Electronic Supplementary Material (ESI) for RSC Advances.

Comprehensive study on the degradation of Ochratoxin A in water by spectroscopic techniques and DFT calculations

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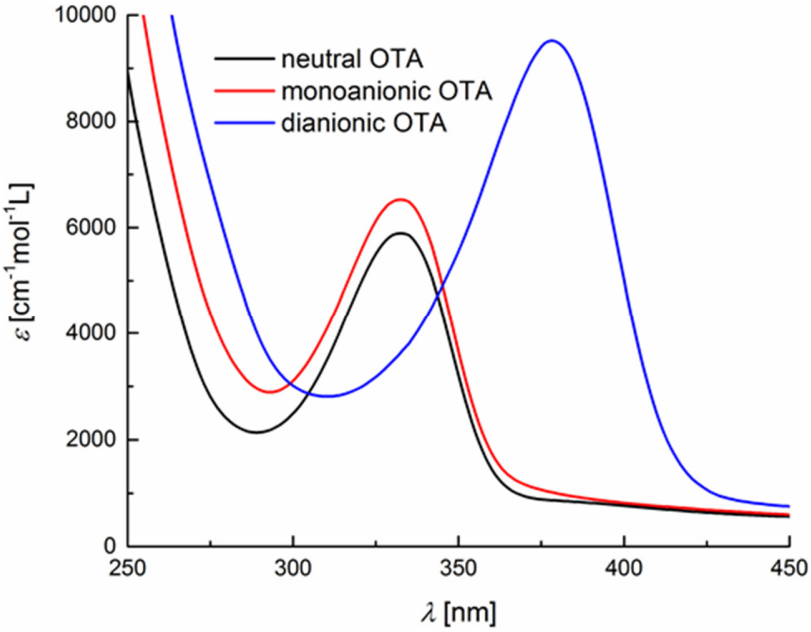


Figure S1. Behavior of ε for the three forms of OTA as a function of λ.

The values of the molar absorptivity (ε) for the three OTA forms, pK_{a1} and pK_{a2} were deduced by the HypSpec® software. The two protonation equilibria had to be considered together to properly model the experimental spectra with the software, because of the correlation between pK_{a1} and pK_{a2}. The optimised values of pK_a derived from the elaboration process are 4.489 and 7.099, with a fit uncertainty of 0.002 and 0.001, respectively. However, the high quality of these elaborations and the very low standard deviations seem to be quite unrealistic, considering the superimposition of the signals of the neutral and the monoanionic forms. For this reason, further evaluations were needed to define more reliable results. In order to verify the stability of the system, pK_{a1} was fixed at different values and the effect of this constraint on the outcome was evaluated. Ten elaborations with fixed and free pK_{a2} were tested and the range of pK_{a1} giving minimum standard deviation was found (4.3 - 4.5). Working in this range, the mean values of the protonation constants, and the corresponding standard deviations, were evaluated: pK_{a1} = 4.4 ± 0.1 and pK_{a2} = 7.09 ± 0.01.

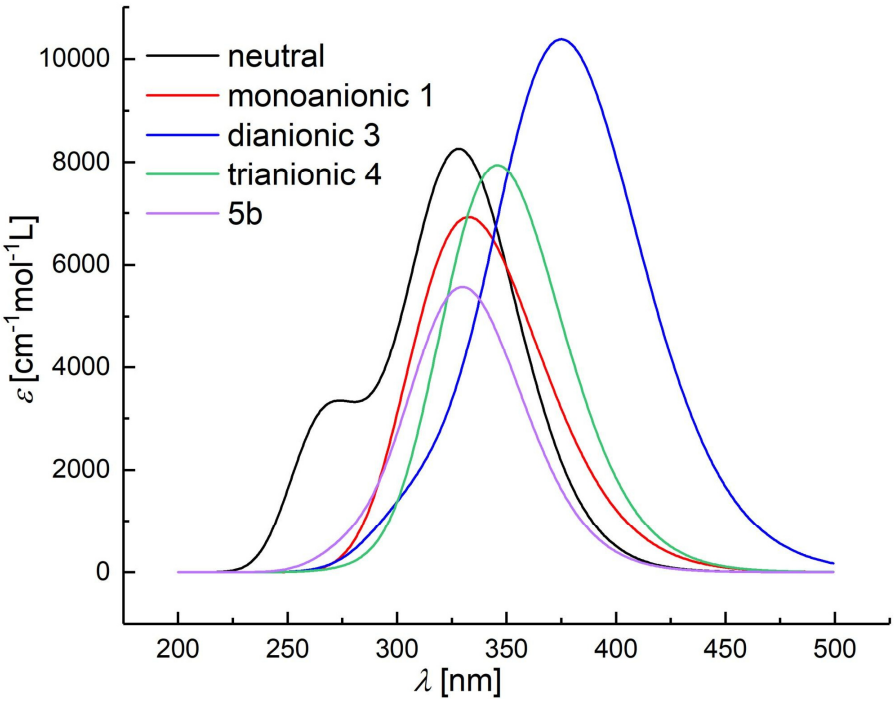


Figure S2. TD-DFT UV spectra of OTA.

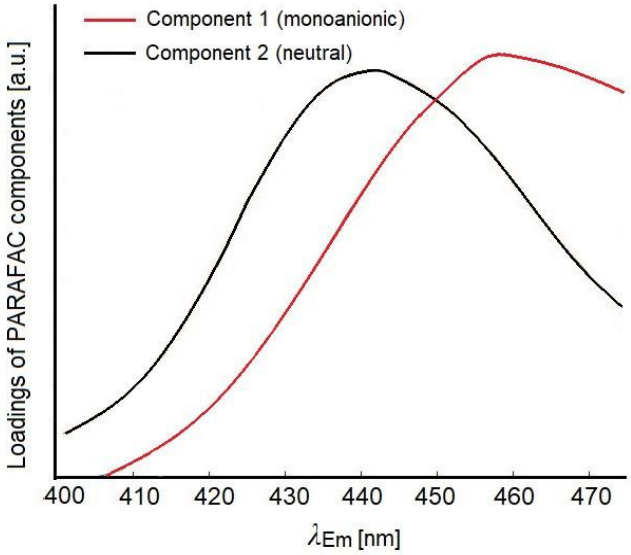


Figure S3. Loadings profiles of the two modeled PARAFAC components for the emission mode.

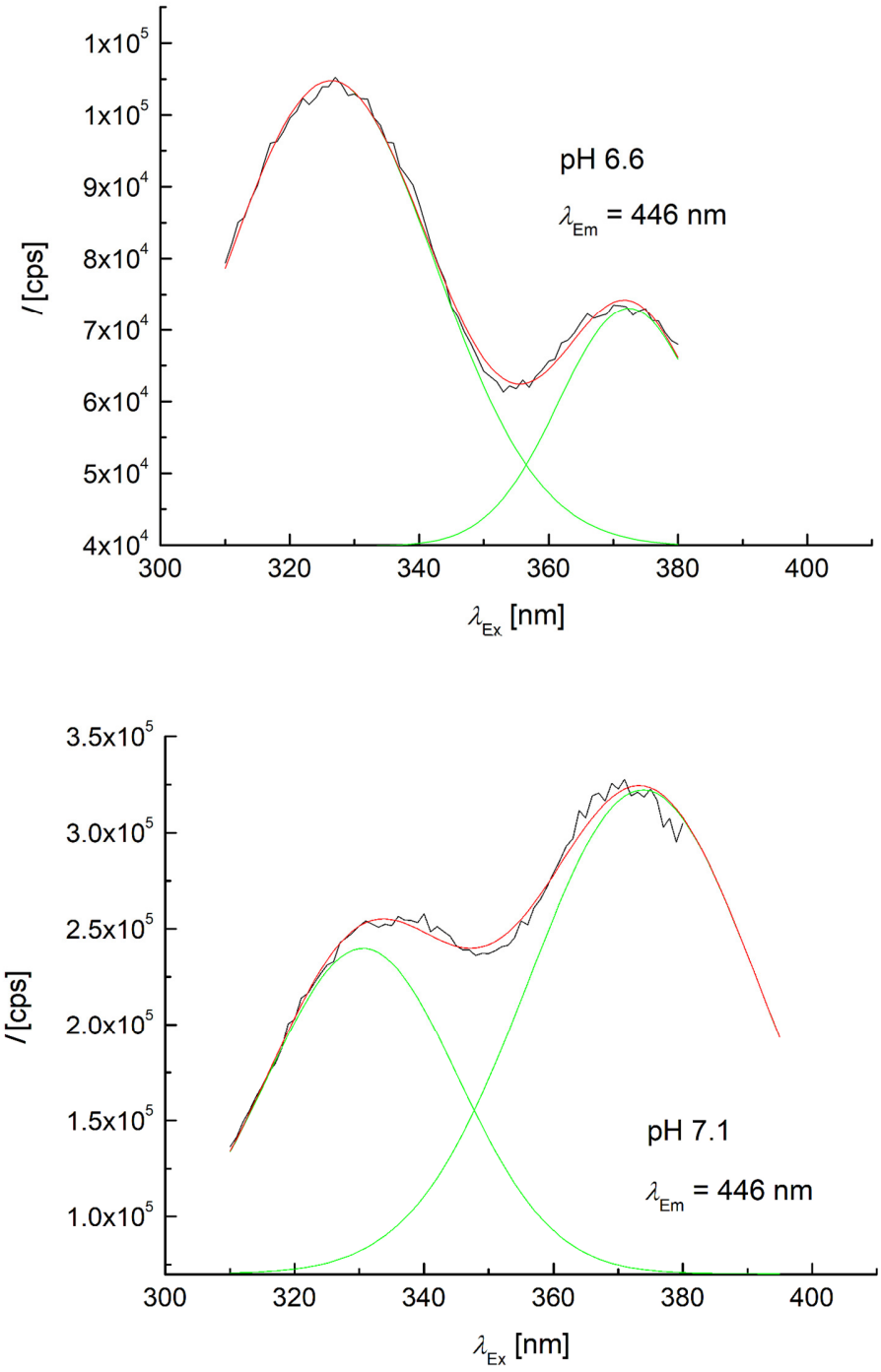
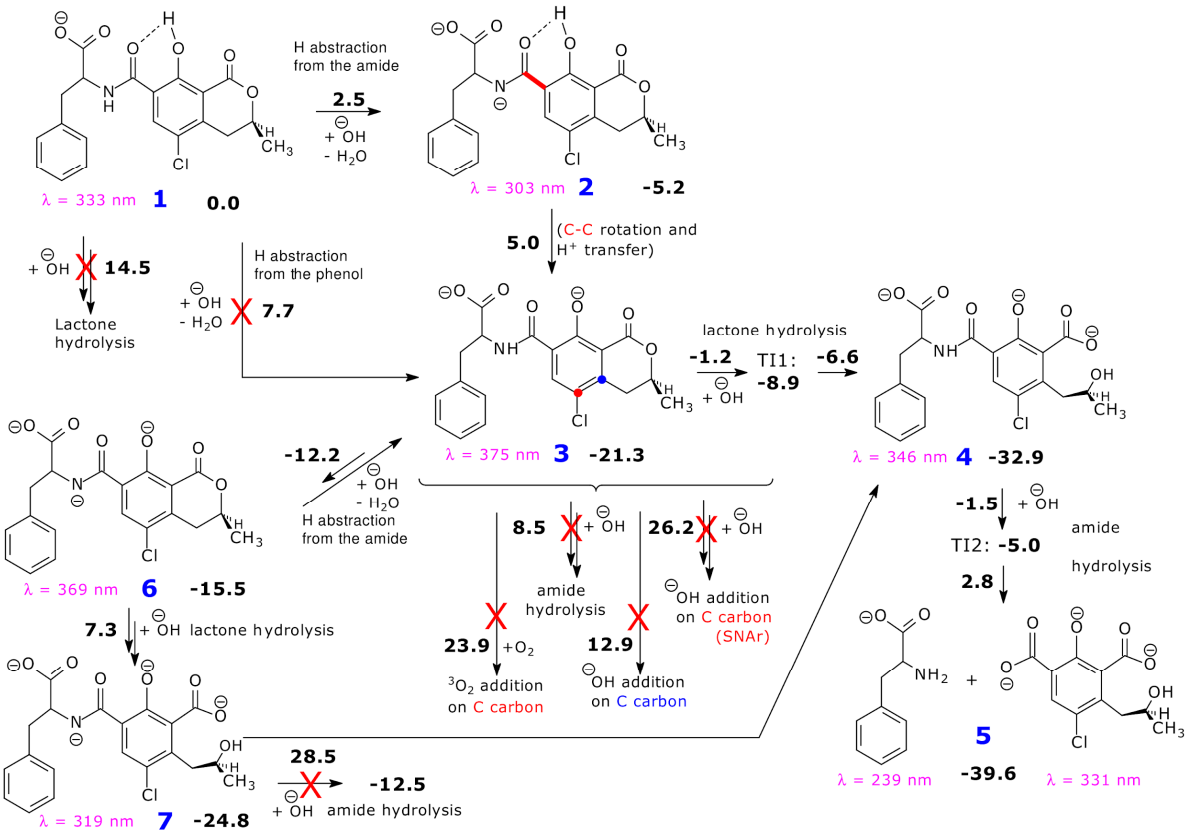


Figure S4. Deconvolutions of the excitation spectra extrapolated from the EEMs reported in Figure 3 c and d, at λ_{Em} of 446 nm.



Scheme S1. The explored reaction pathways that connect the OTA monoanion **1** to the degradation products **5**.

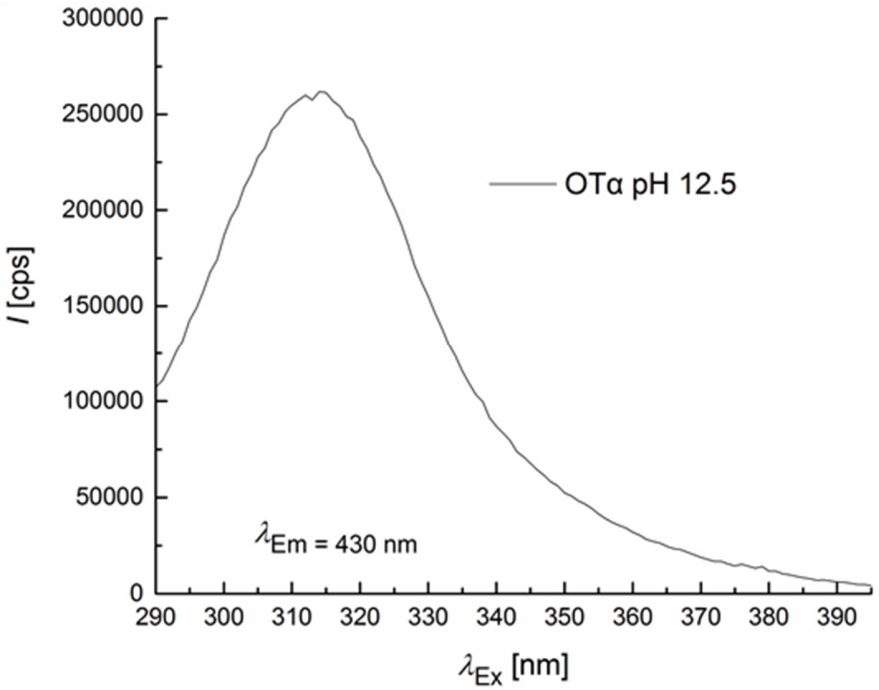


Figure S5. Fluorescence excitation spectra of OTα 1.24·10^{-7} mol L^{-1} at pH 12.5 with λ_{Em} fixed at 430 nm.

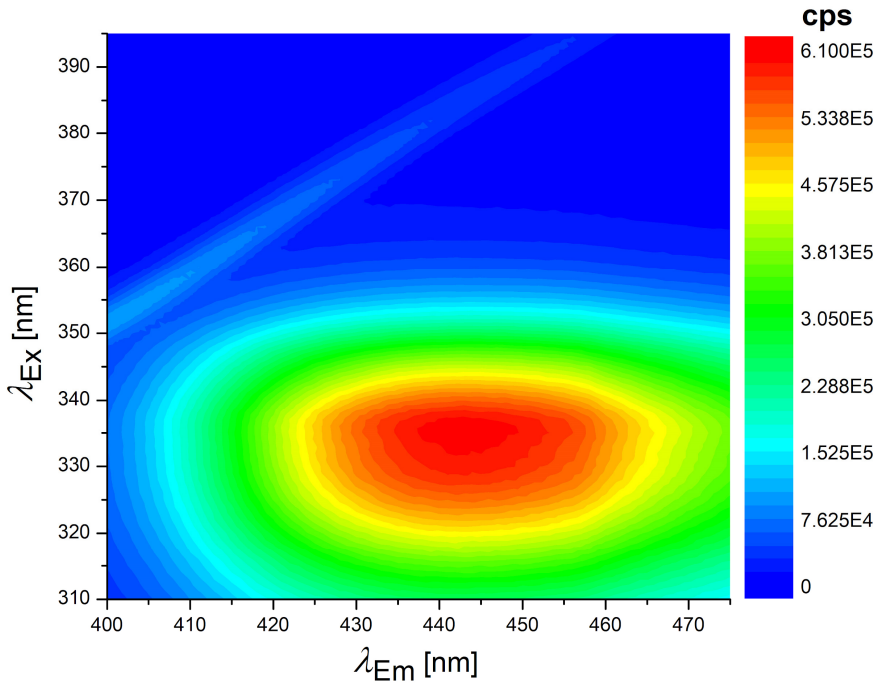
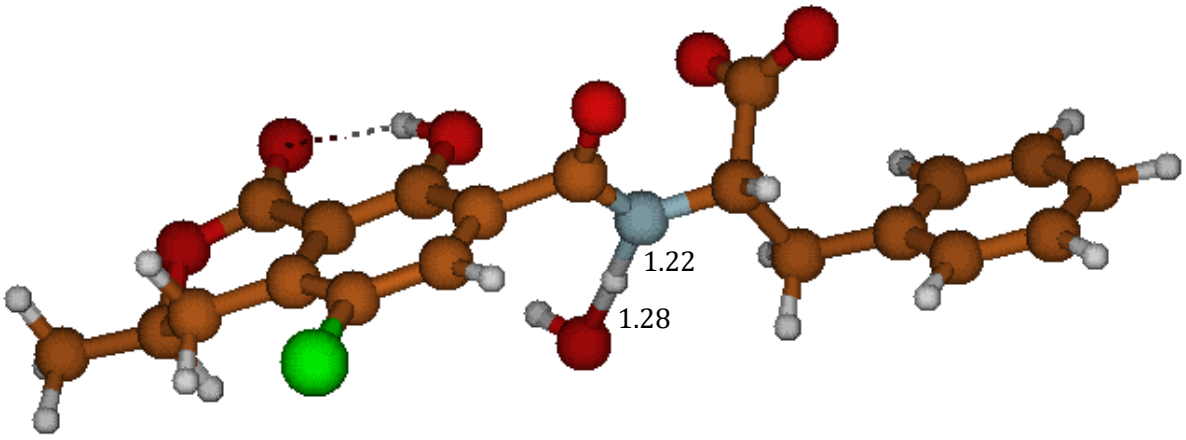
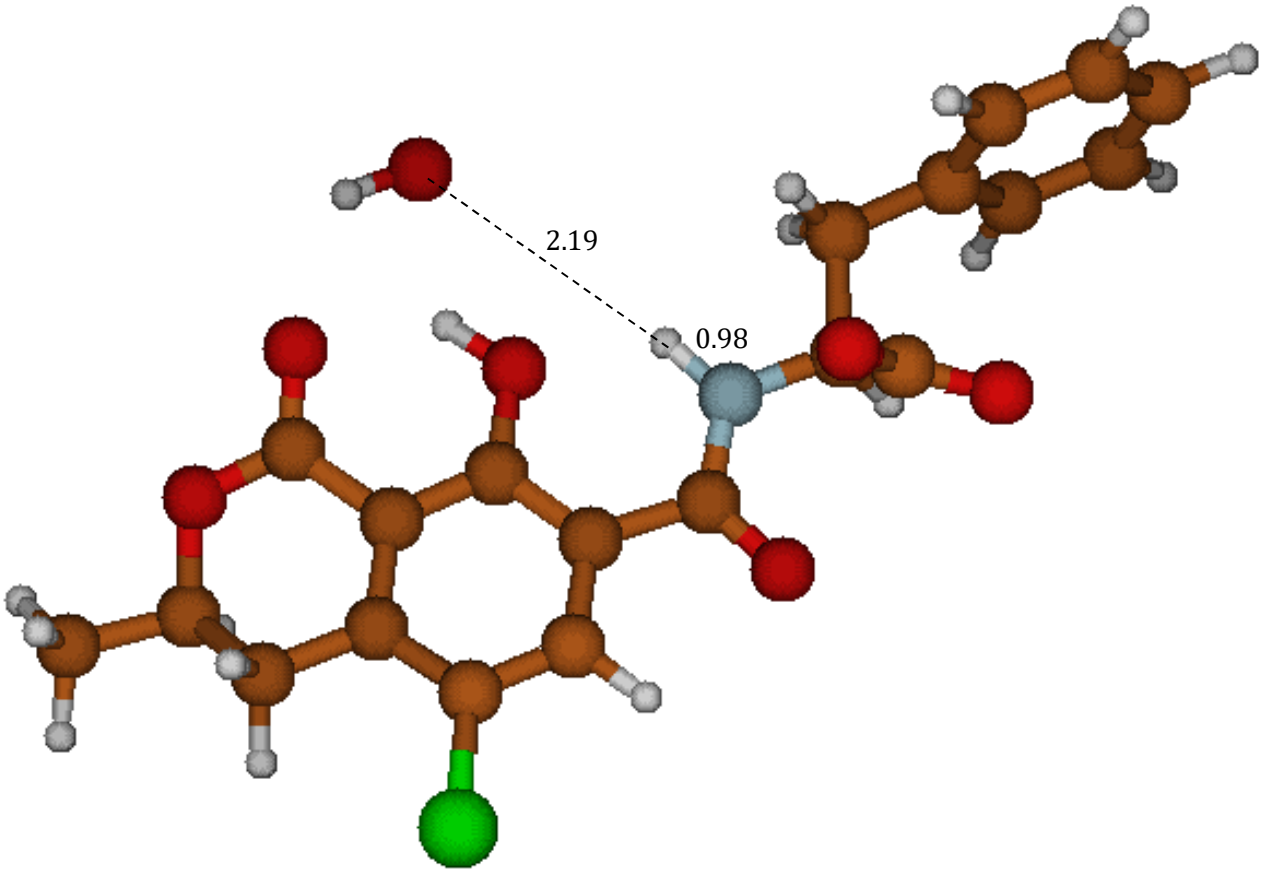


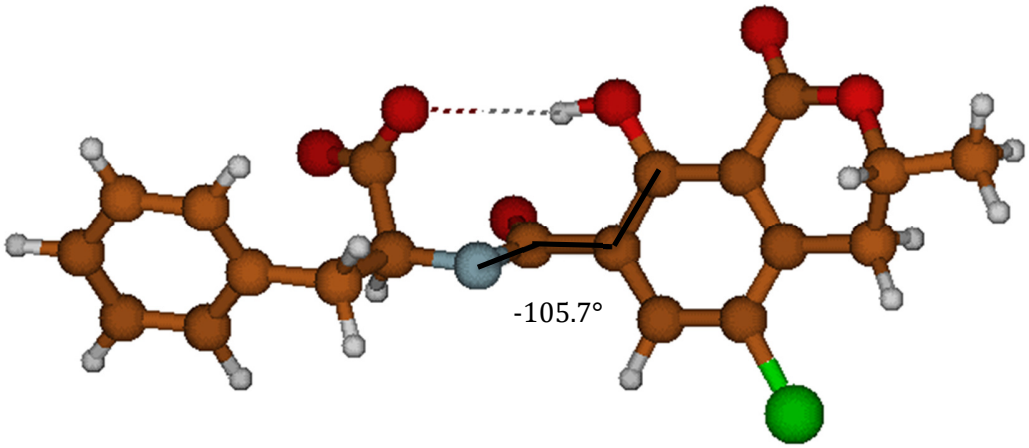
Figure S6. EEM of 1.24·10^{-7} mol L^{-1} OTα solution at pH 1.0.



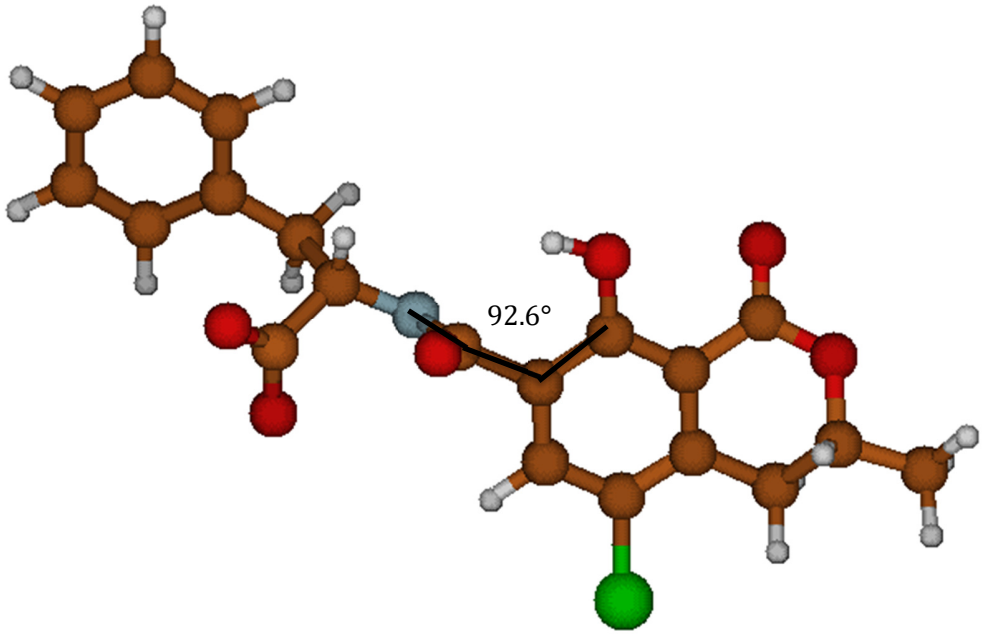
TS 1-2



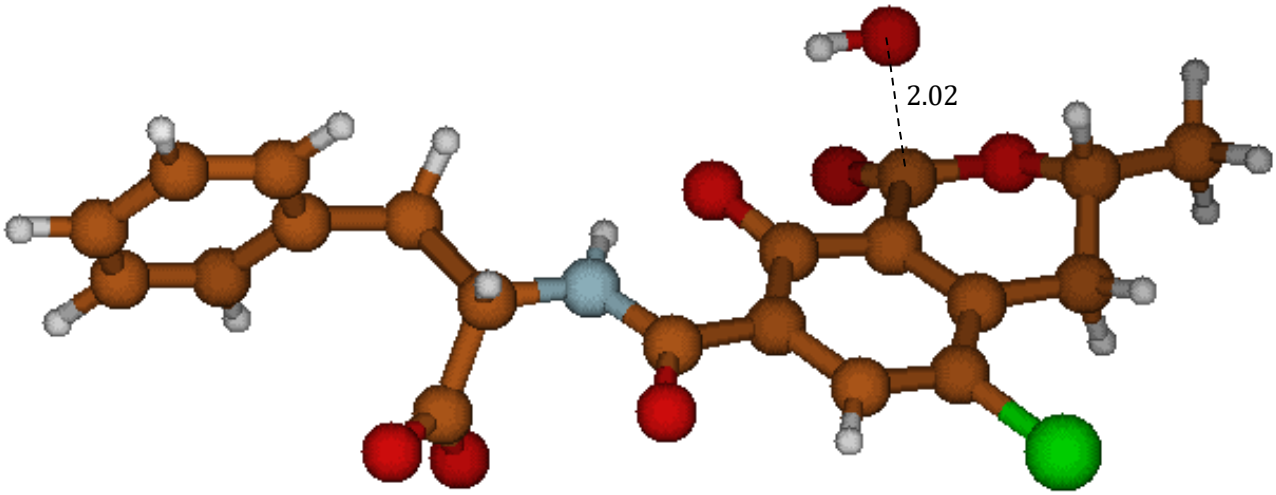
TS 1-3



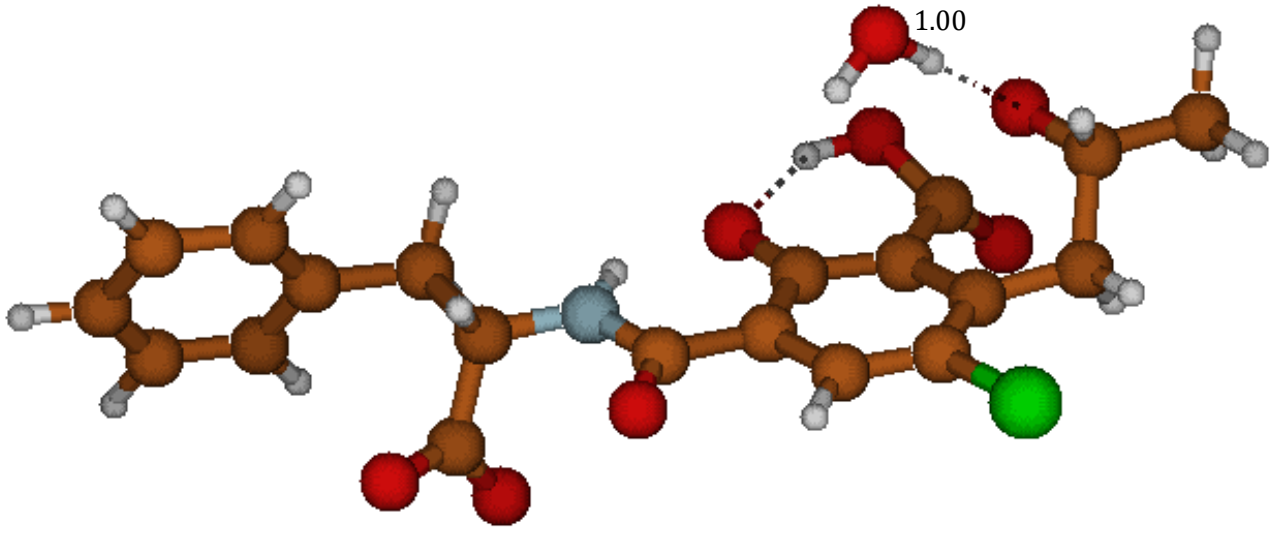
TS 2-3 A



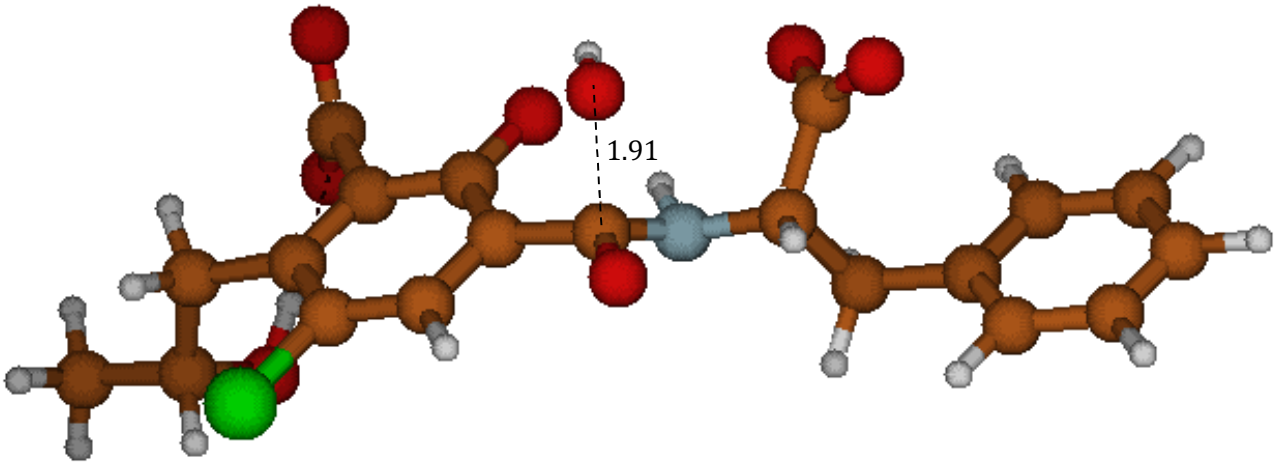
TS 2-3 B



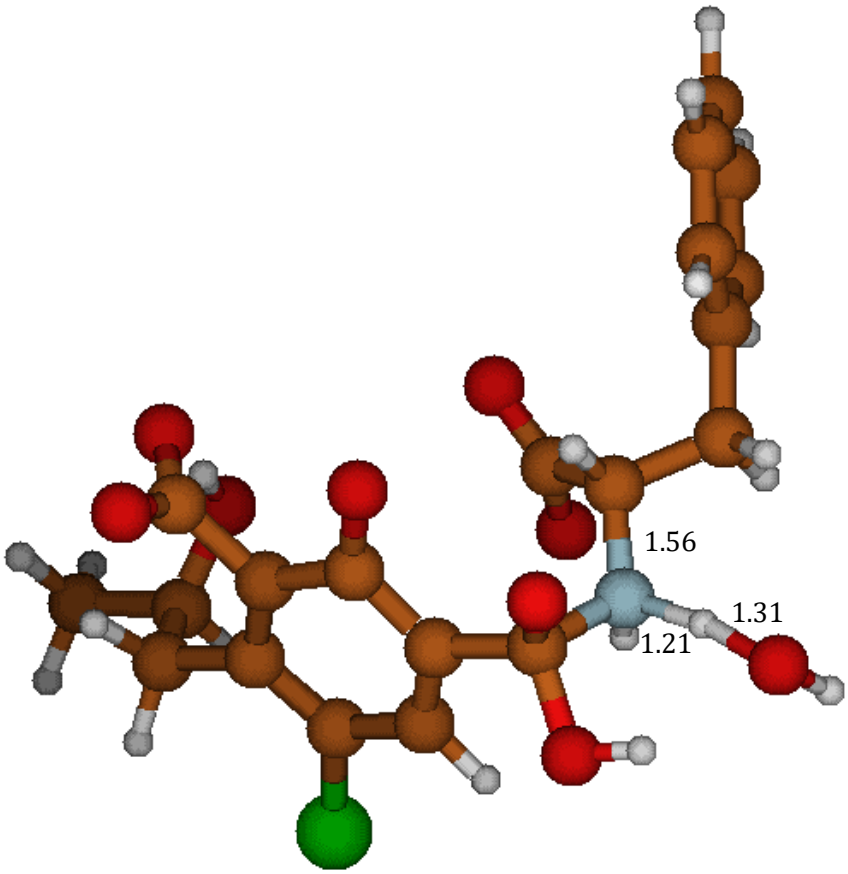
TS 3-TI1



TS TI1-4

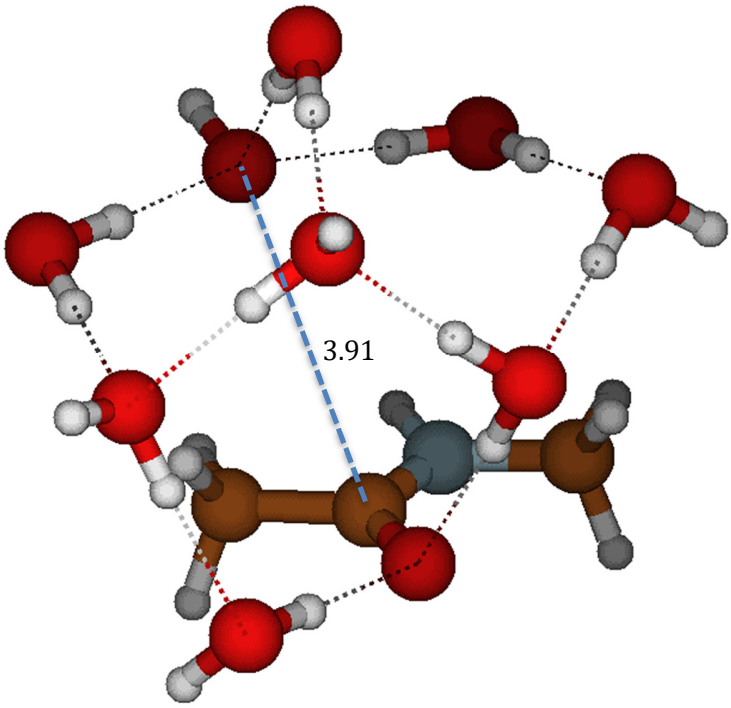


TS 4-TI5

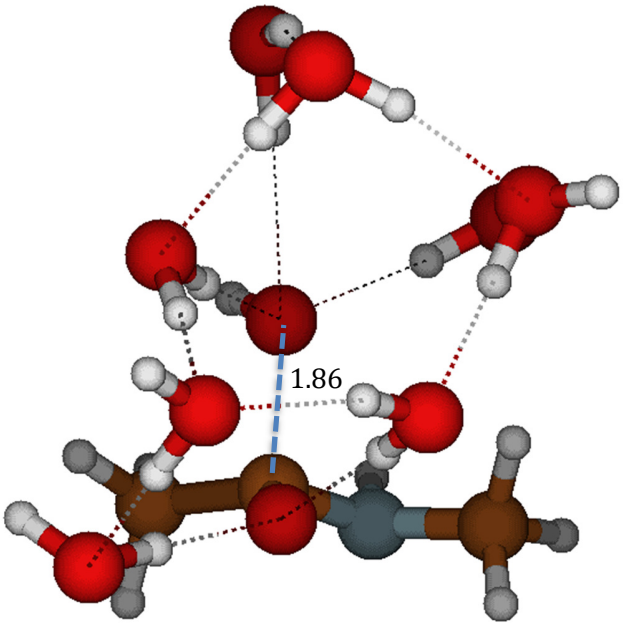


TS TI-5

Figure S7. Transition structures with relevant geometric parameters



N-Methylacetamide + HO^-



Transition structure of HO^- addition on N-Methylacetamide.

Figure S8. N-Methylacetamide + HO^- reaction with 8 explicit water molecules.

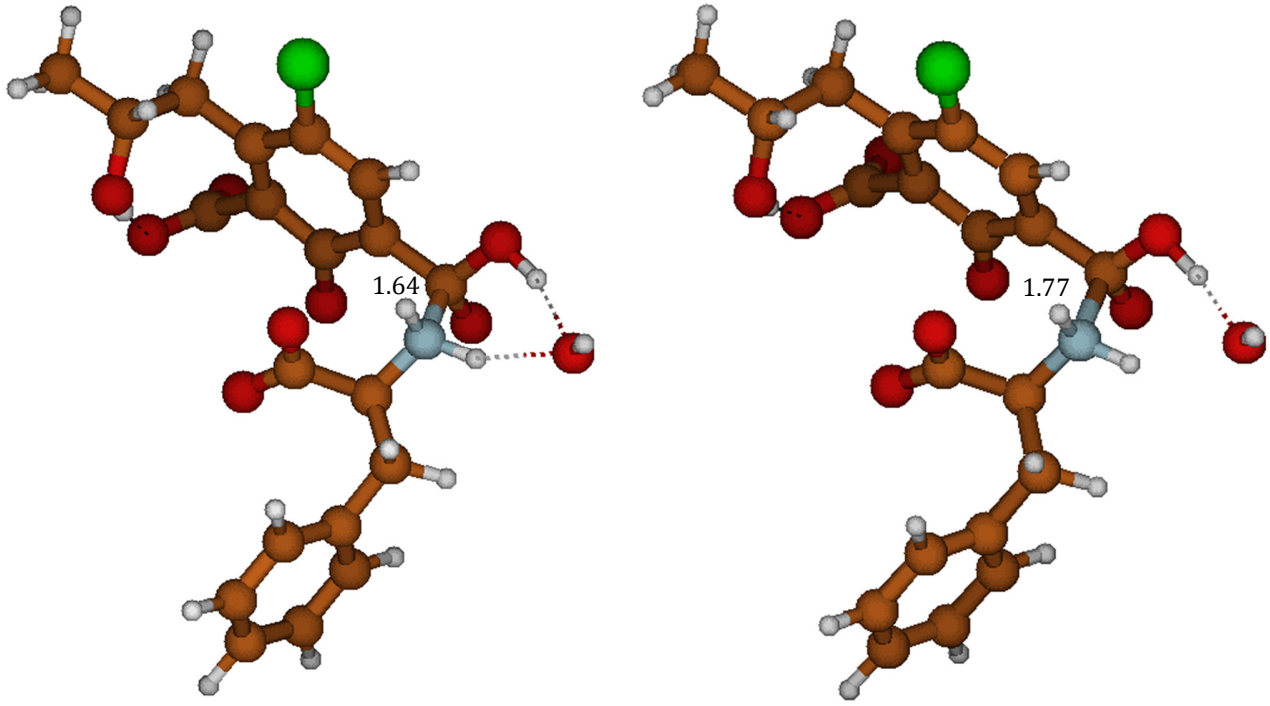


Figure S9. Left: intermediate from TS TI2-5. Right: transition structure for C-N dissociation, leading to **5a + 5b** (see Scheme 1 and note 1).

Geometries and energetics

Neutral OTA

Atom	X	Y	Z (Angstrom)
6	5.290327	0.127966	-0.210037
6	3.812819	0.378056	-0.139324
6	2.979740	-0.702796	0.179067
6	3.565392	-2.031277	0.461741
8	4.854771	-2.228442	0.219148
6	5.565915	-1.300807	-0.635069
6	1.583488	-0.538891	0.298025
6	1.015546	0.721380	0.046863
6	1.857591	1.780638	-0.267319
6	3.230406	1.619552	-0.348135
6	-0.448869	1.048164	0.091606
8	-0.828877	2.191965	-0.167827
17	4.217502	3.014019	-0.716138
8	0.800308	-1.563677	0.646085
8	2.910722	-2.945095	0.931490
6	7.025538	-1.686397	-0.565173
7	-1.318971	0.072642	0.404466
6	-2.761894	0.273319	0.307427
6	-3.269950	1.046529	1.545709
8	-2.880838	2.317027	1.608700
6	-3.469372	-1.071832	0.135727
6	-4.868243	-0.916637	-0.413817
6	-5.059668	-0.760414	-1.787090
6	-6.333537	-0.591902	-2.314088
6	-7.437665	-0.580165	-1.469000
6	-7.257066	-0.736329	-0.100201
6	-5.980582	-0.901916	0.425288
8	-3.953990	0.548125	2.395154
1	-5.837586	-1.001162	1.494993
1	-8.112781	-0.725342	0.565710
1	-8.433573	-0.449622	-1.877302
1	-6.465191	-0.472604	-3.383749
1	-4.201265	-0.775539	-2.453306
1	-2.876123	-1.673538	-0.559756
1	-0.961283	-0.839262	0.654199
1	1.402205	2.747477	-0.443597
1	-2.944031	0.896911	-0.574023
1	-3.492191	-1.589350	1.097607
1	5.182073	-1.455285	-1.650294
1	5.761266	0.809085	-0.920612
1	5.743034	0.322357	0.770038
1	7.608214	-1.053133	-1.238037
1	7.406172	-1.560943	0.451062
1	7.160187	-2.727360	-0.861650
1	1.386734	-2.328310	0.868249
1	-2.246854	2.512121	0.888343

SCF Energy -1739.292094 (Hartree)
zpe 0.358831 (Hartree)
Thermal correction to Enthalpy 0.383886 (Hartree)
Thermal correction to Gibbs Free Energy 0.302873 (Hartree)
Enthalpy -1738.908208 (Hartree)

Free Energy -1738.989221 (Hartree)

1

Atom	X	Y	Z (Angstrom)
6	-5.559377	-0.382644	-1.616957
6	-4.953189	-0.846398	-0.448054
6	-5.756691	-1.133750	0.655136
6	-7.136457	-0.960287	0.594121
6	-7.730544	-0.496251	-0.574632
6	-6.936908	-0.208044	-1.682041
6	-3.455748	-0.994783	-0.374465
6	-2.733988	0.344037	-0.146843
6	-3.199318	0.990102	1.181320
8	-2.694592	0.560342	2.247158
7	-1.305401	0.091428	-0.167366
6	-0.416700	1.090914	-0.120198
8	-0.774232	2.276087	-0.120985
6	1.047574	0.749432	-0.090517
6	1.925675	1.821672	-0.190528
6	3.297075	1.644642	-0.157127
6	3.857330	0.381760	-0.040296
6	2.987732	-0.712957	0.067891
6	1.587405	-0.539992	0.059889
6	3.544823	-2.063780	0.264774
8	4.845894	-2.256572	0.127088
6	5.657156	-1.242894	-0.544301
6	5.332742	0.126771	0.008047
8	2.851581	-3.025493	0.581830
6	7.096214	-1.648565	-0.350744
17	4.320877	3.064462	-0.250352
8	0.763348	-1.587040	0.198108
8	-4.087951	1.874277	1.093784
1	-5.296070	-1.492749	1.570375
1	-7.746768	-1.188921	1.461167
1	-8.805206	-0.359778	-0.624636
1	-7.392555	0.152585	-2.597875
1	-4.944463	-0.155705	-2.482761
1	-3.080387	-1.421481	-1.309003
1	-0.972626	-0.859159	-0.082288
1	1.510546	2.816407	-0.292082
1	-2.983434	1.031453	-0.957778
1	-3.186324	-1.680374	0.434777
1	5.381842	-1.292500	-1.601340
1	5.874031	0.867877	-0.581013
1	5.681497	0.211054	1.044090
1	7.740611	-0.942895	-0.879333
1	7.360359	-1.638357	0.709552
1	7.272302	-2.646496	-0.756304
1	1.308331	-2.383535	0.389281

SCF Energy -1738.865285 (Hartree)
zpe 0.343585 (Hartree)
Thermal correction to Enthalpy 0.368844 (Hartree)
Thermal correction to Gibbs Free Energy 0.287167 (Hartree)
Enthalpy -1738.496441 (Hartree)
Free Energy -1738.578118 (Hartree)

TS 1-3

Atom	X	Y	Z (Angstrom)
6	5.308385	0.354740	0.080233
6	3.828744	0.577403	0.002132
6	2.980778	-0.538245	0.084879
6	3.575001	-1.863806	0.353976
8	4.883789	-2.027594	0.196495
6	5.662051	-1.001304	-0.486638
6	1.578821	-0.397527	0.003267
6	1.023077	0.885735	-0.170934
6	1.879337	1.977725	-0.227292
6	3.250287	1.829493	-0.135189
6	-0.443493	1.205548	-0.291985
8	-0.800404	2.368073	-0.529757
17	4.247925	3.270669	-0.188960
8	0.741202	-1.437423	0.064624
8	2.924482	-2.815856	0.754067
6	7.113119	-1.373368	-0.313320
7	-1.335535	0.221807	-0.135575
6	-2.763280	0.471723	-0.198725
6	-3.245896	1.435219	0.913602
8	-4.146032	2.250953	0.591729
6	-3.484944	-0.882095	-0.088619
6	-4.981124	-0.764971	-0.221349
6	-5.568377	-0.604653	-1.477885
6	-6.945328	-0.463283	-1.605948
6	-7.757450	-0.481249	-0.474820
6	-7.182544	-0.642792	0.781320
6	-5.803256	-0.783012	0.905004
8	-2.744003	1.309978	2.056932
8	0.436375	-4.346642	-0.087748
1	-5.357181	-0.904811	1.887351
1	-7.807675	-0.659672	1.667518
1	-8.831919	-0.372204	-0.573365
1	-7.386110	-0.341136	-2.589465
1	-4.938473	-0.590747	-2.362292
1	-3.095318	-1.532936	-0.876796
1	-1.001691	-0.708056	0.078049
1	1.447178	2.962606	-0.348359
1	-3.002465	0.931327	-1.160639
1	-3.229360	-1.337416	0.872893
1	5.374741	-1.049862	-1.540848
1	5.844282	1.117253	-0.485744
1	5.638025	0.424791	1.123530
1	7.734357	-0.651306	-0.847730
1	7.390596	-1.359871	0.743638
1	7.307167	-2.366377	-0.722986
1	1.178828	-2.303587	0.206400
1	1.362318	-4.471625	0.129197

SCF Energy -1814.814233 (Hartree)
zpe 0.353031 (Hartree)
Thermal correction to Enthalpy 0.381127 (Hartree)
Thermal correction to Gibbs Free Energy 0.291922 (Hartree)
Enthalpy -1814.433106 (Hartree)
Free Energy -1814.522311 (Hartree)

TS 1-2

Atom	X	Y	Z (Angstrom)
6	-5.693631	-1.069018	-0.841253
6	-4.921651	0.087789	-0.950385
6	-5.563984	1.326787	-0.898850
6	-6.942348	1.408399	-0.737381
6	-7.702682	0.246896	-0.625845
6	-7.074271	-0.992605	-0.680820
6	-3.422831	0.008584	-1.079735
6	-2.687851	0.281833	0.246123
6	-3.130236	-0.751418	1.309705
8	-2.603454	-1.892355	1.280544
7	-1.256999	0.272661	-0.005892
6	-0.446686	0.597082	0.980235
8	-0.790379	0.945908	2.135533
6	1.025092	0.572516	0.646305
6	1.725330	-0.633494	0.539359
6	3.097338	-0.612208	0.225885
6	3.782388	0.604489	0.056079
6	3.066796	1.778412	0.208022
6	1.704943	1.765639	0.492298
6	3.835606	-1.881940	0.130462
8	5.076866	-1.878464	-0.333599
6	5.581038	-0.699198	-1.034134
6	5.250424	0.548795	-0.245755
8	3.358954	-2.954876	0.485973
6	7.059366	-0.920925	-1.230213
8	1.050609	-1.776321	0.749466
17	3.863224	3.334076	0.051374
8	-4.028909	-0.389435	2.114250
8	-0.305878	-0.526876	-2.170802
1	-5.205938	-2.038363	-0.878585
1	-7.657654	-1.903262	-0.597417
1	-8.777828	0.309643	-0.498519
1	-7.425022	2.378989	-0.698324
1	-4.976110	2.235902	-0.984159
1	-3.075745	0.745460	-1.809598
1	-0.794639	-0.126126	-1.060077
1	1.167368	2.701591	0.593167
1	-2.990219	1.267230	0.615349
1	-3.131526	-0.979484	-1.446786
1	5.063045	-0.677653	-1.996914
1	5.561288	1.414549	-0.831670
1	5.819355	0.563166	0.691251
1	7.477382	-0.082834	-1.791863
1	7.570016	-0.985628	-0.266177
1	7.239485	-1.838786	-1.792921
1	0.250408	-1.278567	-1.952663
1	1.695149	-2.512884	0.722263

SCF Energy -1814.820150 (Hartree)
zpe 0.349827 (Hartree)
Thermal correction to Enthalpy 0.377547 (Hartree)
Thermal correction to Gibbs Free Energy 0.289449 (Hartree)
Enthalpy -1814.442603 (Hartree)
Free Energy -1814.530701 (Hartree)

2

Atom	X	Y	Z (Angstrom)
6	5.736322	0.357625	-1.433359
6	5.143821	0.775067	-0.238912
6	5.930741	0.818477	0.913013
6	7.274387	0.456763	0.875565
6	7.852575	0.042619	-0.319838
6	7.077907	-0.005272	-1.476138
6	3.679320	1.126856	-0.191678
6	2.746937	-0.099361	-0.143182
6	3.115422	-0.965227	1.086563
8	2.729668	-0.580746	2.222376
7	1.371030	0.370670	-0.150224
6	0.468023	-0.552773	-0.237058
8	0.679448	-1.830772	-0.320083
6	-0.978279	-0.123474	-0.243203
6	-1.321784	1.218238	-0.212645
6	-2.647980	1.618306	-0.182063
6	-3.682736	0.696264	-0.171363
6	-3.357552	-0.669570	-0.252182
6	-2.010288	-1.088889	-0.278826
6	-4.459634	-1.648030	-0.395749
8	-5.687284	-1.273722	-0.009840
6	-5.874844	-0.009870	0.683923
6	-5.129994	1.074184	-0.063159
8	-4.345547	-2.755776	-0.884992
6	-7.363303	0.220511	0.772898
17	-2.991984	3.342479	-0.152442
8	-1.702882	-2.386869	-0.313473
8	3.825201	-1.987045	0.881877
1	5.483656	1.139163	1.849125
1	7.869026	0.498894	1.781904
1	8.899716	-0.237730	-0.352406
1	7.521187	-0.325129	-2.413159
1	5.138449	0.318729	-2.339218
1	3.411385	1.707101	-1.079497
1	-0.530205	1.956172	-0.200760
1	2.950782	-0.716639	-1.026907
1	3.474545	1.751466	0.682990
1	-5.445775	-0.132041	1.683083
1	-5.245546	2.014714	0.475904
1	-5.566799	1.208350	-1.059851
1	-7.551803	1.143235	1.326241
1	-7.800477	0.316710	-0.224285
1	-7.850519	-0.603041	1.298622
1	-0.674326	-2.392018	-0.321246

SCF Energy -1738.372715 (Hartree)
zpe 0.328506 (Hartree)
Thermal correction to Enthalpy 0.353502 (Hartree)
Thermal correction to Gibbs Free Energy 0.272200 (Hartree)
Enthalpy -1738.019213 (Hartree)
Free Energy -1738.100515 (Hartree)

TS 2-3 A

Atom	X	Y	Z (Angstrom)
6	-5.643322	-0.623209	-1.415357
6	-5.021774	0.492385	-0.853004

6	-5.797879	1.375934	-0.098531
6	-7.156034	1.148848	0.091987
6	-7.764378	0.030316	-0.472523
6	-7.003310	-0.854603	-1.228767
6	-3.542009	0.720360	-1.021294
6	-2.701670	0.362607	0.220480
6	-2.966954	-1.110690	0.614554
8	-2.337230	-2.017063	0.005881
7	-1.303749	0.636706	-0.075335
6	-0.487550	0.373012	0.902437
8	-0.765551	-0.036302	2.082036
6	0.984106	0.480385	0.583710
6	1.721965	-0.703045	0.435972
6	3.100960	-0.642332	0.177296
6	3.743069	0.604859	0.039259
6	2.990123	1.753894	0.208333
6	1.627030	1.698048	0.474856
6	3.927869	-1.873278	0.125965
8	5.136359	-1.797327	-0.442897
6	5.541442	-0.589083	-1.144626
6	5.206846	0.613190	-0.290788
8	3.605463	-2.941102	0.609007
6	7.013740	-0.737292	-1.440068
8	1.109561	-1.907287	0.507355
17	3.741425	3.337859	0.093292
8	-3.838273	-1.323334	1.501267
1	-5.052974	-1.319505	-2.003332
1	-7.467565	-1.728054	-1.674083
1	-8.823827	-0.147598	-0.324054
1	-7.742568	1.845532	0.681432
1	-5.330267	2.250351	0.344367
1	-3.358294	1.774756	-1.247678
1	1.061142	2.614714	0.593374
1	-3.055628	0.973190	1.060170
1	-3.172938	0.135221	-1.869010
1	4.964455	-0.557251	-2.073695
1	5.475257	1.515502	-0.840806
1	5.804054	0.596145	0.628553
1	7.357813	0.132503	-2.003994
1	7.587633	-0.802455	-0.512130
1	7.198733	-1.631907	-2.037777
1	0.160755	-1.794188	0.659516

SCF Energy -1738.361916 (Hartree)
zpe 0.328967 (Hartree)
Thermal correction to Enthalpy 0.353645 (Hartree)
Thermal correction to Gibbs Free Energy 0.274055 (Hartree)
Enthalpy -1738.008271 (Hartree)
Free Energy -1738.087861 (Hartree)

TS 2-3 B

Atom	X	Y	Z (Angstrom)
6	5.943776	0.497260	-1.065929
6	5.005809	-0.505016	-0.815313
6	5.451986	-1.711875	-0.270858
6	6.797451	-1.912627	0.015461
6	7.723927	-0.904850	-0.240197
6	7.292573	0.301071	-0.782886

6	3.540752	-0.290032	-1.091927
6	2.706367	0.047862	0.159038
6	3.232714	1.359365	0.784078
8	2.846449	2.453496	0.293741
7	1.303706	0.094639	-0.225807
6	0.463447	0.219626	0.759501
8	0.702607	0.301879	2.012686
6	-0.996995	0.272471	0.362495
6	-1.773054	-0.891180	0.318385
6	-3.137737	-0.813518	-0.007120
6	-3.739372	0.435425	-0.255477
6	-2.939660	1.565642	-0.229231
6	-1.586599	1.489758	0.073729
6	-3.958050	-2.038209	-0.179823
8	-5.289027	-1.915235	-0.133667
6	-5.893494	-0.645612	0.239087
6	-5.214567	0.467848	-0.526828
8	-3.506312	-3.143474	-0.407447
6	-7.369944	-0.770897	-0.044295
8	-1.225742	-2.097122	0.601061
17	-3.618766	3.146204	-0.583637
8	4.060800	1.257614	1.730615
1	5.611824	1.441538	-1.487150
1	8.007352	1.091157	-0.986956
1	8.774735	-1.061125	-0.022178
1	7.125422	-2.857335	0.435904
1	4.733699	-2.501827	-0.071826
1	3.116002	-1.199599	-1.526321
1	-0.983690	2.390685	0.094424
1	2.879482	-0.738893	0.903756
1	3.412881	0.512101	-1.825477
1	-5.718969	-0.516474	1.311415
1	-5.646257	1.418299	-0.211995
1	-5.407924	0.354785	-1.599883
1	-7.874950	0.146188	0.266998
1	-7.547145	-0.923706	-1.111909
1	-7.799488	-1.606414	0.511834
1	-0.296067	-1.989642	0.834593

SCF Energy -1738.361063 (Hartree)
zpe 0.329385 (Hartree)
Thermal correction to Enthalpy 0.354098 (Hartree)
Thermal correction to Gibbs Free Energy 0.273689 (Hartree)
Enthalpy -1738.006965 (Hartree)
Free Energy -1738.087374 (Hartree)

3

Atom	X	Y	Z (Angstrom)
6	-5.524361	-0.447113	-1.625030
6	-4.912154	-0.869746	-0.443590
6	-5.713247	-1.139771	0.665997
6	-7.095405	-0.988623	0.599207
6	-7.694979	-0.564611	-0.581970
6	-6.904274	-0.294774	-1.696089
6	-3.412647	-0.990827	-0.364223
6	-2.713131	0.364171	-0.163365
6	-3.198095	1.028373	1.148388
8	-2.707247	0.617085	2.228538

7	-1.284072	0.136155	-0.176434
6	-0.400403	1.140946	-0.131235
8	-0.768025	2.331332	-0.145134
6	1.045233	0.773655	-0.078421
6	1.941658	1.825042	-0.149903
6	3.310583	1.617343	-0.123523
6	3.837190	0.340122	-0.008845
6	2.953789	-0.747036	0.119558
6	1.518294	-0.586370	0.050982
6	3.530051	-2.068334	0.419700
8	4.830943	-2.282141	0.136119
6	5.572827	-1.292664	-0.617666
6	5.313264	0.070426	-0.019509
8	2.943905	-2.993462	0.957914
6	7.023127	-1.710051	-0.579717
17	4.367894	3.023547	-0.227543
8	0.718550	-1.577261	0.083301
8	-4.089199	1.909253	1.039331
1	-5.248433	-1.466688	1.591124
1	-7.703225	-1.202822	1.471687
1	-8.771456	-0.445092	-0.636404
1	-7.364167	0.033778	-2.621859
1	-4.911803	-0.234556	-2.496147
1	-3.027651	-1.430429	-1.288745
1	-0.888854	-0.801314	-0.087827
1	1.551785	2.831971	-0.241597
1	-2.978477	1.030642	-0.987682
1	-3.132595	-1.654569	0.459426
1	5.193934	-1.322794	-1.644377
1	5.838259	0.821175	-0.611179
1	5.715279	0.114452	0.999789
1	7.616586	-1.013815	-1.176696
1	7.401604	-1.701328	0.445756
1	7.148176	-2.711393	-0.997040

SCF Energy -1738.398554 (Hartree)
zpe 0.329872 (Hartree)
Thermal correction to Enthalpy 0.355133 (Hartree)
Thermal correction to Gibbs Free Energy 0.272432 (Hartree)
Enthalpy -1738.043421 (Hartree)
Free Energy -1738.126122 (Hartree)

TS 3-8

Atom	X	Y	Z (Angstrom)
6	-5.306531	0.084971	-0.390931
6	-3.842511	0.318542	-0.154443
6	-2.983621	-0.806221	-0.073663
6	-3.545133	-2.122768	-0.392032
8	-4.886713	-2.283577	-0.340582
6	-5.711092	-1.235114	0.223406
6	-1.580719	-0.675108	0.226683
6	-1.081857	0.675622	0.357261
6	-1.929534	1.746003	0.228997
6	-3.295513	1.572971	-0.013703
6	0.387189	0.975866	0.619575
8	0.743986	2.169988	0.844682
17	-4.296016	3.021134	-0.154771
8	-0.808815	-1.678154	0.401291

8	-2.911992	-3.104340	-0.754610
6	-7.147676	-1.618345	-0.039382
7	1.238927	0.164978	-0.147336
6	2.668160	0.303001	0.067359
6	3.276949	1.512626	-0.673389
8	4.103156	2.215136	-0.029833
6	3.355680	-0.989336	-0.409288
6	4.849239	-0.973641	-0.212851
6	5.399173	-1.194076	1.051975
6	6.774450	-1.145654	1.248812
6	7.624374	-0.874979	0.179237
6	7.087911	-0.654736	-1.084890
6	5.709978	-0.703732	-1.277027
8	2.967308	1.696834	-1.879007
1	5.295392	-0.528879	-2.265113
1	7.741943	-0.444346	-1.924282
1	8.697544	-0.838144	0.331166
1	7.184571	-1.321137	2.237561
1	4.740141	-1.405359	1.888796
1	2.920664	-1.822270	0.152487
1	0.918792	-0.797984	-0.119484
1	-1.524601	2.746594	0.328893
1	2.885712	0.435965	1.132919
1	3.120591	-1.145123	-1.466244
1	-5.513045	-1.216031	1.300242
1	-5.903477	0.880804	0.056089
1	-5.524482	0.073240	-1.465839
1	-7.809127	-0.873687	0.409367
1	-7.345712	-1.658877	-1.113794
1	-7.374752	-2.591266	0.401598
8	0.469511	0.176521	2.349709
1	0.184601	-0.722241	2.154661

SCF Energy -1814.318623 (Hartree)
zpe 0.341565 (Hartree)
Thermal correction to Enthalpy 0.368215 (Hartree)
Thermal correction to Gibbs Free Energy 0.283503 (Hartree)
Enthalpy -1813.950408 (Hartree)
Free Energy -1814.035120 (Hartree)

TS 3-6

Atom	X	Y	Z (Angstrom)
6	5.750985	-0.213273	1.383897
6	4.986007	0.631086	0.579055
6	5.628124	1.352367	-0.430576
6	6.997394	1.229064	-0.634284
6	7.750767	0.381162	0.174065
6	7.123269	-0.338269	1.185382
6	3.493614	0.733825	0.758791
6	2.703777	-0.047255	-0.309803
6	3.107613	-1.540383	-0.257875
8	2.617704	-2.252350	0.655748
7	1.284779	0.172362	-0.093445
6	0.435116	-0.274769	-0.999012
8	0.749908	-0.896487	-2.048958
6	-1.014536	0.013314	-0.723753
6	-1.893123	-1.089570	-0.421052
6	-3.275572	-0.741186	-0.201661

6	-3.719678	0.605162	-0.219759
6	-2.814215	1.600649	-0.511574
6	-1.469262	1.306219	-0.763277
6	-4.273933	-1.798751	-0.027887
8	-5.484968	-1.472371	0.476988
6	-5.692719	-0.155733	1.042234
6	-5.165501	0.881288	0.077350
8	-4.132275	-2.972200	-0.341582
6	-7.170616	-0.029931	1.326314
8	-1.431271	-2.271914	-0.326496
17	-3.311209	3.291967	-0.586348
8	3.941668	-1.939036	-1.114188
8	0.469907	1.320901	1.964381
1	5.264908	-0.780910	2.171572
1	7.702717	-0.998976	1.821250
1	8.819133	0.282799	0.016026
1	7.478753	1.795550	-1.424321
1	5.044565	2.013404	-1.064506
1	3.187114	1.782061	0.701031
1	0.869122	0.746242	0.930461
1	-0.777735	2.113549	-0.980055
1	2.992669	0.327689	-1.297384
1	3.211460	0.362015	1.747840
1	-5.121279	-0.114348	1.975381
1	-5.289638	1.869731	0.521191
1	-5.754589	0.859213	-0.847589
1	-7.369082	0.938804	1.790472
1	-7.747832	-0.099198	0.400454
1	-7.500689	-0.813661	2.011369
1	-0.482962	1.383620	1.862239

SCF Energy -1814.344813 (Hartree)
zpe 0.336193 (Hartree)
Thermal correction to Enthalpy 0.363850 (Hartree)
Thermal correction to Gibbs Free Energy 0.276617 (Hartree)
Enthalpy -1813.980963 (Hartree)
Free Energy -1814.068196 (Hartree)

6

Atom	X	Y	Z (Angstrom)
6	5.224129	0.723011	-0.232996
6	3.754889	0.612549	0.058097
6	3.179331	-0.685287	0.128966
6	4.067024	-1.844161	0.029242
8	5.308869	-1.671914	-0.482616
6	5.650738	-0.420155	-1.124499
6	1.770933	-0.877998	0.366855
6	0.993397	0.323401	0.555504
6	1.574094	1.562205	0.511031
6	2.948424	1.705863	0.264741
6	-0.476219	0.184057	0.864229
8	-0.777176	-0.047402	2.088901
17	3.607972	3.343813	0.241342
8	1.196194	-2.015938	0.394420
8	3.806887	-2.980172	0.402556
6	7.135633	-0.459105	-1.398203
7	-1.292923	0.319268	-0.144935
6	-2.706098	0.190268	0.173615

6	-3.127293	-1.190404	0.728605
8	-3.973570	-1.202262	1.665657
6	-3.515973	0.478112	-1.107138
6	-5.009182	0.430091	-0.913018
6	-5.684433	1.497853	-0.316308
6	-7.055547	1.439941	-0.092257
6	-7.777771	0.308653	-0.463784
6	-7.117557	-0.759870	-1.061346
6	-5.744792	-0.696780	-1.282826
8	-2.653040	-2.226090	0.190352
1	-5.234011	-1.535970	-1.745468
1	-7.670756	-1.645489	-1.355549
1	-8.847227	0.261502	-0.289743
1	-7.562096	2.279446	0.372011
1	-5.127299	2.383024	-0.023534
1	-3.221774	1.469407	-1.464197
1	0.965705	2.448257	0.663920
1	-3.004081	0.925152	0.932352
1	-3.219215	-0.246298	-1.871634
1	5.092259	-0.379767	-2.065649
1	5.452303	1.663786	-0.735143
1	5.801138	0.698529	0.699527
1	7.433571	0.456455	-1.914474
1	7.697522	-0.530666	-0.463081
1	7.391244	-1.310308	-2.032816

SCF Energy -1737.889227 (Hartree)
zpe 0.316015 (Hartree)
Thermal correction to Enthalpy 0.341270 (Hartree)
Thermal correction to Gibbs Free Energy 0.258253 (Hartree)
Enthalpy -1737.547957 (Hartree)
Free Energy -1737.630974 (Hartree)

TS 6-7

Atom	X	Y	Z (Angstrom)
6	-6.185872	0.682039	0.864649
6	-5.217793	-0.322396	0.899215
6	-5.614390	-1.636303	0.635926
6	-6.939749	-1.938585	0.345901
6	-7.896953	-0.927383	0.315862
6	-7.515371	0.384577	0.576563
6	-3.770294	-0.008079	1.176716
6	-2.884409	0.018088	-0.085010
6	-3.419894	1.104970	-1.042779
8	-3.138939	2.309933	-0.797818
7	-1.498856	0.195991	0.321686
6	-0.627317	0.136802	-0.650025
8	-0.870062	-0.043081	-1.897338
6	0.821669	0.299874	-0.267334
6	1.653506	-0.861178	-0.200297
6	3.030834	-0.641421	0.131642
6	3.555505	0.652517	0.289482
6	2.687904	1.734802	0.218567
6	1.333612	1.562595	-0.044449
6	3.927153	-1.824352	0.382546
8	5.271947	-1.552769	0.533807
6	5.787615	-0.356922	-0.066342
6	5.035552	0.829370	0.500988

8	3.543124	-2.810445	1.040807
6	7.272398	-0.317027	0.219263
8	1.162074	-2.032373	-0.443156
17	3.282965	3.382942	0.468251
8	-4.160234	0.731983	-1.994816
8	4.035869	-2.487577	-1.497469
1	-5.894487	1.708908	1.064169
1	-8.253687	1.179069	0.556405
1	-8.932475	-1.160592	0.093457
1	-7.226910	-2.965605	0.146917
1	-4.872575	-2.429117	0.660241
1	-3.358607	-0.765651	1.849610
1	0.678463	2.426710	-0.093635
1	-3.015681	-0.939250	-0.605908
1	-3.687505	0.958264	1.683464
1	5.615454	-0.417897	-1.146173
1	5.382634	1.738698	0.005865
1	5.266492	0.934340	1.568321
1	7.712673	0.572470	-0.237786
1	7.457163	-0.279874	1.296735
1	7.769730	-1.197729	-0.193525
1	3.088433	-2.601990	-1.618874

SCF Energy -1813.820831 (Hartree)
zpe 0.327800 (Hartree)
Thermal correction to Enthalpy 0.354495 (Hartree)
Thermal correction to Gibbs Free Energy 0.269640 (Hartree)
Enthalpy -1813.466336 (Hartree)
Free Energy -1813.551191 (Hartree)

TS 3-TI1

Atom	X	Y	Z (Angstrom)
6	5.176085	0.286364	0.030403
6	3.689710	0.514766	0.026269
6	2.826630	-0.564804	0.196012
6	3.403254	-1.900128	0.591984
8	4.771585	-2.019289	0.525036
6	5.481040	-1.144060	-0.362539
6	1.396441	-0.426767	0.067361
6	0.900672	0.904750	-0.141197
6	1.783628	1.978445	-0.247136
6	3.142670	1.787722	-0.175199
6	-0.546741	1.232395	-0.259728
8	-0.941547	2.403574	-0.435641
17	4.197211	3.195846	-0.332936
8	0.616666	-1.448851	0.111487
8	2.878980	-2.605137	1.470338
6	6.948052	-1.494559	-0.260840
7	-1.411298	0.213132	-0.169638
6	-2.844779	0.403336	-0.213933
6	-3.360944	1.336895	0.908435
8	-4.281423	2.134490	0.593845
6	-3.509326	-0.979842	-0.102212
6	-5.009906	-0.928730	-0.226101
6	-5.612776	-0.838500	-1.482280
6	-6.995534	-0.759190	-1.603687
6	-7.798275	-0.769690	-0.465944
6	-7.207988	-0.860711	0.790327

6	-5.823373	-0.939601	0.907061
8	-2.867270	1.209002	2.055701
1	-5.365953	-1.007362	1.889481
1	-7.825534	-0.870738	1.681965
1	-8.877076	-0.709479	-0.559086
1	-7.447823	-0.691735	-2.587274
1	-4.990330	-0.831206	-2.372049
1	-3.096805	-1.612396	-0.893561
1	-0.986803	-0.704238	-0.012121
1	1.381442	2.972323	-0.401029
1	-3.123868	0.857955	-1.168623
1	-3.227675	-1.424721	0.856878
1	5.120171	-1.327836	-1.379754
1	5.662683	0.961598	-0.676030
1	5.595617	0.496447	1.021858
1	7.525875	-0.858448	-0.935711
1	7.312071	-1.339528	0.758795
1	7.116025	-2.536720	-0.541708
8	3.006689	-2.859914	-1.144847
1	2.053804	-2.734776	-1.104357

SCF Energy -1814.332560 (Hartree)
zpe 0.340866 (Hartree)
Thermal correction to Enthalpy 0.367735 (Hartree)
Thermal correction to Gibbs Free Energy 0.281933 (Hartree)
Enthalpy -1813.964825 (Hartree)
Free Energy -1814.050627 (Hartree)

TI1

Atom	X	Y	Z (Angstrom)
6	-5.804390	-1.180246	0.632446
6	-4.999269	-0.862084	-0.461195
6	-5.610056	-0.422419	-1.637320
6	-6.992319	-0.300232	-1.718425
6	-7.787125	-0.617955	-0.619907
6	-7.189096	-1.059599	0.555492
6	-3.497897	-0.947584	-0.369154
6	-2.835520	0.421652	-0.142683
6	-3.350689	1.054739	1.172862
8	-2.868801	0.634444	2.253629
7	-1.401381	0.234009	-0.147795
6	-0.545469	1.264999	-0.096102
8	-0.953065	2.445177	-0.098519
6	0.902975	0.936807	-0.049504
6	1.407809	-0.394371	0.061115
6	2.833738	-0.548479	0.143694
6	3.694795	0.522883	-0.026289
6	3.145713	1.812114	-0.137624
6	1.789725	2.017104	-0.129948
6	3.360315	-1.960914	0.474794
8	4.791405	-2.040479	0.338639
6	5.401704	-1.167754	-0.607187
6	5.170991	0.265928	-0.159018
8	3.030721	-2.362583	1.687818
6	6.869966	-1.527446	-0.689831
8	0.639388	-1.441349	0.070078
17	4.210881	3.215252	-0.287191
8	-4.254188	1.923946	1.066467

8	2.867780	-2.862913	-0.561598
1	-5.341043	-1.521793	1.552984
1	-7.800262	-1.311407	1.415547
1	-8.865525	-0.521835	-0.682117
1	-7.450762	0.042870	-2.639636
1	-4.994179	-0.171999	-2.495997
1	-3.092731	-1.363912	-1.296032
1	-0.975286	-0.692912	-0.075746
1	1.386564	3.019116	-0.212233
1	-3.113369	1.092588	-0.959441
1	-3.209221	-1.616204	0.447436
1	4.934221	-1.315222	-1.590433
1	5.604594	0.953630	-0.889147
1	5.687311	0.436893	0.793513
1	7.375799	-0.871691	-1.403213
1	7.350400	-1.411212	0.286207
1	6.998459	-2.560253	-1.022593
1	1.908392	-2.696814	-0.541699

SCF Energy -1814.349196 (Hartree)
zpe 0.344235 (Hartree)
Thermal correction to Enthalpy 0.370427 (Hartree)
Thermal correction to Gibbs Free Energy 0.286337 (Hartree)
Enthalpy -1813.978769 (Hartree)
Free Energy -1814.062859 (Hartree)

TS TI1-4

Atom	X	Y	Z (Angstrom)
6	-5.855024	-1.027607	0.697042
6	-5.015917	-0.891036	-0.409189
6	-5.590439	-0.664852	-1.661341
6	-6.970503	-0.575500	-1.805003
6	-7.798644	-0.711577	-0.693869
6	-7.236674	-0.938047	0.558177
6	-3.518832	-0.954753	-0.255177
6	-2.858246	0.431589	-0.159973
6	-3.415972	1.209607	1.056893
8	-2.969986	0.918113	2.193833
7	-1.426670	0.232431	-0.091708
6	-0.553580	1.248541	-0.094781
8	-0.932418	2.431898	-0.195207
6	0.891201	0.898943	0.010475
6	1.372211	-0.426419	0.228740
6	2.783915	-0.594858	0.373310
6	3.684582	0.451501	0.163628
6	3.156387	1.723607	-0.090795
6	1.798328	1.947028	-0.136767
6	3.342436	-1.949737	0.743635
8	4.538942	-2.064647	-0.836161
6	5.392398	-0.969872	-0.984792
6	5.144969	0.128748	0.088615
8	4.103251	-2.097876	1.721201
6	6.863743	-1.381808	-0.944056
8	0.574190	-1.459232	0.285667
17	4.220130	3.109564	-0.363602
8	-4.316544	2.054549	0.818523
8	2.543291	-3.010915	0.409715
1	-5.419273	-1.201623	1.676207

1	-7.874198	-1.045717	1.429067
1	-8.875133	-0.642423	-0.805428
1	-7.401575	-0.403473	-2.785373
1	-4.948075	-0.560012	-2.530529
1	-3.081055	-1.472281	-1.113394
1	-1.024193	-0.695684	0.045704
1	1.415524	2.945102	-0.311108
1	-3.101298	1.006742	-1.057321
1	-3.259670	-1.524473	0.642593
1	5.210691	-0.481738	-1.961984
1	5.729450	1.011013	-0.170965
1	5.503259	-0.234579	1.053640
1	7.526066	-0.521893	-1.093446
1	7.098870	-1.836537	0.024451
1	7.076864	-2.115625	-1.727187
1	1.644400	-2.612511	0.219092

SCF Energy -1814.331686 (Hartree)
zpe 0.341762 (Hartree)
Thermal correction to Enthalpy 0.367949 (Hartree)
Thermal correction to Gibbs Free Energy 0.283336 (Hartree)
Enthalpy -1813.963737 (Hartree)
Free Energy -1814.048350 (Hartree)

TI1 with H_2O

Atom	X	Y	Z (Angstrom)
6	-5.752972	-0.843512	-1.404682
6	-5.154165	-0.955402	-0.148079
6	-5.972621	-1.017922	0.979471
6	-7.358401	-0.968898	0.857266
6	-7.944222	-0.853808	-0.398546
6	-7.136106	-0.791925	-1.531231
6	-3.653552	-0.975694	-0.016082
6	-3.007299	0.409059	-0.197415
6	-3.566261	1.403133	0.850979
8	-3.083149	1.369745	2.009414
7	-1.573100	0.243577	-0.102363
6	-0.715840	1.255410	-0.292582
8	-1.114076	2.392496	-0.615938
6	0.731249	0.958133	-0.102918
6	1.610448	2.034029	-0.246880
6	2.966646	1.865414	-0.090987
6	3.511506	0.609311	0.202033
6	2.652005	-0.473610	0.333440
6	1.236566	-0.338759	0.217967
8	0.457352	-1.372345	0.396001
6	3.320782	-1.831566	0.628132
8	3.711386	-1.987723	1.873896
6	4.975216	0.356912	0.422415
6	5.457052	-0.929051	-0.266044
8	4.442144	-1.936128	-0.342588
17	4.007001	3.284669	-0.255150
8	2.503207	-2.900704	0.152903
6	6.718143	-1.472455	0.383547
8	-4.503926	2.150770	0.471916
8	3.223255	-1.341273	-2.793594
1	-5.518371	-1.105085	1.961719
1	-7.979648	-1.019201	1.745042

1	-9.023514	-0.814008	-0.496876
1	-7.585605	-0.703842	-2.514459
1	-5.127381	-0.796279	-2.291069
1	-3.227068	-1.644208	-0.769771
1	-1.150640	-0.644543	0.175857
1	1.204429	3.011470	-0.476565
1	-3.263686	0.798857	-1.186108
1	-3.371856	-1.365838	0.966558
1	5.678566	-0.683933	-1.310546
1	5.585270	1.184273	0.060977
1	5.147613	0.276934	1.500640
1	7.509887	-0.717586	0.352636
1	6.530660	-1.735171	1.427911
1	7.070899	-2.360903	-0.146293
1	1.580659	-2.558047	0.230138
1	2.594921	-0.669015	-2.513300
1	3.638964	-1.629756	-1.957300

SCF Energy -1890.801337 (Hartree)
zpe 0.368784 (Hartree)
Thermal correction to Enthalpy 0.398106 (Hartree)
Thermal correction to Gibbs Free Energy 0.307178 (Hartree)
Enthalpy -1890.403231 (Hartree)
Free Energy -1890.494159 (Hartree)

TS TI1-4 with H_2O

Atom	X	Y	Z (Angstrom)
6	5.975798	-1.014847	-0.899383
6	5.145671	-0.934526	0.218490
6	5.730933	-0.786509	1.477745
6	7.112215	-0.717163	1.615928
6	7.932020	-0.797253	0.492813
6	7.359687	-0.947770	-0.765481
6	3.646618	-0.973387	0.071723
6	2.987453	0.409904	0.209852
6	3.555969	1.382806	-0.852894
8	3.097245	1.312689	-2.019519
7	1.555065	0.234101	0.097447
6	0.697625	1.257357	0.210657
8	1.091924	2.406754	0.488821
6	-0.746831	0.958873	0.000046
6	-1.246910	-0.329982	-0.354460
6	-2.656007	-0.450394	-0.557082
6	-3.535936	0.605409	-0.317220
6	-2.991683	1.840695	0.053016
6	-1.633077	2.018631	0.186725
6	-5.006335	0.321396	-0.352130
6	-5.348197	-0.855470	0.599726
8	-4.454207	-1.929307	0.468727
6	-3.252543	-1.773956	-0.996366
8	-3.959492	-1.853648	-2.027497
8	-2.482169	-2.872849	-0.688815
6	-6.790939	-1.296657	0.376673
8	-0.469508	-1.373304	-0.471789
17	-4.034379	3.231904	0.372640
8	4.477579	2.150645	-0.475054
8	-2.808052	-1.734875	2.521205
1	5.532008	-1.129227	-1.883643

1	7.990072	-1.011839	-1.645874
1	9.009784	-0.743174	0.600453
1	7.551323	-0.601436	2.601017
1	5.096133	-0.724523	2.356631
1	3.218690	-1.626802	0.837582
1	1.143997	-0.660293	-0.173605
1	-1.234502	2.988146	0.458848
1	3.225092	0.825331	1.192689
1	3.380005	-1.391385	-0.903507
1	-5.268053	-0.452191	1.624177
1	-5.583971	1.193474	-0.047532
1	-5.311198	0.060616	-1.367388
1	-7.485291	-0.458085	0.495382
1	-6.908204	-1.704023	-0.632989
1	-7.068474	-2.072864	1.095555
1	-1.576326	-2.506991	-0.477939
1	-2.153644	-1.090177	2.239674
1	-3.418181	-1.827417	1.734570

SCF Energy -1890.793696 (Hartree)
zpe 0.365807 (Hartree)
Thermal correction to Enthalpy 0.395077 (Hartree)
Thermal correction to Gibbs Free Energy 0.303210 (Hartree)
Enthalpy -1890.398619 (Hartree)
Free Energy -1890.490486 (Hartree)

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Atom	X	Y	Z (Angstrom)
6	-3.586532	-0.262996	0.382090
6	-2.745823	0.838651	0.305773
6	-1.316600	0.745325	0.340649
6	-0.768963	-0.569103	0.487652
6	-1.621916	-1.673189	0.577553
6	-2.987137	-1.526576	0.523626
6	-3.332929	2.229870	0.168474
8	-3.291042	2.986878	1.165928
8	-0.595604	1.812552	0.228483
6	0.690905	-0.848223	0.555611
7	1.503298	0.217584	0.535576
6	2.948535	0.118653	0.559725
6	3.539737	1.436651	1.093448
8	4.474608	1.352247	1.929683
17	-3.984599	-2.981490	0.653605
6	-5.082497	-0.098106	0.285052
6	-5.646172	-0.373373	-1.119817
6	-7.124780	-0.020220	-1.176239
8	-3.842367	2.542193	-0.947899
8	1.131638	-2.013798	0.642859
6	3.502498	-0.185222	-0.850925
6	4.995674	-0.379656	-0.863780
6	5.553798	-1.586443	-0.435639
6	6.932415	-1.763012	-0.408960
6	7.776996	-0.731376	-0.811237
6	7.231941	0.474761	-1.238952
6	5.851071	0.647610	-1.263374
8	3.063393	2.504823	0.633805
8	-4.921466	0.318564	-2.137009
1	1.043280	1.123378	0.408718

1	3.006724	-1.091370	-1.208847
1	3.220728	0.635345	-1.516474
1	4.898263	-2.393620	-0.122287
1	5.429223	1.591115	-1.596228
1	7.349510	-2.707310	-0.075803
1	8.852574	-0.869022	-0.792399
1	7.882414	1.283198	-1.555090
1	3.236172	-0.688993	1.233972
1	-1.186527	-2.658249	0.693303
1	-5.363663	0.916298	0.581562
1	-5.582302	-0.775756	0.980978
1	-5.524013	-1.437367	-1.343588
1	-7.533141	-0.241758	-2.165425
1	-7.688254	-0.595874	-0.436042
1	-7.270037	1.045106	-0.970127
1	-4.570450	1.155281	-1.767734

SCF Energy -1814.384313 (Hartree)
zpe 0.343480 (Hartree)
Thermal correction to Enthalpy 0.370807 (Hartree)
Thermal correction to Gibbs Free Energy 0.283144 (Hartree)
Enthalpy -1814.013506 (Hartree)
Free Energy -1814.101169 (Hartree)

TS 4-TI2

Atom	X	Y	Z (Angstrom)
6	-5.778664	-1.021469	-1.220388
6	-5.003947	0.138611	-1.189363
6	-5.653135	1.370973	-1.082501
6	-7.039442	1.442756	-1.007494
6	-7.802180	0.277879	-1.038179
6	-7.167139	-0.954932	-1.145597
6	-3.499097	0.070531	-1.224513
6	-2.843182	0.223210	0.164569
6	-3.399715	-0.861272	1.109860
8	-2.944587	-2.028410	0.983745
7	-1.397723	0.163371	0.024761
6	-0.594107	0.964430	0.857745
8	-0.946536	2.163867	1.073838
6	0.881175	0.646811	0.675285
6	1.377468	-0.690056	0.576344
6	2.782681	-0.836564	0.385769
6	3.660271	0.244064	0.268155
6	3.113237	1.523000	0.381569
6	1.756678	1.717962	0.583089
6	5.126289	0.020658	-0.010633
6	5.496345	0.154907	-1.496989
8	4.637339	-0.614898	-2.339715
6	3.322345	-2.250836	0.313600
8	3.697435	-2.683721	-0.817075
8	0.605514	-1.732837	0.650758
17	4.146342	2.959373	0.276349
8	3.384423	-2.912470	1.377532
8	-4.306872	-0.523990	1.916807
6	6.951348	-0.227403	-1.722716
1	-1.048331	-0.792462	0.025129
1	-3.107407	0.869633	-1.859541
1	-3.179445	-0.882806	-1.656673

1	-5.062698	2.282101	-1.057318
1	-5.287370	-1.986444	-1.300876
1	-7.526289	2.408768	-0.926440
1	-8.883800	0.332163	-0.980446
1	-7.752799	-1.867624	-1.171533
1	-3.109379	1.199641	0.568599
1	1.361483	2.723706	0.665816
1	5.426373	-0.972669	0.335273
1	5.732076	0.739725	0.545852
1	5.350016	1.196555	-1.799736
1	7.220333	-0.104253	-2.774923
1	7.613827	0.403472	-1.122676
1	7.118408	-1.271812	-1.440016
1	4.317177	-1.397891	-1.844006
8	-0.802137	0.170094	2.586423
1	-0.605935	-0.753378	2.398079

SCF Energy -1890.300588 (Hartree)
zpe 0.354545 (Hartree)
Thermal correction to Enthalpy 0.383434 (Hartree)
Thermal correction to Gibbs Free Energy 0.293096 (Hartree)
Enthalpy -1889.917154 (Hartree)
Free Energy -1890.007492 (Hartree)

TI2

Atom	X	Y	Z (Angstrom)
6	-1.694867	1.659488	-0.766221
6	-0.889670	0.549300	-0.946646
6	-1.441345	-0.757087	-0.796013
6	-2.822035	-0.846659	-0.470454
6	-3.631274	0.277005	-0.268199
6	-3.034919	1.526564	-0.430550
6	0.609468	0.745219	-1.280651
8	0.933349	1.949234	-1.740807
8	-0.710798	-1.832856	-0.946665
6	-3.419191	-2.233000	-0.343034
8	-3.589934	-2.899985	-1.391780
6	-5.078567	0.121878	0.131068
6	-5.325606	0.270190	1.641091
6	-6.774468	-0.048760	1.979253
17	-3.983046	3.010701	-0.225283
7	1.347070	0.400196	-0.033943
6	2.796731	0.299334	-0.181768
6	3.284930	-1.022215	-0.810775
8	4.180406	-0.959081	-1.697281
6	3.456932	0.453438	1.205113
6	4.961174	0.365022	1.169642
6	5.622107	-0.822720	1.485433
6	7.008779	-0.912635	1.403913
6	7.757244	0.189316	1.003496
6	7.109589	1.381167	0.688963
6	5.724304	1.465514	0.771758
8	2.797617	-2.093648	-0.361125
8	-4.438840	-0.538222	2.416132
8	-3.726717	-2.640606	0.817015
8	0.920934	-0.242719	-2.326704
1	1.009819	-0.501800	0.295017
1	3.155963	1.422302	1.611509

1	3.055748	-0.321312	1.866577
1	5.224264	2.397161	0.523676
1	5.042538	-1.687766	1.793476
1	7.685077	2.247145	0.379461
1	8.837571	0.120482	0.937339
1	7.504101	-1.845481	1.651450
1	3.131785	1.120227	-0.817671
1	-1.261624	2.645507	-0.889104
1	-5.451831	-0.855171	-0.189753
1	-5.692702	0.869073	-0.377127
1	-5.111343	1.304551	1.928068
1	-6.962630	0.106405	3.044643
1	-7.453662	0.595134	1.412793
1	-7.001153	-1.091406	1.734221
1	-4.196436	-1.333603	1.896731
1	0.522779	-1.073824	-1.996686

SCF Energy -1890.311370 (Hartree)
zpe 0.357898 (Hartree)
Thermal correction to Enthalpy 0.386032 (Hartree)
Thermal correction to Gibbs Free Energy 0.298185 (Hartree)
Enthalpy -1889.925338 (Hartree)
Free Energy -1890.013185 (Hartree)

TI2 with H_2O

Y	Z (Angstrom)		
6	-5.319832	-0.555913	-1.710412
6	-4.868839	-1.004667	-0.465706
6	-5.814014	-1.403785	0.479712
6	-7.175608	-1.358650	0.191111
6	-7.611937	-0.909395	-1.050520
6	-6.677728	-0.507802	-2.002486
6	-3.395795	-0.999031	-0.147600
6	-2.866277	0.418223	0.140590
6	-3.622323	1.036590	1.333825
8	-3.509154	0.474829	2.455300
7	-1.419760	0.430724	0.397446
6	-0.586104	0.836778	-0.778838
8	-0.892648	0.264707	-1.945135
6	0.883673	0.584132	-0.364354
6	1.832883	1.579853	-0.531848
6	3.174313	1.356136	-0.254434
6	3.630113	0.130918	0.226518
6	2.669895	-0.866490	0.424971
6	1.289256	-0.700007	0.118272
8	0.454575	-1.689391	0.273708
6	3.090594	-2.205898	0.993557
8	3.752812	-2.986944	0.245831
6	5.091518	-0.136007	0.492637
6	5.889303	-0.504126	-0.768582
8	5.270478	-1.554733	-1.512741
17	4.302265	2.700467	-0.511018
8	-0.814543	2.271609	-0.919026
8	2.775961	-2.468118	2.179702
6	7.320706	-0.873602	-0.409917
8	-4.312772	2.069588	1.115883
1	-1.100919	-0.511025	0.625238
1	-2.828689	-1.398058	-0.992280

1	-3.193704	-1.635360	0.719699
1	-4.594995	-0.240342	-2.454989
1	-5.478901	-1.753916	1.451226
1	-7.009100	-0.156685	-2.974006
1	-8.672143	-0.871842	-1.275851
1	-7.895716	-1.675402	0.937926
1	-3.067305	1.045308	-0.729196
1	1.524030	2.552727	-0.894434
1	5.198240	-0.944237	1.222132
1	5.562302	0.745304	0.934771
1	5.903163	0.363030	-1.436788
1	7.890080	-1.116441	-1.310807
1	7.818870	-0.041279	0.096183
1	7.336399	-1.742282	0.256383
1	4.751301	-2.121031	-0.903288
1	-0.701303	2.680370	-0.052179
8	-0.694256	2.376837	2.225119
1	-0.970529	1.609444	1.653201
1	-1.517674	2.718119	2.584144

SCF Energy -1966.760484 (Hartree)
zpe 0.382904 (Hartree)
Thermal correction to Enthalpy 0.414159 (Hartree)
Thermal correction to Gibbs Free Energy 0.318319 (Hartree)
Enthalpy -1966.346325 (Hartree)
Free Energy -1966.442165 (Hartree)

TS TI2-intermediate with H_2O

Atom	X	Y	Z (Angstrom)
6	1.264982	-0.141642	1.170990
6	0.955642	1.215616	0.830182
6	1.920934	2.020709	0.230053
6	3.191204	1.543910	-0.032138
6	3.565808	0.236296	0.293704
6	2.603504	-0.570066	0.898069
6	-0.386563	1.801499	1.112782
8	-1.025245	1.549609	2.142399
17	4.352642	2.658681	-0.772137
6	4.942242	-0.299793	-0.015036
6	5.119231	-0.764171	-1.469346
6	6.493727	-1.385838	-1.664279
6	2.956507	-1.986942	1.302929
8	3.106003	-2.228170	2.525218
8	0.401382	-0.966258	1.657936
8	-0.666796	3.002317	0.458169
8	3.094749	-2.849448	0.384982
8	4.094798	-1.672583	-1.876376
7	-1.406285	0.975893	-0.693364
6	-2.683068	0.427779	-0.310660
6	-2.625388	-1.067047	0.061179
8	-3.143652	-1.435472	1.153121
6	-3.778835	0.627640	-1.398479
6	-5.151019	0.173926	-0.976581
6	-5.934184	0.972828	-0.138250
6	-7.182895	0.544056	0.297831
6	-7.672631	-0.698240	-0.097433
6	-6.902862	-1.504209	-0.930144
6	-5.653327	-1.070215	-1.363510

8	-2.079530	-1.855213	-0.760774
1	-0.857093	0.241357	-1.132344
1	-3.797564	1.696713	-1.630518
1	-3.466868	0.096307	-2.303459
1	-5.557916	1.943074	0.172797
1	-5.055536	-1.705399	-2.010481
1	-7.777046	1.180809	0.944800
1	-8.646714	-1.034360	0.241007
1	-7.276735	-2.472867	-1.244722
1	-3.037164	0.959045	0.585664
1	1.672174	3.042043	-0.027179
1	5.175284	-1.137978	0.648099
1	5.695945	0.467276	0.178808
1	5.025856	0.104280	-2.129056
1	6.633846	-1.689623	-2.704726
1	7.280041	-0.669739	-1.408041
1	6.606564	-2.267576	-1.025463
1	3.746466	-2.143922	-1.090950
1	-1.026185	2.546907	-0.372955

SCF Energy -1890.259013 (Hartree)
zpe 0.352263 (Hartree)
Thermal correction to Enthalpy 0.381267 (Hartree)
Thermal correction to Gibbs Free Energy 0.289951 (Hartree)
Enthalpy -1889.877746 (Hartree)
Free Energy -1889.969062 (Hartree)

Intermediate with H_2O

Atom	X	Y	Z (Angstrom)
6	0.969440	0.477556	1.501096
6	0.711735	1.622844	0.679030
6	1.599906	1.933391	-0.349678
6	2.732617	1.185184	-0.595483
6	3.061805	0.078330	0.193164
6	2.190412	-0.231316	1.232460
6	-0.550168	2.494304	0.801922
8	-0.261235	3.784374	0.270764
17	3.779555	1.684714	-1.935414
6	4.283499	-0.764527	-0.079178
6	4.084618	-1.817194	-1.183665
6	5.299868	-2.728875	-1.267127
6	2.506829	-1.395481	2.150868
8	2.865375	-1.138164	3.325671
8	0.184072	0.036084	2.428852
8	-1.192373	2.526972	1.928231
8	2.408109	-2.567374	1.679315
8	2.893976	-2.582031	-0.997280
7	-1.567514	1.950061	-0.363826
6	-2.177884	0.628160	-0.147685
6	-1.313691	-0.469167	-0.801966
8	-1.295203	-1.589347	-0.240552
6	-3.595704	0.630979	-0.752727
6	-4.336871	-0.661541	-0.535855
6	-4.932697	-0.932435	0.697191
6	-5.590461	-2.136843	0.918297
6	-5.661596	-3.090360	-0.093863
6	-5.074013	-2.828540	-1.327214
6	-4.416795	-1.621333	-1.544444

8	-0.735817	-0.168770	-1.877565
8	-2.767401	4.450153	-0.255970
1	-1.067287	1.923886	-1.254888
1	-4.147160	1.453640	-0.288384
1	-3.517447	0.846001	-1.822725
1	-4.878520	-0.191188	1.488790
1	-3.953036	-1.422758	-2.505933
1	-6.050131	-2.330985	1.881339
1	-6.173599	-4.030842	0.077503
1	-5.125389	-3.565357	-2.121463
1	-2.238223	0.458353	0.927756
1	1.384918	2.780355	-0.988144
1	4.593804	-1.276360	0.836095
1	5.120126	-0.128529	-0.378270
1	3.958679	-1.302759	-2.141498
1	5.173923	-3.465930	-2.064430
1	6.204646	-2.150268	-1.475936
1	5.440718	-3.260874	-0.320698
1	2.694058	-2.635387	-0.038047
1	-1.156949	4.208589	0.123568
1	-2.267736	2.725985	-0.407635
1	-2.816345	4.819863	-1.140770

SCF Energy -1966.748835 (Hartree)
zpe 0.382619 (Hartree)
Thermal correction to Enthalpy 0.413584 (Hartree)
Thermal correction to Gibbs Free Energy 0.319488 (Hartree)
Enthalpy -1966.335251 (Hartree)
Free Energy -1966.429347 (Hartree)

TS Intermediate-5 with H_2O

Atom	X	Y	Z (Angstrom)
6	-4.871051	-0.975135	0.709502
6	-4.294529	-0.733344	-0.538952
6	-4.361825	-1.729543	-1.512484
6	-4.989561	-2.942911	-1.246727
6	-5.559432	-3.174471	0.000756
6	-5.499179	-2.185470	0.979185
6	-3.586065	0.567183	-0.810381
6	-2.173892	0.640407	-0.193462
6	-1.274426	-0.466034	-0.778912
8	-0.693903	-0.213268	-1.865459
7	-1.590152	1.958259	-0.457049
6	-0.496299	2.596150	0.784111
8	-1.165066	2.632030	1.873626
6	0.726085	1.689665	0.651950
6	1.573197	1.918426	-0.432808
6	2.674348	1.128442	-0.684056
6	3.015150	0.062487	0.156433
6	2.185687	-0.163773	1.248087
6	0.993542	0.588830	1.528573
8	0.245878	0.225848	2.518448
6	2.521962	-1.275812	2.221562
8	2.344572	-2.471821	1.842989
6	4.204381	-0.825632	-0.113583
6	3.935502	-1.933468	-1.145382
8	2.744660	-2.665834	-0.856070
17	3.666345	1.514680	-2.100737

8	-0.241025	3.840386	0.188774
8	2.974474	-0.953084	3.346841
6	5.130342	-2.870697	-1.238548
8	-1.230303	-1.554466	-0.157099
8	-2.609008	4.732579	-0.247809
1	-1.104615	1.932237	-1.353834
1	-4.165538	1.396285	-0.393156
1	-3.501923	0.732054	-1.888746
1	-4.825908	-0.206479	1.475034
1	-3.911810	-1.554204	-2.484954
1	-5.944844	-2.356833	1.953093
1	-6.049638	-4.119119	0.209073
1	-5.032364	-3.707444	-2.014843
1	-2.242525	0.514588	0.888963
1	1.346217	2.730034	-1.111741
1	4.539175	-1.293019	0.816801
1	5.043448	-0.230373	-0.481556
1	3.768664	-1.469268	-2.122442
1	4.950416	-3.648050	-1.985606
1	6.032200	-2.322056	-1.526135
1	5.310991	-3.352606	-0.272254
1	2.586027	-2.657298	0.111449
1	-1.152514	4.286086	0.053751
1	-2.294764	2.706692	-0.485907
1	-2.633354	5.090643	-1.138246

SCF Energy -1966.748414 (Hartree)
zpe 0.380804 (Hartree)
Thermal correction to Enthalpy 0.411678 (Hartree)
Thermal correction to Gibbs Free Energy 0.317380 (Hartree)
Enthalpy -1966.336736 (Hartree)
Free Energy -1966.431034 (Hartree)

TS TI2-5 with H_2O

Atom	X	Y	Z (Angstrom)
6	0.971659	0.497042	1.504511
6	0.689386	1.627077	0.669925
6	1.564681	1.932715	-0.370991
6	2.707069	1.197536	-0.615572
6	3.057738	0.106239	0.183613
6	2.197854	-0.200609	1.234065
6	-0.592007	2.482396	0.786292
8	-0.242764	3.802835	0.280964
17	3.736660	1.694634	-1.970417
6	4.285919	-0.726524	-0.090546
6	4.087741	-1.790059	-1.184524
6	5.310993	-2.690563	-1.272963
6	2.533642	-1.352566	2.160516
8	2.905289	-1.081502	3.328298
8	0.199816	0.056779	2.446349
8	-1.195627	2.547202	1.945974
8	2.437405	-2.529831	1.701542
8	2.906220	-2.564744	-0.980750
7	-1.592506	2.009365	-0.311030
6	-2.164844	0.667253	-0.121249
6	-1.309951	-0.416039	-0.813711
8	-1.240127	-1.537334	-0.254839
6	-3.596224	0.647518	-0.698051

6	-4.296396	-0.671706	-0.507969
6	-4.868652	-0.992081	0.724778
6	-5.487657	-2.220666	0.923993
6	-5.542535	-3.151408	-0.110158
6	-4.977617	-2.841481	-1.343068
6	-4.360050	-1.609671	-1.538254
8	-0.790385	-0.111458	-1.918846
8	-3.070417	4.028549	-0.303945
1	-1.104654	2.003777	-1.207803
1	-4.161529	1.437888	-0.198053
1	-3.546787	0.898288	-1.762230
1	-4.826660	-0.269161	1.533983
1	-3.913849	-1.375063	-2.499967
1	-5.929777	-2.451287	1.887271
1	-6.024684	-4.110500	0.043904
1	-5.016032	-3.560386	-2.154382
1	-2.207966	0.465143	0.949422
1	1.333916	2.765724	-1.022224
1	4.608899	-1.227408	0.826465
1	5.113570	-0.084804	-0.402348
1	3.947617	-1.284410	-2.145070
1	5.184549	-3.434946	-2.063368
1	6.207646	-2.104465	-1.495693
1	5.466724	-3.213666	-0.323922
1	2.714334	-2.610730	-0.019664
1	-1.095612	4.262206	0.203573
1	-2.391821	2.912789	-0.342909
1	-3.273320	4.256275	-1.214494

SCF Energy −1966.746200 (Hartree)
zpe 0.378622 (Hartree)
Thermal correction to Enthalpy 0.409133 (Hartree)
Thermal correction to Gibbs Free Energy 0.316487 (Hartree)
Enthalpy −1966.337067 (Hartree)
Free Energy −1966.429713 (Hartree)

Phenylalanine

Atom	X	Y	Z (Angstrom)
6	2.743101	0.849346	0.785836
6	3.271755	-0.325402	0.257103
6	2.521802	-1.068790	-0.648043
6	1.251224	-0.639968	-1.021246
6	0.711928	0.536720	-0.499840
6	1.474292	1.274849	0.408709
1	4.262646	-0.657413	0.547162
1	2.926585	-1.983421	-1.067766
1	0.668336	-1.225841	-1.725331
6	-0.678457	0.980422	-0.875528
1	1.067294	2.192027	0.823965
1	3.322684	1.436881	1.489779
1	-0.690363	2.064235	-1.032799
1	-0.981401	0.507314	-1.813815
6	-1.727888	0.654558	0.198689
7	-3.032806	1.149419	-0.249210
6	-1.761645	-0.865346	0.456680
1	-1.409778	1.125545	1.136087
1	-3.713619	1.012386	0.491524
1	-2.961661	2.153832	-0.383601

8	-1.277851	-1.266787	1.549202
8	-2.234368	-1.614440	-0.436063

SCF Energy -554.332810 (Hartree)
zpe 0.177828 (Hartree)
Thermal correction to Enthalpy 0.189590 (Hartree)
Thermal correction to Gibbs Free Energy 0.139775 (Hartree)
Enthalpy -554.143220 (Hartree)
Free Energy -554.193035 (Hartree)

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Atom	X	Y	Z (Angstrom)
6	2.136341	0.237785	0.089007
6	1.450904	-1.014703	0.014714
6	0.048330	-0.950914	-0.269965
6	-0.649408	0.243389	-0.440961
6	0.079858	1.433805	-0.340869
6	1.435758	1.429636	-0.073939
6	-2.138353	0.242656	-0.686899
6	-2.971958	0.505532	0.577510
6	-4.456589	0.364564	0.277266
6	-0.684427	-2.273656	-0.381286
8	-1.481623	-2.587464	0.552355
8	-0.470592	-2.981349	-1.394554
8	-2.593191	-0.347117	1.659176
1	-2.236881	-1.185930	1.298183
1	-4.759108	1.062832	-0.508713
1	-5.049041	0.576387	1.170988
1	-4.682358	-0.652954	-0.057837
1	-2.773290	1.525601	0.921018
1	-2.447591	-0.714862	-1.115369
1	-2.399950	1.009842	-1.419560
17	-0.711706	3.000702	-0.576334
1	1.969854	2.370575	-0.001845
6	3.625687	0.334603	0.327856
8	4.031789	1.220762	1.132380
8	2.026205	-2.153607	0.229414
8	4.389975	-0.441176	-0.309246

SCF Energy -1336.006685 (Hartree)
zpe 0.176794 (Hartree)
Thermal correction to Enthalpy 0.194155 (Hartree)
Thermal correction to Gibbs Free Energy 0.131470 (Hartree)
Enthalpy -1335.812530 (Hartree)
Free Energy -1335.875215 (Hartree)

Acid catalyzed ring closure

Protonated acid

Atom	X	Y	Z (Angstrom)
6	0.735773	-0.236647	-0.391060
6	0.064418	-1.465323	-0.349658
6	-1.291579	-1.551988	-0.110240
6	-2.054557	-0.404560	0.097533
6	-1.427005	0.847552	0.044069
6	-0.048336	0.902246	-0.193240
17	0.935285	-2.956369	-0.642039
6	-3.504506	-0.473595	0.348403

8	-4.199797	0.519878	0.507248
8	-2.065176	2.009772	0.212408
6	0.556033	2.251039	-0.229146
8	0.353548	2.911660	-1.536989
6	2.220426	-0.144915	-0.606853
6	3.035928	-0.502481	0.651033
8	2.806872	0.432853	1.704334
8	-3.995133	-1.702404	0.386253
8	1.171834	2.867872	0.552013
6	4.519316	-0.489084	0.345345
1	1.907106	0.330031	2.028509
1	4.751260	-1.221787	-0.430739
1	5.091532	-0.742183	1.240577
1	4.832126	0.499184	-0.004687
1	2.746533	-1.500327	0.996441
1	2.506496	0.859271	-0.928685
1	2.507846	-0.831069	-1.406400
1	-1.773404	-2.520495	-0.085765
1	-3.016147	1.820077	0.354933
1	-4.949759	-1.661122	0.543274
1	-0.388497	2.635043	-2.108359
1	0.472425	3.881137	-1.523679

SCF Energy −1337.784907 (Hartree)
zpe 0.226780 (Hartree)
Thermal correction to Enthalpy 0.245711 (Hartree)
Thermal correction to Gibbs Free Energy 0.180095 (Hartree)
Enthalpy −1337.539196 (Hartree)
Free Energy −1337.604812 (Hartree)

TS H_2O loss

Atom	X	Y	Z (Angstrom)
6	-0.025591	0.878860	-0.111594
6	0.770517	-0.250358	-0.376368
6	0.102549	-1.473502	-0.373066
6	-1.257834	-1.565707	-0.130750
6	-2.026272	-0.436413	0.129017
6	-1.408715	0.822723	0.133461
6	2.248977	-0.134959	-0.599280
6	3.068370	-0.457931	0.667419
6	4.551255	-0.391154	0.367461
17	0.973308	-2.952726	-0.700701
6	-3.476830	-0.523126	0.383335
8	-3.965520	-1.749466	0.331456
8	-2.041103	1.965024	0.360384
6	0.579092	2.171841	-0.078141
8	1.242051	2.961260	0.390391
8	-4.163872	0.459506	0.619828
8	-0.020839	2.959543	-1.776880
8	2.794511	0.475195	1.711257
1	1.933499	0.279669	2.092303
1	4.811547	-1.112014	-0.410585
1	5.127404	-0.627412	1.264608
1	4.829165	0.609236	0.022929
1	2.812448	-1.464214	1.014351
1	2.515045	0.868438	-0.941104
1	2.546076	-0.829036	-1.387596
1	-1.737303	-2.535956	-0.143159

1	-2.991234	1.768815	0.515325
1	-4.918846	-1.724424	0.500461
1	-0.865477	2.639916	-2.121590
1	-0.123475	3.913194	-1.654465

SCF Energy -1337.777559 (Hartree)
zpe 0.224541 (Hartree)
Thermal correction to Enthalpy 0.243796 (Hartree)
Thermal correction to Gibbs Free Energy 0.176903 (Hartree)
Enthalpy -1337.533763 (Hartree)
Free Energy -1337.600656 (Hartree)

Acyl cation

Atom	X	Y	Z (Angstrom)
6	-1.325689	-1.361504	-0.028682
6	0.044187	-1.402718	-0.266603
6	0.776357	-0.248061	-0.459149
6	0.041956	0.970270	-0.371220
6	-1.358100	1.035374	-0.129555
6	-2.041059	-0.175956	0.040628
17	0.815671	-2.964119	-0.313045
6	2.254251	-0.228013	-0.681317
6	3.016461	-0.065515	0.649937
8	2.670964	1.183229	1.248669
6	0.752853	2.146059	-0.514202
8	1.266485	3.131553	-0.665197
8	-2.052305	2.160196	-0.058058
6	-3.517236	-0.296820	0.296580
8	-4.263036	0.801181	0.311953
6	4.511495	-0.192776	0.435801
8	-4.033441	-1.375352	0.481656
1	-1.578260	2.989349	-0.201221
1	2.674331	-0.830165	1.351042
1	4.866149	0.576197	-0.258150
1	5.037742	-0.080727	1.385977
1	4.751448	-1.172515	0.017210
1	2.564656	-1.154196	-1.164136
1	-1.869673	-2.288353	0.107931
1	2.535700	0.593659	-1.347406
1	-3.735412	1.604231	0.164008
1	3.244707	1.864052	0.881025

SCF Energy -1261.319396 (Hartree)
zpe 0.199779 (Hartree)
Thermal correction to Enthalpy 0.216988 (Hartree)
Thermal correction to Gibbs Free Energy 0.155314 (Hartree)
Enthalpy -1261.102408 (Hartree)
Free Energy -1261.164082 (Hartree)

TS cyclization

Atom	X	Y	Z (Angstrom)
6	0.017630	1.484853	-0.244437
6	-0.790253	0.376457	-0.412861
6	-0.136679	-0.884823	-0.334357
6	1.257291	-1.035482	-0.108194
6	2.019985	0.130615	0.050816
6	1.384176	1.359269	-0.022801
6	-2.271568	0.443994	-0.602068
6	-2.994053	-0.015831	0.675100

6	-4.491461	0.183188	0.577299
6	-0.881862	-2.049790	-0.491403
8	-1.241576	-3.085161	-0.745712
8	1.883004	-2.202421	-0.033340
6	3.502477	0.159859	0.293066
8	4.084170	1.204733	0.479305
17	-0.645755	3.096662	-0.294139
8	-2.658823	-1.390697	0.909117
8	4.184479	-0.979334	0.296237
1	1.357821	-2.997160	-0.189404
1	-2.595191	0.534931	1.529442
1	-4.898051	-0.369965	-0.275081
1	-4.978751	-0.163255	1.491045
1	-4.717502	1.242883	0.442360
1	-2.572241	1.460980	-0.845136
1	1.987862	2.250354	0.097592
1	-2.581260	-0.201673	-1.430623
1	3.610014	-1.749242	0.150295
1	-3.338996	-1.941928	0.504068

SCF Energy -1261.318964 (Hartree)
zpe 0.199182 (Hartree)
Thermal correction to Enthalpy 0.215742 (Hartree)
Thermal correction to Gibbs Free Energy 0.155718 (Hartree)
Enthalpy -1261.103222 (Hartree)
Free Energy -1261.163246 (Hartree)

Protonated lactone

Atom	X	Y	Z (Angstrom)
6	-2.251300	0.920443	-0.123063
6	-0.781672	0.627908	-0.054269
6	-0.317211	-0.703537	-0.043142
6	-1.231154	-1.822040	-0.128864
8	-2.600238	-1.451364	-0.225876
6	-3.102457	-0.170921	0.463610
6	0.167124	1.638154	-0.040720
6	1.522545	1.354934	0.002555
6	1.992934	0.050394	0.029722
6	1.063685	-1.000952	0.005007
6	3.479012	-0.131732	0.070338
8	4.234963	0.815543	0.098198
8	1.528926	-2.251314	0.022743
17	-0.320303	3.314988	-0.091319
8	-0.994516	-2.992192	-0.169736
6	-4.568055	-0.074209	0.173819
8	3.976099	-1.364706	0.074635
1	2.243030	2.163376	0.014896
1	-2.886424	-0.351556	1.516013
1	-2.485417	1.828871	0.434246
1	-2.532734	1.095734	-1.167039
1	-4.939698	0.813967	0.690011
1	-4.752262	0.034976	-0.895920
1	-5.101427	-0.942538	0.564197
1	0.814817	-2.911222	-0.038384
1	-3.186602	-2.229836	-0.142090
1	3.269292	-2.034958	0.046818

SCF Energy -1261.348148 (Hartree)
zpe 0.202016 (Hartree)

Thermal correction to Enthalpy	0.217871	(Hartree)
Thermal correction to Gibbs Free Energy	0.159735	(Hartree)
Enthalpy	-1261.130277	(Hartree)
Free Energy	-1261.188413	(Hartree)