMAGINARY FREQUENCIES = 0
 ZPE ENERGY = -837.056469
 FREE ENERGY = -837.098253

5

RM062X/6-311+G(d,p) (AceticAcid)

O 1

O	2.709210	-1.902696	-0.009508
C	2.023828	-0.723442	-0.003594
C	0.523534	1.625765	0.005403
C	0.634896	-0.796757	-0.013565
C	2.665767	0.512448	0.013283
C	1.910797	1.681264	0.017510
C	-0.107280	0.381524	-0.009059
C	-1.596885	0.353152	-0.013509
O	-2.290685	1.344993	-0.030110
O	-2.098183	-0.880029	0.008400
C	-3.529152	-0.978188	0.024558
H	3.659567	-1.737019	-0.000363
H	-0.072317	2.530179	0.008888
H	0.154288	-1.767246	-0.025561
H	3.750273	0.553407	0.022972
H	2.415540	2.640117	0.031628
H	-3.747988	-2.042349	0.062529
H	-3.946166	-0.536462	-0.880981
H	-3.928969	-0.473368	0.904460

Number of imaginary frequencies = 0
 ZPE Energy = -535.148366
 Free Energy = -535.193480

6

RM062X/6-311+G(d,p) (AceticAcid)

O 1

O	4.009140	1.018284	-0.102977
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C	2.807573	0.381939	-0.084309
C	0.289372	-0.800215	-0.032326
C	2.682181	-0.997918	-0.217937
C	1.673284	1.169154	0.078027
C	0.410660	0.584978	0.086201
C	1.424949	-1.586589	-0.177596
C	-0.747105	1.520021	0.240232
O	-0.804529	2.365804	1.100810
O	-1.667566	1.355562	-0.697042
C	-2.810989	2.221228	-0.616453
Br	-1.394449	-1.671254	0.125469
H	4.727996	0.385320	-0.221905
H	3.566588	-1.614273	-0.339967
H	1.774800	2.243331	0.186996
H	1.336203	-2.663617	-0.251927
H	-3.340126	2.053295	0.322264
H	-2.496679	3.262909	-0.685801
H	-3.438951	1.954142	-1.462432

Number of imaginary frequencies = 0
 ZPE Energy = -3108.723170
 Free Energy = -3108.783655

7

RM062X/6-311+G(d,p) (AceticAcid)

O 1

O	-3.407290	-0.440863	0.000000
C	-2.039510	-0.467395	0.000000
C	0.762512	-0.387262	0.000000
C	-1.382425	0.760204	0.000000
C	-1.307010	-1.645187	0.000000
C	0.085859	-1.603514	0.000000
C	0.000000	0.787907	0.000000
Cl	0.816892	2.328272	0.000000
O	2.113772	-0.254865	0.000000
C	2.888197	-1.446511	0.000000
H	-3.755113	-1.340446	0.000000
H	-1.954552	1.680067	0.000000
H	-1.819999	-2.600855	0.000000
H	0.638019	-2.534088	0.000000
H	3.927667	-1.124849	0.000000
H	2.689608	-2.042035	0.895445
H	2.689608	-2.042035	-0.895445

Number of imaginary frequencies = 0
 ZPE Energy = -881.414913
 Free Energy = -881.462601

8

RM062X/6-311+G(d,p) (AceticAcid)

O 1

O	1.217476	-3.080315	0.000000
C	0.265965	-2.095498	0.000000
C	-1.557143	-0.004619	0.000000
C	0.713983	-0.780472	0.000000
C	-1.097582	-2.382334	0.000000
C	-1.998790	-1.326638	0.000000
C	-0.189414	0.287026	0.000000
C	0.354488	1.717957	0.000000
C	1.217476	1.933580	1.253204
C	1.217476	1.933580	-1.253204
C	-0.763855	2.761799	0.000000
H	0.798678	-3.949326	0.000000
H	-2.291625	0.790195	0.000000
H	1.785198	-0.609497	0.000000
H	-1.437357	-3.412989	0.000000
H	-3.062949	-1.536011	0.000000
H	0.631016	1.774964	2.163037
H	2.073044	1.254269	1.277946
H	1.601722	2.957988	1.269949
H	1.601722	2.957988	-1.269949
H	0.631016	1.774964	-2.163037
H	2.073044	1.254269	-1.277946
H	-1.397948	2.678520	0.887010
H	-1.397948	2.678520	-0.887010
H	-0.323045	3.762374	0.000000

Number of imaginary frequencies = 0
ZPE Energy = -464.437659
Free Energy = -464.487023

HTMA⁺

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	2.440045	-0.000006	-0.796391
C	-1.260906	-1.208440	-0.667630
C	0.853888	-1.273239	0.551550
C	0.853888	1.273245	0.551546
C	-0.966024	0.000012	1.376079
C	-1.260898	1.208435	-0.667653
H	-0.923917	-2.070954	-1.242065
H	2.855287	0.944020	-1.138828
H	-2.048283	0.000014	1.503415
H	-2.324404	-1.329558	-0.449219
H	-0.488694	0.000024	2.357822
H	2.855280	-0.944037	-1.138824
H	1.279437	-1.389848	1.550554
H	1.180576	-2.085248	-0.097778
H	1.180590	2.085253	-0.097775

H	1.279420	1.389849	1.550558
H	-2.324397	1.329567	-0.449252
H	-0.923895	2.070934	-1.242101
N	1.463067	-0.000002	0.009902
N	-1.086322	-0.000011	-1.463252
N	-0.571767	1.201951	0.636905
N	-0.571769	-1.201943	0.636925
H	-0.189426	-0.000018	-1.934885

Number of imaginary frequencies = 0
ZPE Energy = -454.999722
Free Energy = -455.044126

Transition States

TS-1+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.717923	0.894967	-0.969541
C	-2.753561	0.727718	1.389134
C	-1.451086	1.779163	-0.387623
C	-1.204709	-0.499648	-1.507111
C	-3.326902	0.417188	-0.907460
C	-2.582228	-1.509886	0.255467
H	-2.209416	1.344466	2.102352
H	1.301200	0.249667	-1.619895
H	-4.342763	0.160142	-0.606447
H	-3.788763	0.612216	1.711731
H	-3.350821	0.912526	-1.878817
H	1.064074	1.908454	-0.798804
H	-1.613171	2.437899	-1.244586
H	-0.928619	2.323205	0.399460
H	-0.537303	-1.354390	-1.391353
H	-1.303298	-0.250198	-2.567006
H	-3.614287	-1.804568	0.446459
H	-1.933886	-2.383732	0.245004
N	-0.565734	0.670709	-0.839394
N	-2.137576	-0.650192	1.416700
N	-2.523999	-0.801521	-0.995827
N	-2.736453	1.322152	0.078833
H	-2.411434	-1.113070	2.287768
C	1.924241	0.301711	0.820699
C	3.889702	-0.190030	-0.481250
C	3.379108	-1.487686	-0.712806
C	2.192801	-1.907308	-0.161171
C	1.428350	-1.026364	0.664928
O	0.308529	-1.386319	1.177590
H	4.841300	0.100997	-0.911693
H	1.818197	-2.912624	-0.322957
C	3.189920	0.691703	0.315435

H	1.403304	0.952998	1.518710
H	-1.069799	-0.660427	1.398633
H	3.947884	-2.171467	-1.335261
C	3.691179	2.078767	0.597998
H	4.675898	2.242326	0.158123
H	3.004180	2.829368	0.190747
H	3.757200	2.256945	1.674743

Number of imaginary frequencies = 1 (-170.5568)

ZPE Energy = -801.603025

Free Energy = -801.662574

TS-1+HMTA⁺-R₄

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	1.142761	1.690774	-0.001633
C	1.307906	1.409598	1.388481
C	2.110273	0.376230	1.792756
C	2.737212	-0.456923	0.837292
C	2.751197	-0.066631	-0.531808
C	1.948772	0.974427	-0.931957
O	0.277307	2.561034	-0.403023
H	-2.588572	2.291133	-0.546369
H	0.767096	2.022572	2.102276
H	2.213694	0.142211	2.847929
H	3.428870	-1.224886	1.168786
H	1.885267	1.255912	-1.979113
C	1.023730	-1.812533	0.601003
C	-2.156038	0.553748	-1.568219
C	-0.617397	-1.324135	-1.101896
C	-1.092260	-1.048859	1.440191
C	-2.820465	-1.263575	-0.184565
C	-2.597710	0.838170	0.917475
H	-1.422143	0.910140	-2.290133
H	1.172115	-2.161857	1.616555
H	-3.856384	-1.003050	-0.406046
H	-3.162496	0.689097	-1.964669
H	-2.740520	-2.342734	-0.044901
H	1.537088	-2.347897	-0.190350
H	-0.600606	-2.385489	-1.361289
H	0.074785	-0.780862	-1.744449
H	-0.648647	-0.366731	2.164757
H	-1.219816	-2.032706	1.898601
H	-3.671493	1.027702	0.906054
H	-2.140020	1.364838	1.753224
N	-0.119827	-1.228337	0.312036
N	-2.044141	1.446034	-0.351608
N	-2.390163	-0.579380	1.029940
N	-1.963574	-0.842787	-1.287733

H	-1.035826	1.831157	-0.259638
C	3.589239	-0.839609	-1.508201
H	3.361322	-0.562739	-2.538343
H	4.651257	-0.649293	-1.327045
H	3.437191	-1.917586	-1.393606

Number of imaginary frequencies = 1 (-246.8664)

ZPE Energy = -801.590128

Free Energy = -801.649678

TS-1+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.417367	1.259902	0.773592
C	2.806569	0.144594	-1.500880
C	1.866124	1.711881	0.113689
C	1.375263	-0.219257	1.634949
C	3.553366	0.185113	0.762869
C	2.407351	-1.746854	0.012952
H	2.339946	0.728117	-2.295117
H	-1.046121	0.828469	1.549068
H	4.485025	-0.291632	0.455494
H	3.784418	-0.205223	-1.847032
H	3.746501	0.834353	1.618486
H	-0.549365	2.330794	0.643302
H	2.194811	2.455292	0.849068
H	1.395963	2.229272	-0.725026
H	0.590860	-0.962841	1.780684
H	1.618150	0.240579	2.599407
H	3.369059	-2.232351	-0.178950
H	1.668627	-2.510563	0.259409
N	0.861168	0.833010	0.733656
N	1.941765	-1.029641	-1.207117
N	2.587798	-0.848451	1.140000
N	3.033887	0.990146	-0.342336
H	2.030642	-1.675234	-1.992465
C	-1.361135	0.771433	-0.810547
C	-3.718841	1.055101	-0.269387
C	-3.792312	-0.319178	0.126543
C	-2.694113	-1.134316	-0.013473
C	-1.483466	-0.625233	-0.532764
O	-0.468193	-1.431927	-0.644483
H	-4.607088	1.671688	-0.187543
H	-2.734742	-2.183976	0.255781
C	-2.562846	1.563574	-0.766891
H	-0.582918	1.073338	-1.506236
H	0.472880	-1.032445	-0.973371
H	-2.505092	2.600256	-1.081519
C	-5.083489	-0.842265	0.673834

H	-5.367386	-0.283594	1.570240
H	-5.884368	-0.700375	-0.057724
H	-5.017213	-1.900930	0.923559

Number of imaginary frequencies = 1 (-417.4802)

ZPE Energy = -801.599895

Free Energy = -801.658205

TS-1+HMTA⁺-R₂ (no H-Bond)

RM062X/6-311+G(d,p) (AceticAcid)

1 1

O	-2.658888	-2.325129	-0.573840
H	-3.092527	-2.151261	-1.422374
C	-0.842442	-0.049422	-1.623482
C	2.302884	-1.142220	1.151798
C	1.098965	-1.337027	-0.972630
C	1.180084	1.182584	-1.158191
C	3.129068	-0.128129	-0.842890
C	2.409017	1.257507	0.955846
H	1.682884	-1.951108	1.541492
H	-1.017128	0.830720	-2.242113
H	4.131555	-0.126976	-0.412274
H	3.319611	-1.271996	1.531546
H	3.209104	-0.221241	-1.928549
H	-1.064921	-0.972369	-2.162433
H	1.272362	-1.643497	-2.012180
H	0.466896	-2.086370	-0.487328
H	0.600895	2.028276	-0.776458
H	1.349030	1.327296	-2.232641
H	3.439842	1.353061	1.306558
H	1.870612	2.171019	1.211739
N	0.360332	-0.047018	-0.970511
N	1.787039	0.131846	1.647229
N	2.467378	1.132924	-0.506971
N	2.379671	-1.266693	-0.310973
H	0.793663	0.164779	1.453998
C	-2.343835	0.061512	-0.618848
C	-1.664450	1.142605	1.438233
C	-1.476909	-0.140445	2.003423
C	-1.798498	-1.311085	1.342362
C	-2.311989	-1.211180	0.054336
H	-1.445476	2.022381	2.032190
C	-2.162820	1.265379	0.170111
H	-3.056240	0.132621	-1.440842
H	-1.090473	-0.208174	3.015747
H	-1.696588	-2.281770	1.811370
C	-2.466890	2.586143	-0.455706
H	-2.111584	3.407802	0.165872
H	-2.016291	2.671369	-1.449492

H	-3.548173	2.691728	-0.590696
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Number of imaginary frequencies = 1 (-299.0971)

ZPE Energy = -801.587399

Free Energy = -801.647349

TS-1+HMTA⁺-R₄ (no H-Bond)

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.605907	-1.800529	0.929010
C	-1.968856	0.592422	-1.654795
C	-1.059496	-1.509668	-0.788064
C	-1.405221	-0.618380	1.569633
C	-3.150799	-0.693000	-0.030755
C	-2.286296	1.444630	0.576582
H	-1.240865	0.541038	-2.465795
H	0.636339	-2.011132	1.996265
H	-4.076249	-0.210599	-0.349039
H	-2.911137	0.972624	-2.058144
H	-3.378300	-1.701892	0.321801
H	0.845464	-2.674489	0.324752
H	-1.333466	-2.568451	-0.705360
H	-0.287286	-1.406445	-1.556058
H	-0.843114	0.025966	2.251099
H	-1.760307	-1.494988	2.124527
H	-3.257763	1.908663	0.386789
H	-1.784240	2.004790	1.366391
N	-0.467535	-1.083429	0.510712
N	-1.489536	1.529476	-0.644546
N	-2.557971	0.083258	1.058567
N	-2.236799	-0.769567	-1.172034
H	-0.533105	1.286380	-0.413825
C	2.280991	-0.986369	0.785105
C	1.851196	1.348128	1.320204
C	1.805559	1.610785	-0.067426
C	2.064673	0.611060	-1.024965
C	2.373959	-0.663300	-0.614226
H	1.681877	2.164310	2.011895
C	2.143029	0.082857	1.730998
H	2.837421	-1.861147	1.112995
H	2.202223	-0.148676	2.789339
O	1.526334	2.860534	-0.414072
H	1.504415	2.978082	-1.374821
H	2.064499	0.876953	-2.077862
C	2.757873	-1.727774	-1.589559
H	2.577483	-1.413668	-2.617567
H	3.821878	-1.958776	-1.476485
H	2.211335	-2.656155	-1.397660

Number of imaginary frequencies = 1 (-367.3597)

ZPE Energy = -801.589820

Free Energy = -801.649642

TS-1+HMTA⁺-R₆(no H-Bond)

RM062X/6-311+G(d,p) (AceticAcid)

1 1

O	2.697056	-1.592278	-1.566554
H	2.923441	-2.464945	-1.213164
C	0.535856	-1.948805	0.653508
C	-1.840083	0.979954	-1.472211
C	-1.037783	-1.296051	-1.056477
C	-1.526738	-0.937010	1.404077
C	-3.164717	-0.605029	-0.279603
C	-2.330873	1.310719	0.864421
H	-1.047466	1.092496	-2.213928
H	0.511523	-2.346934	1.666418
H	-4.055939	-0.033122	-0.541908
H	-2.739709	1.474137	-1.848632
H	-3.433328	-1.659923	-0.186684
H	0.786903	-2.708667	-0.088484
H	-1.345854	-2.338258	-1.208838
H	-0.218812	-1.069186	-1.745013
H	-1.011795	-0.474034	2.250292
H	-1.915940	-1.912957	1.717965
H	-3.281199	1.827999	0.707523
H	-1.893325	1.665892	1.798565
N	-0.520451	-1.154529	0.329206
N	-1.434319	1.645480	-0.237568
N	-2.645598	-0.117778	1.000310
N	-2.168330	-0.447059	-1.340221
H	-0.504089	1.325377	0.005024
C	2.198697	-1.158123	0.747468
C	1.841105	1.159414	1.389131
C	1.890410	1.537361	0.014141
C	2.154155	0.594345	-0.969642
C	2.391103	-0.726356	-0.606739
H	1.667656	1.925486	2.136347
C	2.046605	-0.135092	1.748833
H	2.734733	-2.059606	1.037930
H	2.227643	0.880210	-2.012935
H	2.032325	-0.436602	2.790730
C	1.720138	2.977292	-0.349865
H	2.691200	3.476941	-0.250883
H	1.382333	3.097830	-1.379260
H	1.026879	3.477572	0.327020

Number of imaginary frequencies = 1 (-372.6181)

ZPE Energy = -801.587259

Free Energy = -801.646695

TS-2+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.461702	-0.339589	1.020511
C	-3.845726	-1.379440	-1.231656
C	-2.279287	-1.864065	0.580007
C	-2.711745	0.461336	1.532682
C	-4.471963	-1.076608	1.048693
C	-4.320404	0.896125	-0.265155
H	-3.153208	-1.863849	-1.918013
H	-0.094401	0.519205	1.575353
H	-5.518572	-1.150850	0.752586
H	-4.873644	-1.590293	-1.528057
H	-4.349747	-1.480545	2.054219
H	0.166687	-1.223210	0.970209
H	-2.236499	-2.476801	1.484016
H	-1.622016	-2.288986	-0.179759
H	-2.327104	1.465372	1.351243
H	-2.732919	0.261642	2.607307
H	-5.393309	0.873715	-0.455540
H	-3.944059	1.915055	-0.330006
N	-1.758893	-0.513680	0.926384
N	-3.656732	0.112928	-1.377712
N	-4.060212	0.326476	1.028982
N	-3.644746	-1.841684	0.115678
H	-4.065946	0.406237	-2.269607
C	0.414415	0.287793	-0.880798
C	2.396870	1.395377	0.025728
C	1.647615	2.604840	0.093341
C	0.356845	2.678182	-0.335900
C	-0.306884	1.521883	-0.884829
O	-1.510598	1.575359	-1.280448
C	1.772190	0.280090	-0.499264
H	0.018457	-0.562452	-1.426247
H	-2.644730	0.423185	-1.404340
C	4.389358	-0.005019	0.304944
C	3.698607	-1.041483	-0.206379
H	-0.199881	3.607697	-0.298467
H	2.144914	3.479604	0.499562
H	5.419240	-0.138652	0.607927
C	4.186280	-2.435929	-0.424676
H	3.528309	-3.102985	0.143255
H	4.024770	-2.673924	-1.481534
C	5.640468	-2.661653	-0.039164
H	5.809227	-2.457367	1.020222
H	5.912754	-3.701058	-0.228565
H	6.309326	-2.027145	-0.624800

C	3.786139	1.307826	0.464322
O	2.400866	-0.917023	-0.601303
O	4.399730	2.269179	0.933159

Number of imaginary frequencies = 1 (-216.2400)

ZPE Energy = -1105.608500

Free Energy = -1105.673300

TS-2+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.840791	1.047335	-0.997266
C	-4.679648	0.500317	0.723409
C	-3.244938	1.305919	-1.070588
C	-2.153920	-0.981222	-1.202961
C	-4.515322	-0.690879	-1.328963
C	-3.624425	-1.780773	0.580924
H	-4.533337	1.454638	1.226181
H	-0.022593	0.433704	-1.364566
H	-5.474356	-1.162215	-1.111190
H	-5.693133	0.138450	0.898647
H	-4.405090	-0.571615	-2.407469
H	-0.840372	2.084283	-1.316067
H	-3.333452	1.583190	-2.125303
H	-3.111276	2.206557	-0.469245
H	-1.343230	-1.502854	-0.690487
H	-2.043956	-1.115646	-2.283874
H	-4.550633	-2.336911	0.725348
H	-2.783419	-2.330011	0.999963
N	-2.034337	0.465649	-0.903635
N	-3.750415	-0.497856	1.378071
N	-3.434413	-1.530755	-0.820976
N	-4.460914	0.623506	-0.688139
H	-4.113522	-0.722154	2.308494
C	-0.038626	1.490539	0.819442
C	2.314231	1.212316	0.289461
C	2.182096	-0.162842	0.644370
C	1.024112	-0.703528	1.138826
C	-0.122295	0.126097	1.325207
O	-1.197086	-0.317956	1.823615
C	3.602579	1.720393	-0.210671
C	1.214906	2.025364	0.428664
H	-0.836889	2.159428	1.125250
H	1.301832	3.075471	0.167746
O	3.241859	-1.007073	0.508773
H	-2.771266	-0.139743	1.516298
C	4.635584	0.713181	-0.363693
C	4.418491	-0.568884	-0.013336
C	5.364233	-1.703730	-0.159232

H	0.990702	-1.745351	1.435587
C	4.724005	-2.845283	-0.957589
O	3.775716	2.905066	-0.486100
H	5.597799	1.004465	-0.763990
H	5.629165	-2.059370	0.842824
H	6.271111	-1.347509	-0.646892
H	4.484507	-2.519613	-1.972608
H	3.804972	-3.187393	-0.477072
H	5.411440	-3.689828	-1.021153

Number of imaginary frequencies = 1 (-358.0582)

ZPE Energy = -1105.600987

Free Energy = -1105.669624

TS-3+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.307503	-0.759110	0.891276
C	-2.948685	-0.524691	-1.587342
C	-1.712589	-1.816843	0.068253
C	-1.881727	0.125448	1.644663
C	-3.798761	-0.841485	0.617403
C	-3.195600	1.357726	-0.023582
H	-2.282383	-0.926485	-2.351248
H	0.724215	-0.186861	1.717770
H	-4.805770	-0.634930	0.252675
H	-3.958911	-0.449770	-2.001048
H	-3.855271	-1.541865	1.452475
H	0.747105	-1.750570	0.781583
H	-1.861055	-2.647376	0.767913
H	-1.064520	-2.154102	-0.743585
H	-1.348139	1.053738	1.853134
H	-2.049455	-0.413116	2.584340
H	-4.240099	1.564166	-0.275296
H	-2.713005	2.286646	0.282953
N	-1.038634	-0.711332	0.767315
N	-2.474228	0.838459	-1.220346
N	-3.186337	0.406722	1.071295
N	-3.006092	-1.437682	-0.458966
H	-2.695880	1.453815	-2.004283
C	1.140354	-0.007199	-0.593325
C	3.443405	0.433315	0.116593
C	3.149416	1.755872	0.434215
C	1.864564	2.226506	0.203798
C	0.874535	1.397809	-0.353402
O	-0.317786	1.879369	-0.552508
H	1.606112	3.253354	0.428894
C	2.503159	-0.386124	-0.430725
H	0.564234	-0.512051	-1.364516

H	-1.113618	1.227896	-0.919931
O	3.019688	-1.604543	-0.683252
O	4.649908	-0.234657	0.176902
H	3.912408	2.406112	0.846871
C	4.307671	-1.601467	-0.024724
H	4.196767	-2.105350	0.939491
H	5.040350	-2.076310	-0.671020

Number of imaginary frequencies = 1 (-415.8955)

ZPE Energy = -950.821928

Free Energy = -950.882201

TS-3+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.009520	-1.167204	0.704410
C	-3.338884	-0.239860	-1.475566
C	-2.244139	-1.779013	0.067777
C	-1.863636	0.147615	1.641675
C	-4.021247	-0.397972	0.803789
C	-3.042054	1.631223	0.076395
H	-2.856404	-0.765943	-2.299898
H	0.631313	-0.716923	1.474695
H	-4.993699	0.013975	0.531510
H	-4.350884	0.045686	-1.781935
H	-4.142953	-1.081900	1.645473
H	0.239574	-2.204607	0.481146
H	-2.496408	-2.573619	0.778478
H	-1.750317	-2.222884	-0.798861
H	-1.129886	0.940945	1.785549
H	-2.050352	-0.348459	2.600203
H	-4.043944	2.043990	-0.079965
H	-2.361473	2.445136	0.329090
N	-1.291241	-0.853756	0.712420
N	-2.549580	0.978912	-1.166156
N	-3.127370	0.694764	1.184276
N	-3.471222	-1.132745	-0.336818
H	-2.688389	1.635257	-1.934902
C	0.932682	-0.506727	-0.903369
C	3.256577	-0.634002	-0.383644
C	3.202814	0.703456	0.093492
C	2.081023	1.477851	0.030377
C	0.934023	0.870573	-0.529072
O	-0.158685	1.589209	-0.591401
H	2.056037	2.503668	0.373195
C	2.179423	-1.235504	-0.925279
H	0.158984	-0.824183	-1.595843
H	-1.032287	1.114786	-0.935334
H	2.218777	-2.245602	-1.313543

O	4.540542	-1.086316	-0.252641
O	4.410171	1.051778	0.558966
C	5.221681	-0.136286	0.558959
H	5.295243	-0.505276	1.583888
H	6.190039	0.093462	0.121937

Number of imaginary frequencies = 1 (-385.5505)

ZPE Energy = -950.828929

Free Energy = -950.888805

TS-4+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.078405	-0.785480	-0.749978
C	3.782494	-0.890636	1.304227
C	2.157240	-1.897628	-0.214631
C	2.106020	0.279949	-1.558673
C	4.133398	-0.870767	-1.053052
C	3.761369	1.241081	-0.024900
H	3.260224	-1.365185	2.133025
H	-0.461009	-0.138293	-1.435850
H	5.200391	-0.736386	-0.874061
H	4.855287	-0.877761	1.497625
H	3.987021	-1.442948	-1.969994
H	-0.385113	-1.716977	-0.442177
H	2.131027	-2.664227	-0.993173
H	1.651261	-2.264556	0.678979
H	1.572131	1.228045	-1.475981
H	2.069218	-0.075401	-2.591640
H	4.834621	1.418834	0.046074
H	3.219934	2.184198	-0.064697
N	1.385421	-0.725172	-0.724073
N	3.337247	0.549468	1.251060
N	3.493934	0.436939	-1.187546
N	3.537138	-1.592466	0.072117
H	3.742892	1.048524	2.047962
C	-0.944701	0.142119	1.022923
C	-2.858549	0.979719	-0.262079
C	-2.126813	2.145404	-0.591168
C	-0.861684	2.323522	-0.099587
C	-0.234508	1.350821	0.757539
O	0.951882	1.532830	1.197880
H	-0.297374	3.220779	-0.329382
C	-2.276023	0.026301	0.567405
H	-0.537050	-0.548054	1.753731
H	2.286485	0.673733	1.325912
H	-2.585717	2.890966	-1.232250
C	-4.559910	-0.433168	-0.229140
N	-4.147304	0.696350	-0.688756

S	-3.392222	-1.281596	0.795758
C	-5.894832	-1.039961	-0.494908
H	-5.788803	-1.998322	-1.008796
H	-6.436370	-1.214645	0.437443
H	-6.475044	-0.362925	-1.121411

Number of imaginary frequencies = 1 (-164.6066)

ZPE Energy = -1292.053326

Free Energy = -1292.109075

TS-4+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.410030	1.289401	0.544579
C	4.229024	0.391123	-1.032824
C	2.774277	1.753860	0.377745
C	1.924973	-0.359331	1.503667
C	4.250569	0.157902	1.337918
C	3.429794	-1.700664	0.109731
H	3.972825	1.034179	-1.872997
H	-0.365138	0.819628	1.143838
H	5.246978	-0.279206	1.266971
H	5.269124	0.073368	-1.109544
H	4.158656	0.705980	2.276088
H	0.306201	2.351342	0.351445
H	2.863814	2.440774	1.224357
H	2.531160	2.319592	-0.522750
H	1.160218	-1.109829	1.296784
H	1.854265	-0.044394	2.549041
H	4.409964	-2.176600	0.144337
H	2.645911	-2.449157	0.011670
N	1.647134	0.827530	0.654684
N	3.389354	-0.859553	-1.147505
N	3.249549	-0.907794	1.295630
N	4.038686	1.074678	0.218373
H	3.736860	-1.420084	-1.930497
C	-0.485544	0.834793	-1.307349
C	-2.758112	0.714323	-0.531268
C	-2.534252	-0.664922	-0.215699
C	-1.352262	-1.310713	-0.481329
C	-0.291840	-0.579144	-1.100233
O	0.820120	-1.130994	-1.383596
H	-1.206887	-2.364583	-0.273896
C	-1.751876	1.438314	-1.117921
H	0.258958	1.345423	-1.909534
H	2.368431	-0.667659	-1.345409
H	-1.910549	2.480099	-1.375506
C	-4.762522	0.280551	0.309374
N	-4.031292	1.190100	-0.218202

S	-3.987649	-1.313180	0.499675
C	-6.170993	0.457827	0.757178
H	-6.475090	1.489461	0.583551
H	-6.835439	-0.210138	0.203499
H	-6.270444	0.225981	1.820233

Number of imaginary frequencies = 1 (-286.5792)

ZPE Energy = -1292.048428

Free Energy = -1292.105380

TS-5+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.184770	-0.314523	-1.069636
C	3.101252	-1.270121	1.377432
C	1.600673	-1.820882	-0.469130
C	2.092071	0.446799	-1.512275
C	3.818052	-1.077508	-0.888197
C	3.629973	0.952868	0.327810
H	2.381583	-1.720846	2.058563
H	-0.511857	0.482947	-1.731109
H	4.852454	-1.146604	-0.550747
H	4.116622	-1.467077	1.722469
H	3.728582	-1.525429	-1.878544
H	-0.803520	-1.204718	-1.009607
H	1.584331	-2.471833	-1.347489
H	0.911031	-2.208794	0.282001
H	1.712521	1.463288	-1.400289
H	2.156336	0.194314	-2.574620
H	4.693312	0.930920	0.566146
H	3.261612	1.976838	0.330143
N	1.112161	-0.481385	-0.887359
N	2.910339	0.226416	1.442793
N	3.420524	0.328702	-0.950013
N	2.949518	-1.794665	0.045799
H	3.273425	0.565102	2.338468
C	-1.171515	0.434991	0.656059
C	-3.023052	1.566046	-0.444388
C	-2.219497	2.731593	-0.535364
C	-0.957309	2.774016	-0.007933
C	-0.394850	1.634337	0.663860
O	0.771445	1.669636	1.169463
H	-0.359913	3.678533	-0.053704
C	-2.511426	0.455249	0.177372
H	-0.849704	-0.386187	1.288431
H	1.897877	0.534668	1.398540
C	-3.273095	-0.818906	0.255261
H	-4.024175	1.560186	-0.855630
O	-2.754724	-1.886094	0.508788

O	-4.568948	-0.680491	0.001804
C	-5.351265	-1.884218	0.027735
H	-2.624813	3.609394	-1.026992
H	-5.324548	-2.323677	1.025302
H	-6.363258	-1.580997	-0.227576
H	-4.969336	-2.596367	-0.704370

Number of imaginary frequencies = 1 (-253.6348)

ZPE Energy = -990.142428

Free Energy = -990.199155

TS-5+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.405544	1.277691	-0.991268
C	-4.155610	0.346802	0.784381
C	-2.825829	1.311359	-1.021065
C	-1.527318	-0.866150	-1.210653
C	-3.907000	-0.790202	-1.294183
C	-2.889743	-1.818469	0.591079
H	-4.100368	1.303170	1.301357
H	0.466888	0.773812	-1.398909
H	-4.816936	-1.350288	-1.075875
H	-5.124956	-0.119371	0.962199
H	-3.820920	-0.642479	-2.371276
H	-0.506056	2.333912	-1.216974
H	-2.955759	1.592712	-2.069930
H	-2.765991	2.212967	-0.409737
H	-0.661884	-1.314579	-0.719155
H	-1.426126	-0.976133	-2.294702
H	-3.759374	-2.458411	0.741499
H	-1.994612	-2.290552	0.990893
N	-1.534677	0.585202	-0.896352
N	-3.121498	-0.562742	1.405716
N	-2.746833	-1.535682	-0.810918
N	-3.966141	0.513310	-0.631040
H	-3.434382	-0.829394	2.343722
C	0.472670	1.718344	0.851885
C	2.777948	1.584816	0.109190
C	2.737562	0.180729	0.345271
C	1.635847	-0.428970	0.885384
C	0.466961	0.334377	1.226561
O	-0.553082	-0.212938	1.740490
H	3.679265	2.041246	-0.277034
H	1.637070	-1.493307	1.094885
C	1.674624	2.335046	0.404337
H	-0.338722	2.335335	1.224899
H	-2.184372	-0.101537	1.521060
H	1.684907	3.407345	0.240987

C	3.915190	-0.687517	0.026854
O	3.956065	-1.875782	0.245996
O	4.916749	-0.015180	-0.530531
C	6.085183	-0.784589	-0.856182
H	5.828622	-1.568562	-1.569160
H	6.504564	-1.225219	0.048543
H	6.785677	-0.079691	-1.296319

Number of imaginary frequencies = 1 (-332.2469)

ZPE Energy = -990.138117

Free Energy = -990.195256

TS-6+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.551473	0.176894	-1.040796
C	-4.114460	1.060593	1.002933
C	-2.591279	1.451769	-0.863376
C	-2.648661	-1.026058	-1.405419
C	-4.633632	0.279980	-1.187439
C	-4.215322	-1.393327	0.444351
H	-3.520472	1.755081	1.594510
H	-0.059157	-0.675231	-1.501401
H	-5.686511	0.244030	-0.906470
H	-5.168866	1.156265	1.263130
H	-4.549149	0.519399	-2.247959
H	-0.090616	1.148835	-1.182578
H	-2.616381	1.890697	-1.864880
H	-2.025483	2.104131	-0.195830
H	-2.126522	-1.924049	-1.072846
H	-2.677182	-1.001447	-2.498897
H	-5.282718	-1.504997	0.635411
H	-3.687448	-2.314479	0.683617
N	-1.872882	0.154881	-0.946509
N	-3.701941	-0.337758	1.400942
N	-4.017620	-1.021503	-0.929821
N	-3.953480	1.311917	-0.403604
H	-4.073589	-0.533038	2.334772
C	0.374941	0.017303	0.827605
C	2.497318	-0.901543	0.127720
C	1.930859	-2.204150	0.213229
C	0.658356	-2.397934	0.662997
C	-0.167458	-1.286006	1.047807
O	-1.348426	-1.449144	1.473260
H	0.251049	-3.397975	0.763489
C	1.752878	0.194537	0.482976
H	-0.152424	0.855471	1.270498
H	-2.657122	-0.471614	1.461342
C	2.290018	1.587620	0.484184

Br	4.279040	-0.799566	-0.515607
O	3.418459	1.900722	0.761802
O	1.340478	2.471955	0.162707
C	1.735687	3.853109	0.195645
H	2.536351	-3.056320	-0.073127
H	0.846426	4.418209	-0.072430
H	2.071045	4.121581	1.197771
H	2.533122	4.032507	-0.525572

Number of imaginary frequencies = 1 (-329.9057)

ZPE Energy = -3563.716707

Free Energy = -3563.796897

TS-6+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.960668	-1.018344	-0.922000
C	4.869241	-0.741727	0.711254
C	3.335780	-1.464098	-1.043014
C	2.426337	0.902443	-1.207904
C	4.754166	0.418978	-1.365565
C	3.990186	1.610101	0.542850
H	4.666674	-1.673433	1.236517
H	0.170290	-0.371655	-1.294677
H	5.753378	0.813477	-1.178680
H	5.909767	-0.449985	0.855826
H	4.610087	0.287049	-2.438417
H	0.870563	-2.075219	-1.149767
H	3.378359	-1.761244	-2.094705
H	3.142325	-2.342582	-0.425941
H	1.666254	1.496389	-0.697751
H	2.312449	1.018484	-2.290008
H	4.962223	2.089255	0.660711
H	3.205297	2.232015	0.968362
N	2.193288	-0.526988	-0.875379
N	4.029367	0.334891	1.360230
N	3.755076	1.355044	-0.852420
N	4.607088	-0.873435	-0.695370
H	4.419854	0.546373	2.283018
C	0.110555	-1.312302	0.958327
C	-2.176043	-0.851146	0.339006
C	-1.939216	0.537762	0.560751
C	-0.742390	0.973479	1.057686
C	0.330191	0.054080	1.333026
O	1.439212	0.450549	1.789505
H	-0.587741	2.026527	1.269549
C	-1.188474	-1.757857	0.588279
H	0.833488	-2.044537	1.303255
H	3.034175	0.042514	1.514687

H	-1.367689	-2.818921	0.458307
C	-2.986670	1.575839	0.287325
O	-3.424404	2.316702	1.132338
O	-3.338541	1.604578	-0.988826
C	-4.383205	2.531202	-1.335159
H	-4.066075	3.551161	-1.117777
H	-5.288027	2.292639	-0.774970
H	-4.547821	2.398431	-2.401074
Br	-3.907098	-1.457384	-0.163977

Number of imaginary frequencies = 1 (-344.4168)

ZPE Energy = -3563.713384

Free Energy = -3563.793547

TS-7+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.046644	0.654401	0.948308
C	3.650417	0.900656	-1.074861
C	2.149391	1.635941	0.703989
C	1.855149	-0.786418	1.423463
C	4.002911	0.227062	1.185201
C	3.405248	-1.490463	-0.339091
H	3.174901	1.624606	-1.734351
H	-0.643851	-0.075956	1.487322
H	5.048299	0.029660	0.946128
H	4.714358	0.829962	-1.302710
H	3.923232	0.557282	2.221497
H	-0.384291	1.685802	0.965797
H	2.208185	2.149332	1.667807
H	1.695598	2.298228	-0.034372
H	1.224582	-1.624830	1.123248
H	1.851859	-0.699261	2.513729
H	4.454421	-1.747971	-0.484956
H	2.770312	-2.353443	-0.529608
N	1.257116	0.458287	0.871612
N	3.054466	-0.451994	-1.382535
N	3.223550	-0.996652	0.999514
N	3.489111	1.276060	0.304299
H	3.404872	-0.770226	-2.290555
C	-1.073184	0.387220	-0.902248
C	-3.198217	-0.372844	0.024562
C	-2.672963	-1.691974	0.022965
C	-1.423058	-1.976344	-0.463828
C	-0.583031	-0.952639	-1.003976
O	0.575780	-1.201474	-1.472975
H	-1.059722	-2.997805	-0.477582
C	-2.401163	0.629165	-0.476805
H	-0.542390	1.169471	-1.434195

H	1.998555	-0.445204	-1.454477
H	-3.279951	-2.501401	0.409778
Cl	-2.977675	2.270897	-0.483055
O	-4.437526	-0.050444	0.478795
C	-5.278861	-1.105458	0.930930
H	-4.847064	-1.610109	1.799371
H	-6.214348	-0.630273	1.219273
H	-5.468786	-1.827506	0.132344

Number of imaginary frequencies = 1 (-248.2234)

ZPE Energy = -1336.408275

Free Energy = -1336.473527

TS-7+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.137771	1.105661	-0.788377
C	-3.886003	0.668922	1.096613
C	-2.462211	1.732192	-0.579116
C	-1.784403	-0.572497	-1.423053
C	-4.066037	0.097088	-1.211026
C	-3.263965	-1.607380	0.233786
H	-3.544165	1.411425	1.815469
H	0.589911	0.505196	-1.327130
H	-5.076862	-0.267194	-1.026375
H	-4.934177	0.429716	1.278111
H	-4.003728	0.499027	-2.222945
H	0.045826	2.171319	-0.716324
H	-2.571882	2.289291	-1.513503
H	-2.133524	2.407830	0.211446
H	-1.044731	-1.324238	-1.142856
H	-1.760618	-0.419969	-2.505760
H	-4.266299	-2.026847	0.322332
H	-2.514292	-2.378965	0.396398
N	-1.396016	0.713690	-0.781948
N	-3.103647	-0.597159	1.347770
N	-3.117583	-1.006540	-1.064349
N	-3.742996	1.153290	-0.251445
H	-3.430987	-1.018000	2.222059
C	0.893073	0.885960	1.118007
C	3.106375	0.493537	0.203676
C	2.749305	-0.884060	0.082446
C	1.546833	-1.371796	0.505150
C	0.572509	-0.499919	1.096412
O	-0.551240	-0.950577	1.500498
H	1.318428	-2.428118	0.424726
C	2.186095	1.347789	0.755313
H	0.233625	1.548437	1.668816
H	-2.060990	-0.438309	1.462402

H	2.413527	2.399379	0.876417
Cl	3.909870	-1.971900	-0.624261
O	4.346612	0.834783	-0.225770
C	4.708823	2.205121	-0.127241
H	4.699760	2.538175	0.914263
H	5.719600	2.275252	-0.523997
H	4.036769	2.828591	-0.724670

Number of imaginary frequencies = 1 (-221.9056)

ZPE Energy = -1336.408197

Free Energy = -1336.472324

TS-8+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.177531	-0.361328	-1.069881
C	3.203210	-1.277267	1.274997
C	1.745976	-1.753310	-0.622372
C	2.010449	0.653860	-1.400654
C	3.879834	-0.756935	-0.950968
C	3.513040	1.091409	0.490919
H	2.535065	-1.870435	1.896901
H	-0.580432	0.444759	-1.677260
H	4.918409	-0.765999	-0.619640
H	4.234949	-1.416517	1.598895
H	3.826436	-1.094496	-1.986482
H	-0.716565	-1.301825	-1.055776
H	1.782786	-2.298264	-1.569579
H	1.105703	-2.287393	0.080941
H	1.536615	1.611130	-1.177184
H	2.089180	0.528668	-2.484539
H	4.576849	1.139129	0.723951
H	3.051291	2.068723	0.614961
N	1.126425	-0.427170	-0.888563
N	2.872418	0.176810	1.511803
N	3.349129	0.601306	-0.851436
N	3.090544	-1.656500	-0.108251
H	3.204662	0.440748	2.443631
C	-1.298715	0.275134	0.679439
C	-2.981060	1.412530	-0.600967
C	-2.149322	2.553829	-0.639107
C	-0.940509	2.594815	0.011672
C	-0.486735	1.455401	0.740649
O	0.636318	1.447991	1.352493
H	-3.940269	1.448953	-1.104115
H	-0.322933	3.486766	0.007620
C	-2.594318	0.283907	0.095305
H	-0.992119	-0.543690	1.320960
H	1.834300	0.398074	1.490037

C	-3.522030	-0.932274	0.168930
C	-3.825207	-1.433469	-1.252726
C	-2.916672	-2.085097	0.974404
C	-4.837285	-0.512803	0.844636
H	-2.910996	-1.737222	-1.771763
H	-4.315974	-0.663702	-1.852551
H	-4.490956	-2.300432	-1.207864
H	-1.983959	-2.451297	0.534345
H	-3.621934	-2.920031	0.991250
H	-2.719212	-1.797842	2.010959
H	-5.346236	0.272071	0.280610
H	-4.654793	-0.140736	1.856826
H	-5.511171	-1.372185	0.911975
H	-2.487597	3.427599	-1.187575

Number of imaginary frequencies = 1 (-211.4309)

ZPE Energy = -919.430642

Free Energy = -919.493553

TS-8+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.479106	1.284972	0.816903
C	3.809088	0.223917	-1.336597
C	2.845287	1.602824	0.424962
C	2.046649	-0.483716	1.565239
C	4.326020	-0.164545	0.958823
C	3.105562	-1.832051	-0.196893
H	3.474471	0.967846	-2.060087
H	-0.249166	0.823415	1.480270
H	5.241483	-0.676392	0.659476
H	4.783500	-0.163278	-1.651585
H	4.483354	0.319612	1.924234
H	0.458810	2.371625	0.833403
H	3.156746	2.193487	1.294153
H	2.503041	2.282683	-0.358210
H	1.192233	-1.160151	1.520910
H	2.234149	-0.209437	2.609540
H	4.040270	-2.369924	-0.383424
H	2.287719	-2.551756	-0.144013
N	1.714625	0.741490	0.810018
N	2.822295	-0.890159	-1.315744
N	3.244814	-1.143281	1.073802
N	3.990348	0.851471	-0.039869
H	2.932972	-1.408071	-2.188055
C	-0.367476	1.110387	-0.872967
C	-2.728998	1.491760	-0.412247
C	-2.927533	0.084758	-0.201589
C	-1.877775	-0.778640	-0.415683

C	-0.608756	-0.295552	-0.809286
O	0.348323	-1.157780	-0.992535
H	-3.561961	2.173002	-0.291685
H	-1.979361	-1.850050	-0.299713
C	-1.515595	1.974215	-0.780847
H	0.475367	1.444137	-1.472457
H	1.335683	-0.793762	-1.196893
H	-1.372203	3.036851	-0.945536
C	-4.302730	-0.396079	0.241625
C	-5.330444	-0.017146	-0.838947
C	-4.351380	-1.909502	0.457477
C	-4.667358	0.301139	1.563789
H	-6.322342	-0.359687	-0.531366
H	-5.382399	1.062464	-0.995659
H	-5.086551	-0.491700	-1.793507
H	-5.353774	-2.191355	0.788664
H	-4.139870	-2.459597	-0.463445
H	-3.643672	-2.231952	1.226203
H	-5.650051	-0.042818	1.897940
H	-3.940338	0.063014	2.345540
H	-4.711256	1.386940	1.455554

Number of imaginary frequencies = 1 (-405.0519)

ZPE Energy = -919.429126

Free Energy = -919.491586

Products

P-1+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-1.681800	0.325708	-0.440207
C	-3.064495	0.862470	-0.212360
C	-4.015221	0.059518	0.297848
C	-3.756844	-1.348712	0.531594
C	-2.600211	-1.950634	0.178487
C	-1.558389	-1.177113	-0.476150
O	-0.567277	-1.713086	-0.974531
C	-0.777910	0.772809	0.768684
N	0.617037	0.502332	0.502756
C	1.352879	-0.092603	1.621043
N	2.704725	-0.461599	1.208698
C	3.392433	0.728778	0.702982
N	2.688326	1.268116	-0.463464
C	1.333961	1.645367	-0.067119
C	2.725242	0.311538	-1.535785
N	2.190650	-1.050116	-1.126354
C	2.738983	-1.502007	0.217646
H	1.157035	-1.022705	-1.069555

H	-1.237789	0.751190	-1.345185
H	-5.004333	0.446748	0.515900
H	-4.549017	-1.940778	0.979668
H	-2.439299	-3.015304	0.302228
H	-1.101900	0.228767	1.660774
H	-0.954033	1.838087	0.957323
H	0.817798	-0.984953	1.953023
H	1.447692	0.604455	2.466379
H	4.414050	0.468134	0.422888
H	3.413139	1.485612	1.487413
H	1.419662	2.465997	0.660370
H	0.786703	2.006676	-0.941344
H	3.757046	0.151541	-1.849122
H	2.125347	0.645745	-2.380982
H	2.452321	-1.736929	-1.838997
H	2.142879	-2.359620	0.526588
H	3.770659	-1.805389	0.038684
C	-3.296071	2.303339	-0.537130
H	-4.293918	2.623870	-0.236167
H	-2.559016	2.947613	-0.047400
H	-3.187316	2.464054	-1.614896

Number of imaginary frequencies = 0
 ZPE Energy = -801.622003
 Free Energy = -801.682022

P-1+HMTA⁺-R₄
 RM062X/6-311+G(d,p) (AceticAcid)

1 1			
C	0.580965	-1.810828	0.962927
C	-2.030687	0.230743	-1.737360
C	-1.488957	-1.677600	-0.339080
C	-1.219409	-0.279281	1.604491
C	-3.197770	-0.133749	0.292260
C	-1.696071	1.704510	0.291901
H	-1.452863	-0.209897	-2.548759
H	0.459456	-2.092578	2.016171
H	-3.978821	0.530951	-0.079501
H	-2.859181	0.816407	-2.135523
H	-3.645155	-0.900764	0.924161
H	0.588225	-2.738929	0.386709
H	-1.994877	-2.474851	0.223898
H	-0.957567	-2.122264	-1.182577
H	-0.500446	0.280269	2.202329
H	-1.730845	-1.004174	2.253891
H	-2.488246	2.404817	0.027185
H	-0.890115	2.222795	0.811813
N	-0.514766	-0.963486	0.506947
N	-1.111791	1.212553	-1.026640
N	-2.233899	0.633150	1.083903

N	-2.524256	-0.775097	-0.839550
H	-0.243286	0.707494	-0.813567
C	1.970418	-1.118481	0.791654
C	2.052519	1.323021	1.270754
C	1.996745	1.605397	-0.170189
C	2.212761	0.478324	-1.084895
C	2.208232	-0.795273	-0.655120
H	2.052791	2.174404	1.943198
C	2.048772	0.059327	1.705033
H	2.707136	-1.865322	1.113519
H	2.044917	-0.154035	2.771094
O	1.747133	2.733505	-0.593859
H	-0.894404	2.012526	-1.628859
H	2.345499	0.724320	-2.134637
C	2.379471	-1.947637	-1.595164
H	1.437329	-2.493463	-1.711802
H	2.701317	-1.608524	-2.580090
H	3.113128	-2.657896	-1.203672

Number of imaginary frequencies = 0
 ZPE Energy = -801.620777
 Free Energy = -801.680723

P-1+HMTA⁺-R₆
 RM062X/6-311+G(d,p) (AceticAcid)

1 1			
C	1.395098	-0.801558	-0.661542
C	2.653416	-1.600255	-0.582009
C	3.809317	-1.066099	-0.175876
C	3.909316	0.354827	0.162348
C	2.844684	1.177541	0.007128
C	1.587338	0.689552	-0.527034
O	0.674511	1.465414	-0.823196
C	0.455474	-1.261309	0.504264
N	-0.872828	-0.703914	0.368854
C	-1.475875	-0.242084	1.620544
N	-2.743375	0.436893	1.360387
C	-3.641073	-0.481570	0.655565
N	-3.059259	-0.882896	-0.627451
C	-1.790572	-1.564109	-0.379681
C	-2.932127	0.265258	-1.483586
N	-2.154713	1.396010	-0.832236
C	-2.598930	1.649224	0.600500
H	-1.142551	1.170827	-0.831783
H	0.866854	-1.003353	-1.599341
H	2.581811	-2.658157	-0.816095
H	4.704743	-1.672300	-0.087098
H	2.913949	2.239373	0.219036
H	0.897295	-0.936833	1.451029
H	0.438732	-2.359159	0.514340

H	-0.784945	0.450732	2.105279
H	-1.686737	-1.075175	2.307524
H	-4.600949	0.007617	0.483005
H	-3.793327	-1.369832	1.268710
H	-2.015398	-2.487604	0.174436
H	-1.330717	-1.831753	-1.333868
H	-2.408247	0.010499	-2.403816
H	-3.920113	0.665712	-1.712051
H	-2.290364	2.251754	-1.377222
H	-1.853691	2.306635	1.046763
H	-3.560591	2.158531	0.535771
C	5.229150	0.849234	0.659543
H	5.525855	0.289208	1.551680
H	6.001395	0.673108	-0.096051
H	5.200839	1.912293	0.897456

Number of imaginary frequencies = 0
 ZPE Energy = -801.623131
 Free Energy = -801.683037

P-1+HMTA⁺-R₂ (no H-Bond)
 RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.699203	0.580953	0.637542
C	-1.917581	0.218243	-0.226456
C	-4.616436	-0.691116	0.024778
C	-3.056600	1.185680	0.001583
C	-2.267573	-1.261394	-0.120393
C	-3.665010	-1.640532	-0.088665
C	-4.315121	0.725944	0.085892
O	-1.364961	-2.098372	-0.090420
N	0.518094	-0.215856	0.296447
C	1.591206	0.016322	1.317429
C	0.986479	-0.000443	-1.152256
N	2.396157	-0.214632	-1.292975
N	2.822130	-0.720753	1.001826
C	2.785335	-1.270503	-0.355456
C	4.011698	0.160314	1.074147
C	3.217521	1.024638	-1.048706
N	4.360009	0.779921	-0.203246
H	5.036737	0.209771	-0.698243
H	0.219740	-1.202208	0.355429
H	-0.921938	0.393599	1.690198
H	-0.429221	1.628578	0.508851
H	-1.649696	0.353520	-1.288803
H	-5.658843	-0.988380	0.083573
H	-3.896381	-2.699098	-0.102680
H	-5.139433	1.421504	0.194473
H	1.752385	1.096298	1.363435
H	1.169887	-0.314474	2.267742

H	0.415217	-0.725901	-1.733969
H	0.707966	1.013265	-1.441629
H	2.082006	-2.100614	-0.437055
H	3.771268	-1.664669	-0.591033
H	4.866679	-0.429087	1.404900
H	3.819624	0.926157	1.828474
H	3.564969	1.404585	-2.008315
H	2.591837	1.796508	-0.587782
C	-2.738049	2.648677	0.040980
H	-2.219415	2.917976	0.966862
H	-2.085703	2.929542	-0.791976
H	-3.652729	3.238648	-0.015970

Number of imaginary frequencies = 0
 ZPE Energy = -801.587941
 Free Energy = -801.649428

P-1+HMTA⁺-R₄ (no H-Bond)
 RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.576929	-1.774063	0.938925
C	-1.773163	0.875978	-1.558780
C	-0.961350	-1.336285	-0.886554
C	-1.600411	-0.836788	1.424803
C	-3.155605	-0.634922	-0.347756
C	-2.425324	1.358898	0.718072
H	-2.647056	1.321333	-2.041746
H	0.427856	-2.024284	1.991805
H	-4.028655	-0.086602	-0.706543
H	-0.926207	0.950318	-2.243543
H	-3.428623	-1.682587	-0.202224
H	0.657047	-2.716507	0.386281
H	-1.275813	-2.391799	-0.878976
H	-0.134782	-1.230391	-1.594734
H	-1.210166	-0.374156	2.335834
H	-1.976264	-1.840167	1.677405
H	-3.373519	1.847497	0.478492
H	-2.046423	1.782294	1.649523
N	-0.486180	-0.939765	0.454476
N	-1.470090	1.649478	-0.352619
N	-2.723608	-0.064678	0.928299
N	-2.089017	-0.545659	-1.345642
H	-0.562432	1.340861	-0.022190
C	2.023591	-1.079374	0.860397
C	1.891527	1.339069	1.333959
C	1.971604	1.562875	-0.076702
C	2.224716	0.517974	-0.998313
C	2.320641	-0.763906	-0.554745
H	1.778337	2.189419	1.997240
C	1.965869	0.069699	1.778343

H	2.698477	-1.854963	1.237236
H	2.363459	0.781438	-2.040692
H	1.897637	-0.143362	2.840784
O	1.841291	2.757446	-0.583840
H	1.663386	3.437719	0.085815
C	2.678309	-1.884704	-1.467233
H	2.691088	-1.566567	-2.509055
H	3.672842	-2.256283	-1.197455
H	1.987757	-2.725124	-1.350625

Number of imaginary frequencies = 0

ZPE Energy = -801.592647

Free Energy = -801.652148

P-1+HMTA⁺-R₆ (no H-Bond)

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.420861	0.817780	0.637890
C	-1.650312	0.589218	-0.250147
C	-4.453352	-0.065887	0.014824
C	-2.691452	1.627841	0.033344
C	-2.147893	-0.845763	-0.186221
C	-3.574476	-1.082650	-0.149791
C	-3.985833	1.317242	0.133541
O	-1.331838	-1.769357	-0.189231
N	0.728415	-0.063431	0.270145
C	1.794924	0.006444	1.324338
C	1.238347	0.186127	-1.158538
N	2.626042	-0.142436	-1.292084
N	2.975949	-0.796243	0.979650
C	2.913098	-1.272129	-0.404107
C	4.226373	-0.005559	1.107535
C	3.538980	1.011391	-0.975318
N	4.648109	0.631903	-0.137456
H	5.274504	0.022739	-0.652401
H	0.337162	-1.019292	0.268197
H	-0.668936	0.603361	1.679373
H	-0.078581	1.850604	0.556779
H	-1.360742	0.735015	-1.304235
H	-2.354423	2.656970	0.111293
H	-3.902660	-2.115391	-0.197829
H	-4.728487	2.089567	0.303345
H	2.037535	1.064026	1.453359
H	1.323886	-0.358187	2.238219
H	0.615261	-0.453767	-1.785498
H	1.055686	1.234180	-1.397341
H	2.144909	-2.035451	-0.534541
H	3.865778	-1.735295	-0.651030
H	5.030232	-0.663948	1.435883
H	4.070835	0.747469	1.882914

H	3.921944	1.415684	-1.911302
H	2.972533	1.803608	-0.473548
C	-5.925943	-0.298018	0.101888
H	-6.311346	0.100707	1.045263
H	-6.434518	0.243753	-0.701871
H	-6.175061	-1.356270	0.031618

Number of imaginary frequencies = 0

ZPE Energy = -801.590561

Free Energy = -801.652086

P-2+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.411749	-0.453141	-0.522912
C	-1.879621	-0.309948	-0.338722
C	-2.683219	-1.320961	0.069251
C	-2.106326	-2.640855	0.255074
C	-0.818067	-2.920173	-0.017852
C	0.066381	-1.888758	-0.548238
O	1.195010	-2.148578	-0.952164
C	0.295543	0.247515	0.692157
N	1.716972	0.353924	0.468361
C	2.103869	1.600239	-0.200929
N	3.526964	1.599251	-0.527343
C	4.298258	1.398354	0.701557
N	3.956755	0.111666	1.312656
C	2.538347	0.108805	1.658765
C	4.335042	-0.960822	0.432936
N	3.743366	-0.811013	-0.959899
C	3.891934	0.602887	-1.496006
H	4.214171	-1.461551	-1.594776
O	-2.318817	0.937504	-0.548249
C	-3.633809	1.241261	-0.343304
C	-4.513447	0.306794	0.062828
C	-4.107700	-1.067051	0.299786
O	-4.883562	-1.948188	0.666161
C	-3.913069	2.681811	-0.601718
C	-3.161471	3.591380	0.374680
H	-0.098148	0.057160	-1.438054
H	-2.777070	-3.416271	0.611497
H	-0.411029	-3.918774	0.087876
H	0.101950	-0.344977	1.591026
H	-0.175630	1.228056	0.837281
H	1.520513	1.709430	-1.118162
H	1.910044	2.470473	0.443016
H	4.063612	2.198302	1.403583
H	5.363746	1.420396	0.469294
H	2.384884	0.880205	2.427077
H	2.266047	-0.863869	2.073343

H	3.994418	-1.921847	0.815686
H	5.417325	-0.967104	0.303536
H	2.741459	-1.064059	-0.924751
H	4.942158	0.718582	-1.763978
H	3.268437	0.670103	-2.386164
H	-5.549612	0.580607	0.215971
H	-3.615880	2.909076	-1.630464
H	-4.989702	2.836746	-0.522697
H	-2.081086	3.465574	0.279137
H	-3.399791	4.635985	0.168062
H	-3.445629	3.371034	1.406134

Number of imaginary frequencies = 0

ZPE Energy = -1105.625973

Free Energy = -1105.691938

P-2+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	1.246986	-1.076175	-0.887353
C	2.330994	-0.354935	-0.517144
C	2.302872	1.085933	-0.309443
C	1.134907	1.737158	-0.435126
C	-0.144762	1.030629	-0.679778
C	-0.012371	-0.409384	-1.114112
O	-0.979783	-1.004942	-1.594389
C	-0.924581	1.033218	0.691973
N	-2.252275	0.486247	0.549429
C	-3.293915	1.505056	0.393077
N	-4.591162	0.891368	0.122978
C	-4.913117	-0.039649	1.208289
N	-3.906824	-1.099150	1.284210
C	-2.606612	-0.503965	1.571037
C	-3.932826	-1.883029	0.080682
N	-3.778604	-1.034512	-1.172546
C	-4.654826	0.204287	-1.137570
H	-4.029818	-1.599754	-1.988121
O	3.497010	-1.026750	-0.356349
C	4.649955	-0.383788	-0.004795
C	4.722938	0.945237	0.193339
C	3.560461	1.797203	0.043363
O	3.586124	3.009044	0.201438
C	5.776203	-1.348939	0.129832
C	5.504858	-2.399424	1.210926
H	1.328581	-2.138941	-1.080072
H	1.107954	2.811254	-0.274033
H	-0.765781	1.575793	-1.396538
H	-0.945941	2.065210	1.061147
H	-0.347042	0.442546	1.408890
H	-3.021396	2.162383	-0.436112

H	-3.399073	2.112050	1.304265
H	-5.894698	-0.481405	1.030064
H	-4.928634	0.506798	2.151164
H	-2.665566	-0.053690	2.572840
H	-1.842478	-1.284625	1.577047
H	-4.895383	-2.386733	-0.008978
H	-3.121984	-2.610344	0.067057
H	-2.783076	-0.764184	-1.265652
H	-4.328285	0.847270	-1.953629
H	-5.674306	-0.138838	-1.315256
H	5.668771	1.392366	0.469064
H	5.914543	-1.839450	-0.839384
H	6.682548	-0.786136	0.354988
H	4.622760	-2.995332	0.970787
H	6.358924	-3.073813	1.290039
H	5.351646	-1.925503	2.183151

Number of imaginary frequencies = 0

ZPE Energy = -1105.614098

Free Energy = -1105.679395

P-3+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	1.181295	-0.100998	-0.541457
C	2.601175	-0.434086	-0.331871
C	3.502287	0.415646	0.167836
C	3.187784	1.773506	0.474079
C	1.943708	2.242122	0.200786
C	0.937423	1.398139	-0.432984
O	-0.128173	1.864220	-0.835045
C	0.346882	-0.788352	0.601089
N	-1.068981	-0.579849	0.417263
C	-1.770015	-0.048694	1.589451
N	-3.154172	0.277265	1.259145
C	-3.818867	-0.921618	0.744736
N	-3.155523	-1.386178	-0.476152
C	-1.770352	-1.726864	-0.164188
C	-3.288115	-0.396113	-1.509179
N	-2.792303	0.971711	-1.074521
C	-3.288210	1.349876	0.312588
H	-1.757952	0.994208	-1.058540
O	3.121090	-1.689934	-0.425065
C	4.538710	-1.478245	-0.273244
O	4.684778	-0.253763	0.440313
H	0.803307	-0.464742	-1.500561
H	3.946494	2.413098	0.912331
H	1.678107	3.276632	0.380017
H	0.676195	-0.375925	1.559528

H	0.607391	-1.852979	0.599577
H	-1.793193	-0.776585	2.413606
H	-1.253680	0.853230	1.925315
H	-4.863800	-0.694751	0.527765
H	-3.765977	-1.708333	1.497385
H	-1.254039	-2.029047	-1.078325
H	-1.788529	-2.579546	0.530079
H	-4.340843	-0.270653	-1.763266
H	-2.719063	-0.674028	-2.394971
H	-3.115122	1.675189	-1.744234
H	-2.712615	2.221906	0.620811
H	-4.340711	1.611227	0.200930
H	4.970471	-2.296355	0.295991
H	4.976622	-1.373278	-1.271055

Number of imaginary frequencies = 0

ZPE Energy = -950.841995

Free Energy = -950.903377

P-3+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.937289	-0.582706	-0.742574
C	2.250268	-1.309285	-0.738911
C	3.323351	-0.663041	-0.300697
C	3.288353	0.730960	0.111373
C	2.197959	1.518561	0.025425
C	1.004825	0.924901	-0.540127
O	0.018758	1.616702	-0.807834
C	0.055750	-1.162081	0.412086
N	-1.313622	-0.700991	0.332104
C	-1.895255	-0.279630	1.607031
N	-3.215278	0.311742	1.400385
C	-4.074891	-0.664836	0.728373
N	-3.519669	-1.020517	-0.579476
C	-2.199433	-1.615929	-0.388435
C	-3.510022	0.136418	-1.431280
N	-2.789990	1.319240	-0.806211
C	-3.188917	1.534600	0.644737
H	-3.010133	2.163460	-1.341469
O	4.613650	-1.093903	-0.180661
C	5.322647	-0.107993	0.553980
O	4.507387	1.075224	0.531823
H	0.404723	-0.764742	-1.681321
H	2.283108	-2.350813	-1.036218
H	2.209654	2.568476	0.287758
H	0.495368	-0.855512	1.366401
H	0.117753	-2.257333	0.368848
H	-2.020714	-1.123763	2.301474
H	-1.233854	0.458763	2.064980

H	-4.140136	-1.562623	1.342979
H	-5.072723	-0.242885	0.597750
H	-2.338949	-2.558325	0.162441
H	-1.759191	-1.842672	-1.362449
H	-3.009827	-0.075737	-2.375214
H	-4.533539	0.464046	-1.614662
H	-1.764605	1.174105	-0.846792
H	-2.473527	2.240798	1.064179
H	-4.186152	1.974669	0.625249
H	5.442824	-0.425526	1.590832
H	6.269937	0.105481	0.065111

Number of imaginary frequencies = 0

ZPE Energy = -950.857321

Free Energy = -950.918637

P-4+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.723844	0.199954	-0.490446
C	2.186877	-0.002061	-0.298490
C	3.024258	0.968528	0.169453
C	2.530459	2.305908	0.415638
C	1.252771	2.636786	0.141479
C	0.330610	1.667502	-0.446492
O	-0.775405	2.014677	-0.851609
C	-0.047975	-0.508367	0.677086
N	-1.473761	-0.495240	0.452265
C	-2.279435	-0.219880	1.644697
N	-3.691511	-0.094875	1.293716
C	-4.133376	-1.328440	0.639140
N	-3.373348	-1.550737	-0.592722
C	-1.958090	-1.681176	-0.260117
C	-3.652656	-0.499287	-1.529794
N	-3.402485	0.883416	-0.949174
C	-3.977408	1.033614	0.450541
H	-2.385178	1.069984	-0.916289
H	0.370500	-0.224995	-1.433767
H	3.225419	3.039176	0.812483
H	0.877709	3.643489	0.283193
H	0.190423	0.010014	1.610829
H	0.342878	-1.530571	0.767624
H	-2.195930	-1.024547	2.389780
H	-1.931406	0.713871	2.091190
H	-5.196266	-1.255441	0.404089
H	-3.969873	-2.166734	1.316058
H	-1.379033	-1.807691	-1.177815
H	-1.845842	-2.587544	0.353317
H	-4.706009	-0.527031	-1.808771
H	-3.027939	-0.585575	-2.417625

H	-3.831647	1.583147	-1.560794
H	-3.558285	1.949447	0.864905
H	-5.055573	1.135544	0.325370
C	4.519532	-0.648636	0.068858
S	3.068367	-1.466860	-0.494008
N	4.337777	0.595717	0.369680
C	5.811863	-1.383118	0.179150
H	6.602473	-0.672508	0.418325
H	5.759986	-2.135460	0.969979
H	6.058636	-1.890177	-0.755649

Number of imaginary frequencies = 0
 ZPE Energy = -1292.073704
 Free Energy = -1292.129188

P-4+HMTA⁺-R₆
 RM062X/6-311+G(d,p) (AceticAcid)

1 1			
C	0.366635	-0.617830	-0.814488
C	1.678496	-1.322898	-0.796359
C	2.790524	-0.690643	-0.400241
C	2.748702	0.735499	-0.052216
C	1.633547	1.496259	-0.155281
C	0.421938	0.887284	-0.665826
O	-0.569674	1.572146	-0.931501
C	-0.479776	-1.170838	0.389864
N	-1.847278	-0.707761	0.339687
C	-2.390834	-0.271399	1.627484
N	-3.719454	0.309097	1.455150
C	-4.595619	-0.680077	0.825150
N	-4.082624	-1.047556	-0.496199
C	-2.753527	-1.632978	-0.343903
C	-4.112300	0.098700	-1.361064
N	-3.380264	1.294808	-0.775724
C	-3.726541	1.523378	0.686826
H	-3.628580	2.130635	-1.311779
H	-0.188162	-0.855920	-1.727585
H	1.703360	-2.379979	-1.040844
H	1.620953	2.558041	0.059732
H	-0.008337	-0.839816	1.319904
H	-0.418218	-2.266206	0.367108
H	-2.487808	-1.106889	2.336367
H	-1.718680	0.476411	2.053327
H	-4.636382	-1.570777	1.452094
H	-5.599482	-0.264612	0.723301
H	-2.868144	-2.570820	0.219992
H	-2.344816	-1.866463	-1.329908
H	-3.643977	-0.119951	-2.319769
H	-5.144224	0.416026	-1.512265
H	-2.356572	1.157386	-0.857280

H	-3.000371	2.237198	1.073451
H	-4.726082	1.958470	0.699207
N	4.057977	-1.274344	-0.270687
S	4.337365	1.231949	0.450352
C	4.928738	-0.444078	0.145844
C	6.362614	-0.739285	0.396578
H	6.560694	-1.787187	0.175378
H	6.994756	-0.108133	-0.233373
H	6.615530	-0.532047	1.439520

Number of imaginary frequencies = 0
 ZPE Energy = -1292.063305
 Free Energy = -1292.118534

P-5+HMTA⁺-R₂
 RM062X/6-311+G(d,p) (AceticAcid)

1 1			
C	1.013125	0.494168	-0.318448
C	2.485394	0.407115	-0.072518
C	3.206842	1.477084	0.293950
C	2.582381	2.788702	0.393097
C	1.300532	2.998271	0.041262
C	0.488882	1.896845	-0.479891
O	-0.615196	2.101962	-0.974771
C	0.246997	-0.112951	0.914096
N	-1.143895	-0.323816	0.588632
C	-2.092304	0.011652	1.651756
N	-3.464829	-0.088328	1.159912
C	-3.697616	-1.446340	0.661792
N	-2.788205	-1.748496	-0.445472
C	-1.411126	-1.651886	0.030797
C	-3.072256	-0.882471	-1.556028
N	-3.040006	0.588456	-1.172480
C	-3.776739	0.864216	0.130095
H	-3.470643	1.137824	-1.921178
C	3.082506	-0.948044	-0.209480
O	2.435835	-1.919108	-0.538801
O	4.382136	-0.989173	0.058911
C	5.012693	-2.274542	-0.055796
H	0.732926	-0.097834	-1.193457
H	4.264702	1.387989	0.508417
H	3.192633	3.617071	0.736310
H	0.846971	3.982472	0.069439
H	0.333439	0.579919	1.756332
H	0.747593	-1.044669	1.203857
H	-2.002001	-0.666725	2.512633
H	-1.897400	1.033615	1.983633
H	-4.729687	-1.536917	0.319953
H	-3.522084	-2.155673	1.470368
H	-1.266111	-2.437419	0.786674

H	-0.722762	-1.836347	-0.797232
H	-2.343768	-1.016404	-2.354398
H	-4.078019	-1.077822	-1.928143
H	-2.059201	0.899991	-1.067844
H	-4.839912	0.815386	-0.105368
H	-3.504042	1.874143	0.433788
H	6.061634	-2.103365	0.171430
H	4.900588	-2.658727	-1.069790
H	4.575632	-2.971578	0.659616

Number of imaginary frequencies = 0

ZPE Energy = -990.159276

Free Energy = -990.216287

P-5+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.339483	1.342826	-0.631117
C	-1.491870	2.262461	-0.394923
C	-2.727531	1.809526	-0.160317
C	-2.999932	0.376902	-0.188596
C	-2.062814	-0.530474	-0.529373
C	-0.722180	-0.084150	-0.918022
O	0.078995	-0.870123	-1.412839
C	0.532832	1.328331	0.673130
N	1.767827	0.599458	0.484132
C	2.216647	-0.130587	1.673600
N	3.404967	-0.923101	1.370444
C	4.463647	-0.032538	0.891093
N	4.039909	0.643323	-0.336076
C	2.845754	1.435552	-0.056726
C	3.857573	-0.322468	-1.382409
N	2.894889	-1.432775	-0.988095
C	3.176048	-1.966807	0.410417
H	2.976001	-2.199501	-1.661329
C	-4.392806	-0.049579	0.172883
O	-5.254784	0.733382	0.491936
O	-4.571354	-1.360886	0.110504
C	-5.883790	-1.835333	0.455241
H	0.294259	1.706193	-1.445411
H	-1.275891	3.325407	-0.358152
H	-3.548930	2.480457	0.057737
H	-2.272065	-1.592188	-0.581209
H	-0.049625	0.858250	1.471025
H	0.710277	2.371339	0.968218
H	2.477266	0.549671	2.497808
H	1.411139	-0.790246	2.002253
H	5.366809	-0.611912	0.693875
H	4.673333	0.714748	1.656242
H	3.129823	2.223313	0.656647

H	2.503392	1.908445	-0.979638
H	3.453549	0.141168	-2.281054
H	4.807410	-0.808700	-1.605245
H	1.928411	-1.070481	-1.028774
H	4.068902	-2.585943	0.321747
H	2.319821	-2.578463	0.690544
H	-5.841071	-2.915293	0.341895
H	-6.623588	-1.408143	-0.221912
H	-6.117801	-1.567415	1.485788

Number of imaginary frequencies = 0

ZPE Energy = -990.153455

Free Energy = -990.212284

P-6+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.532236	1.449680	1.356316
C	-1.209903	0.316207	0.631837
C	-1.949525	0.531686	-0.459774
C	-2.140142	1.872867	-1.008930
C	-1.529936	2.942316	-0.477811
C	-0.619160	2.802466	0.665908
O	0.039476	3.741275	1.072902
C	0.910082	1.065341	1.746551
N	1.617643	0.414437	0.650196
C	2.800114	-0.301689	1.155356
N	3.530991	-0.960550	0.079679
C	3.925863	0.040980	-0.911765
N	2.738089	0.676082	-1.481299
C	1.993031	1.349485	-0.422521
C	1.966019	-0.292192	-2.206962
N	1.611550	-1.502775	-1.358491
C	2.802699	-2.018035	-0.561010
H	0.866513	-1.259811	-0.692202
Br	-2.872635	-0.866335	-1.355069
C	-1.001552	-1.043679	1.221643
O	-0.471556	-1.963943	0.641924
O	-1.423882	-1.099404	2.471372
C	-1.196716	-2.343837	3.162080
H	-1.081588	1.602505	2.298724
H	-2.790183	1.983330	-1.869648
H	-1.649909	3.934218	-0.898400
H	1.429366	1.963901	2.107222
H	0.862338	0.356358	2.577715
H	3.499156	0.385204	1.654737
H	2.464065	-1.049877	1.877179
H	4.501095	-0.436878	-1.705985
H	4.539007	0.800697	-0.427243
H	2.618889	2.166638	-0.034254

H	1.089132	1.778487	-0.861140
H	1.026976	0.133951	-2.558343
H	2.545925	-0.672168	-3.048158
H	1.260714	-2.252572	-1.961285
H	2.406755	-2.725318	0.166641
H	3.447082	-2.529474	-1.276262
H	-1.718702	-3.151301	2.649204
H	-0.126714	-2.550435	3.202794
H	-1.599734	-2.199067	4.160437

Number of imaginary frequencies = 0

ZPE Energy = -3563.734904

Free Energy = -3563.812736

P-6+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.273626	-0.833417	-0.594567
C	1.053128	-1.487624	-0.389020
C	2.172589	-0.770893	-0.275669
C	2.152105	0.687928	-0.406515
C	1.034070	1.341024	-0.768818
C	-0.210281	0.609603	-1.018044
O	-1.184068	1.178466	-1.494522
C	-1.073072	-0.881358	0.756287
N	-2.446865	-0.475644	0.564412
C	-2.986388	0.368513	1.634807
N	-4.328624	0.831558	1.296292
C	-5.193579	-0.327559	1.064894
N	-4.687150	-1.122181	-0.055925
C	-3.344245	-1.596141	0.264607
C	-4.752053	-0.348723	-1.265128
N	-4.035427	0.986571	-1.143912
C	-4.368309	1.703458	0.155412
H	-3.014422	0.834688	-1.189176
C	3.384156	1.508988	-0.148461
O	3.885726	2.227105	-0.975245
O	3.809528	1.370029	1.094477
C	5.000605	2.103294	1.438036
Br	3.854523	-1.631285	-0.064542
H	-0.852318	-1.394060	-1.334819
H	1.065844	-2.568847	-0.304214
H	1.027492	2.416352	-0.910492
H	-0.583513	-0.213156	1.470889
H	-0.994223	-1.900192	1.156551
H	-2.326880	1.229183	1.763338
H	-3.056277	-0.174736	2.588501
H	-6.206214	0.011252	0.841298
H	-5.208904	-0.944792	1.962933
H	-2.945203	-2.154863	-0.585068

H	-3.428556	-2.277303	1.124017
H	-5.791474	-0.116213	-1.496546
H	-4.291271	-0.879453	-2.096763
H	-4.304256	1.581109	-1.932640
H	-3.648674	2.514593	0.258548
H	-5.374798	2.103866	0.033578
H	5.206743	1.853606	2.475149
H	4.820798	3.172717	1.328221
H	5.824167	1.791727	0.794961

Number of imaginary frequencies = 0

ZPE Energy = -3563.728129

Free Energy = -3563.808481

P-7+HMTA⁺-R₂

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	-0.895852	0.146954	-0.451046
C	-2.306754	0.591467	-0.266092
C	-3.299878	-0.239470	0.096874
C	-3.002483	-1.659721	0.245025
C	-1.799778	-2.190395	-0.044989
C	-0.723463	-1.349193	-0.552378
O	0.318509	-1.830132	-0.987497
C	-0.039538	0.596755	0.787841
N	1.369180	0.407461	0.536841
C	2.120678	-0.187015	1.644651
N	3.493190	-0.476129	1.237253
C	4.126768	0.761980	0.780136
N	3.410315	1.302815	-0.377863
C	2.034720	1.601341	0.010662
C	3.513008	0.387202	-1.479753
N	3.043400	-1.014357	-1.123998
C	3.592439	-1.481927	0.215460
H	2.010044	-1.043519	-1.083880
H	-0.460606	0.613699	-1.339424
H	-3.796779	-2.312197	0.588828
H	-1.615001	-3.255122	0.032878
H	-0.352710	0.009063	1.655775
H	-0.279671	1.645324	1.001773
H	1.625977	-1.113952	1.942321
H	2.171529	0.486092	2.512788
H	5.163582	0.561763	0.505736
H	4.099414	1.492593	1.588608
H	2.070915	2.401920	0.764172
H	1.479647	1.963212	-0.858511
H	4.556741	0.290954	-1.779580
H	2.909842	0.717192	-2.324266
H	3.351181	-1.662911	-1.853688
H	3.033104	-2.375931	0.487899

H	4.640007	-1.729285	0.043393
Cl	-2.604486	2.290742	-0.445968
O	-4.537671	0.254229	0.338942
C	-5.646663	-0.646303	0.339940
H	-5.644843	-1.274492	1.233322
H	-6.533331	-0.015650	0.350319
H	-5.651288	-1.262701	-0.562179

Number of imaginary frequencies = 0
ZPE Energy = -1336.424936
Free Energy = -1336.490070

P-7+HMTA⁺-R₆
RM062X/6-311+G(d,p) (AceticAcid)

1 1			
C	-0.672678	0.606504	-0.600848
C	-2.007422	1.264122	-0.471694
C	-3.115751	0.575913	-0.163024
C	-3.028448	-0.882674	0.008737
C	-1.904061	-1.582530	-0.219230
C	-0.703051	-0.895627	-0.680451
O	0.274008	-1.534333	-1.062074
C	0.196975	0.969164	0.652553
N	1.578580	0.584984	0.464118
C	2.231912	0.021788	1.648145
N	3.572779	-0.456808	1.316159
C	4.355227	0.653532	0.765903
N	3.730501	1.160977	-0.457077
C	2.390625	1.645320	-0.137438
C	3.745837	0.144568	-1.471882
N	3.109245	-1.153868	-1.004207
C	3.576783	-1.554201	0.386732
H	2.079191	-1.054526	-0.994630
H	-0.145611	0.986066	-1.481349
H	-2.032448	2.340599	-0.587980
H	-1.871037	-2.660639	-0.119812
H	-0.218626	0.452615	1.523032
H	0.091088	2.046552	0.834679
H	1.628356	-0.811009	2.015357
H	2.338486	0.765838	2.450951
H	5.366540	0.310637	0.542688
H	4.399764	1.457424	1.500851
H	2.503761	2.497849	0.548546
H	1.903308	1.993639	-1.050803
H	3.197807	0.463709	-2.357276
H	4.775796	-0.098291	-1.733772
H	3.351779	-1.901774	-1.659852
H	2.916193	-2.353269	0.720497
H	4.592770	-1.930868	0.268285
Cl	-4.461692	-1.706814	0.514201

O	-4.355410	1.078332	0.013057
C	-4.504685	2.485058	-0.134291
H	-5.557377	2.691888	0.045272
H	-3.892603	3.016494	0.599892
H	-4.232482	2.798285	-1.146097

Number of imaginary frequencies = 0
ZPE Energy = -1336.428003
Free Energy = -1336.492920

P-8+HMTA⁺-R₂
RM062X/6-311+G(d,p) (AceticAcid)

1 1			
C	1.103149	0.353673	-0.345847
C	2.565507	0.221081	-0.021823
C	3.217490	1.303135	0.447513
C	2.579776	2.601557	0.530463
C	1.337163	2.842148	0.059427
C	0.594091	1.759216	-0.557589
O	-0.461582	1.954946	-1.162867
C	0.275445	-0.172186	0.889329
N	-1.129580	-0.282614	0.566206
C	-2.035944	0.202341	1.609138
N	-3.419791	0.169338	1.143497
C	-3.760170	-1.200518	0.753896
N	-2.900243	-1.647650	-0.344973
C	-1.508100	-1.617753	0.097409
C	-3.146133	-0.842072	-1.509858
N	-2.987252	0.642579	-1.233613
C	-3.683281	1.064931	0.050945
H	-1.981986	0.879246	-1.156689
C	3.269583	-1.133563	-0.155993
C	3.632274	-1.666187	1.241802
C	2.414079	-2.180247	-0.880343
C	4.565524	-0.948285	-0.964127
H	0.816128	-0.252534	-1.207204
H	4.255071	1.237979	0.754436
H	3.154518	3.418733	0.955739
H	0.894621	3.831375	0.061483
H	0.415524	0.529066	1.717475
H	0.690419	-1.133652	1.210372
H	-1.760486	1.229299	1.858803
H	-1.982418	-0.411572	2.520165
H	-4.803563	-1.241758	0.438322
H	-3.614453	-1.860544	1.608984
H	-1.397651	-2.367490	0.895163
H	-0.859613	-1.896094	-0.736559
H	-4.174190	-0.982413	-1.844204
H	-2.453239	-1.089113	-2.312855
H	-3.380795	1.172962	-2.015826

H	-3.337365	2.072921	0.276191
H	-4.751005	1.071563	-0.168707
H	2.740922	-1.836054	1.851787
H	4.280793	-0.965757	1.773490
H	4.163184	-2.618102	1.147129
H	2.177642	-1.874308	-1.903312
H	2.977189	-3.115218	-0.938848
H	1.479341	-2.397331	-0.357505
H	4.355105	-0.534294	-1.954156
H	5.269156	-0.284077	-0.458390
H	5.055146	-1.917591	-1.096226

Number of imaginary frequencies = 0

ZPE Energy = -919.447469

Free Energy = -919.511185

P-8+HMTA⁺-R₆

RM062X/6-311+G(d,p) (AceticAcid)

1 1

C	0.405872	-1.092350	-0.721243
C	1.606744	-1.967238	-0.587672
C	2.817897	-1.480025	-0.302119
C	3.050447	-0.038283	-0.144647
C	2.035660	0.831849	-0.368330
C	0.720847	0.380403	-0.792086
O	-0.137317	1.185346	-1.162473
C	-0.505185	-1.329086	0.527340
N	-1.788281	-0.671527	0.393209
C	-2.346412	-0.184571	1.657779
N	-3.574528	0.570104	1.417798
C	-4.540533	-0.292985	0.734654
N	-4.007570	-0.733983	-0.556199
C	-2.773465	-1.482539	-0.328984
C	-3.832062	0.401074	-1.421306
N	-2.969366	1.481805	-0.791390
C	-3.368412	1.767229	0.648983
H	-1.979442	1.178478	-0.819503
C	4.449404	0.405353	0.253350
C	4.557827	1.921773	0.415338
C	4.814223	-0.258679	1.592774
C	5.440078	-0.046808	-0.834125
H	-0.171617	-1.365818	-1.610231
H	1.449100	-3.037697	-0.679134
H	3.653145	-2.158141	-0.177840
H	2.166287	1.904972	-0.301783
H	0.011654	-0.936662	1.408286
H	-0.613586	-2.413582	0.669932
H	-1.610236	0.462364	2.138943
H	-2.595519	-1.010272	2.340651
H	-5.470146	0.255490	0.575110

H	-4.738887	-1.167196	1.354594
H	-3.034559	-2.386567	0.240945
H	-2.355207	-1.785939	-1.290821
H	-3.345409	0.113425	-2.352348
H	-4.798800	0.860775	-1.627555
H	-3.057722	2.342705	-1.338116
H	-2.575611	2.377548	1.079078
H	-4.297121	2.335879	0.599805
H	3.877017	2.296392	1.184574
H	4.347760	2.446856	-0.520360
H	5.576338	2.177576	0.717670
H	4.810556	-1.348935	1.528966
H	4.116312	0.041796	2.379504
H	5.818299	0.054994	1.891095
H	5.451820	-1.131656	-0.959815
H	6.449906	0.267153	-0.556033
H	5.194855	0.407804	-1.797986

Number of imaginary frequencies = 0

ZPE Energy = -919.452385

Free Energy = -919.517084