

Supplementary material for "Nucleophilic identity substitution reactions. I. The reaction between water and protonated alcohols" by Jon K. Laerdahl and Einar Uggerud.

SUPPLEMENTARY MATERIAL, H₂O + ROH₂⁺ :

Cartesian coordinates:

H₂O:

O	-0.119316	0.000000	0.000000
H	0.477265	-0.763209	0.000000
H	0.477265	0.763209	0.000000

H₃O⁺:

O	0.011734	-0.048487	0.064009
H	0.461905	0.812945	0.256757
H	0.410264	-0.495887	-0.725217
H	-0.966043	0.070839	-0.043616

H₂O--H--OH₂⁺:

O	1.028975	-0.616657	0.142979
O	-0.987107	0.681234	-0.145049
H	1.531261	-0.377966	0.948953
H	1.021829	-1.591236	0.056477
H	-0.998126	1.200264	-0.975317
H	-1.870744	0.281884	-0.014498
H	-0.019159	-0.029560	0.000948

H₂O--HOH:

O	1.409003	-0.080272	0.122312
O	-1.492123	0.077422	-0.118988
H	1.590244	-0.368836	-0.786669
H	1.583384	0.874589	0.108335
H	-1.959741	-0.419175	0.567344
H	-0.548927	-0.063778	0.084400

A1, CH₃OH₂⁺:

C	-0.036026	-0.020800	-0.794276
O	-0.034120	-0.019699	0.723653
H	0.856361	0.494420	-1.140501
H	-0.059146	-1.073022	-1.060546
H	-0.958837	0.485290	-1.060546
H	0.726991	-0.507778	1.119013
H	-0.076252	0.883482	1.119013

A2, H₂O--CH₃OH₂⁺:

C	-0.413711	0.012141	-0.000669
O	-1.950082	-0.114211	0.000671
O	2.202169	0.026611	0.000213
H	-0.109578	-0.501686	0.902090
H	-0.110791	-0.507751	-0.900371
H	-0.169102	1.068427	-0.004469
H	-2.372409	0.277597	0.799707
H	-2.373426	0.272576	-0.800273
H	2.778502	-0.754803	-0.003865
H	2.822373	0.773594	0.004126

A3, CH₃OH₂--OH₂⁺:

C	0.817411	1.357908	0.032633
H	1.708787	1.771217	-0.430328
H	0.827484	1.455870	1.116266
H	-0.083929	1.774793	-0.406225
O	0.790266	-0.083695	-0.334998
H	-0.120080	-0.567126	-0.064035
H	1.571783	-0.569791	0.003975
O	-1.437583	-1.046793	0.217146
H	-1.957368	-1.443863	-0.505724
H	-1.672607	-1.524644	1.033091

TS(A2,A3), H₂O--CH₃OH₂⁺:

C	0.544050	-0.419849	0.234096
H	-0.322503	0.191950	0.000594

H	0.609700	-1.322645	-0.364665
H	1.477576	0.133667	0.230235
O	-0.817569	1.215421	-1.782627
H	-0.649598	2.146938	-1.999065
H	-1.388210	0.907523	-2.505366
O	0.435816	-0.941376	1.668690
H	-0.354745	-1.513271	1.807919
H	0.417503	-0.217427	2.337268

Imaginary Frequency: 88.18i cm⁻¹

TS(A3,A3'), CH3(OH2)2+:

C	-0.022673	1.343784	0.051601
H	-0.211419	1.291650	1.113706
H	-0.842384	1.531808	-0.622821
H	0.974633	1.559277	-0.293992
O	-1.204820	-0.573674	-0.214292
H	-1.028919	-1.215176	0.496903
H	-2.172100	-0.571388	-0.343420
O	1.216909	-0.554483	0.161910
H	2.163038	-0.531654	0.401156
H	1.156470	-1.101966	-0.642073

Imaginary Frequency: 577.62i cm⁻¹

TS(A2,A2'), H2O--CH3--OH2+:

C	0.000000	0.010425	0.000000
O	1.945258	-0.037044	-0.168398
O	-1.945258	-0.037044	0.168398
H	0.037452	0.541634	0.936118
H	-0.037452	0.541634	-0.936118
H	0.000000	-1.066806	0.000000
H	2.429897	-0.561190	0.498301
H	2.412579	0.818034	-0.234065
H	-2.412579	0.818034	0.234065
H	-2.429897	-0.561190	-0.498301

Imaginary Frequency: 498.89i cm⁻¹

A6, CH3+:

C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.089010
H	0.943109	0.000000	-0.544506
H	-0.943109	0.000002	-0.544506

B1, CH3CH2OH2+:

C	-0.472275	0.365934	-0.189949
C	-0.651449	-1.118561	-0.080305
O	1.004665	0.667977	0.165870
H	-0.536544	0.750224	-1.205867
H	-1.072283	0.954731	0.503515
H	-0.525565	-1.474346	0.945407
H	0.022479	-1.652066	-0.751873
H	-1.680067	-1.344487	-0.378284
H	1.263257	0.310377	1.048448
H	1.233742	1.627510	0.133220

B2, H2O--CH2(CH3)OH2+:

C	-0.360859	1.282486	-0.006613
C	-0.393493	-0.214044	-0.012753
O	-1.904298	-0.618409	-0.107819
O	2.402697	-0.320680	0.048251
H	0.011083	-0.676613	-0.907081
H	-0.017434	-0.694703	0.886483
H	-2.051244	-1.592209	-0.068336
H	-2.449726	-0.191045	0.592802
H	3.002089	-0.361267	-0.714864
H	3.001389	-0.339593	0.812706
H	-0.834105	1.702332	0.885073
H	0.695956	1.558171	0.011648
H	-0.819089	1.696989	-0.905691

B3, CH3CH3OH2--OH2+:

C	-0.850244	-0.514861	0.093855
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O	0.103453	0.646733	-0.042677
O	2.463843	-0.210484	-0.028376
C	-2.250952	0.001981	-0.088093
H	-0.668022	-0.967732	1.069410
H	-0.528152	-1.183586	-0.701993
H	1.115879	0.354917	0.015069
H	-0.095757	1.354936	0.607486
H	3.026067	-0.040670	-0.805802
H	3.057720	-0.266716	0.741385
H	-2.938754	-0.846107	-0.033022
H	-2.530861	0.702746	0.702991
H	-2.369315	0.479501	-1.061675

B4, CH2CH2:

C	0.000003	0.000006	-0.668193
C	-0.000004	-0.000007	0.668193
H	0.922647	0.034076	1.238285
H	-0.922657	-0.034095	1.238281
H	-0.922645	-0.034071	-1.238291
H	0.922659	0.034100	-1.238276

TS(B2,B2'), H2O--CH2(CH3)--OH2+:

C	0.000000	-0.217980	-0.009316
C	0.000000	1.267845	0.013656
O	-2.047913	-0.435974	-0.054159
O	2.047913	-0.435975	-0.054159
H	0.000000	-0.815094	0.887861
H	0.000000	-0.734821	-0.957564
H	2.429980	-1.324039	-0.188519
H	2.571509	-0.026688	0.660181
H	-2.571509	-0.026687	0.660181
H	-2.429981	-1.324039	-0.188519
H	0.874956	1.630093	-0.530250
H	-0.874956	1.630093	-0.530250
H	0.000000	1.667586	1.027382

Imaginary Frequency: 427.57i cm-1

TS(B3,B3'), CH3CH2(OH2)2+:

C	-0.884335	-0.342099	0.731467
C	-1.680522	-0.286436	-0.449947
O	1.470974	-1.021868	-0.139921
O	0.592620	1.595778	-0.037109
H	-0.498858	-1.286400	1.097773
H	-0.784432	0.528528	1.367469
H	1.640053	-1.499647	-0.970906
H	2.197115	-1.295552	0.447983
H	1.378857	1.093822	-0.309750
H	0.886065	2.512416	0.095271
H	-2.671352	-0.469210	0.050817
H	-1.734260	0.702451	-0.901156
H	-1.532796	-1.106478	-1.150377

Imaginary Frequency: 332.84i cm-1

TS(B2,B3), H2O--CH2(CH3)OH2+:

C	-0.185765	0.623381	-0.188655
C	-0.242757	0.629025	1.307847
H	0.793396	0.603104	1.657571
H	0.209624	1.539524	-0.622667
H	0.270537	-0.271448	-0.609238
H	-0.733221	-0.265689	1.700776
H	-0.723960	1.526549	1.698139
O	1.903395	-1.570079	-0.298766
H	2.743415	-1.497507	-0.780489
H	1.986423	-2.405321	0.189338
O	-1.659920	0.660008	-0.695920
H	-2.195330	-0.073659	-0.312743
H	-1.727554	0.610580	-1.678358

Imaginary Frequency: 45.44i cm-1

B5, CH2CH2--OH3--OH2+:

C	-1.689216	-1.310941	-0.332597
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C	-1.358789	-1.610245	0.937870
O	0.177537	1.000219	0.524851
O	2.178582	1.281160	-0.931831
H	-1.958430	-1.268948	1.776931
H	-0.514832	-2.253543	1.170108
H	1.021229	1.054121	-0.127212
H	-0.383961	1.799583	0.439016
H	2.320797	0.870536	-1.803248
H	3.049102	1.345901	-0.498758
H	-1.130791	-1.711933	-1.173880
H	-2.575273	-0.727163	-0.566546
H	-0.388759	0.167524	0.407796

TS(B3,B5), CH2CH2--H--OH2--OH2+:

C	-0.958588	-1.809543	-0.457417
C	-0.035071	-1.292910	0.449634
O	0.991575	0.397911	-0.934122
O	-0.185698	1.996202	0.968657
H	0.958086	-1.719566	0.545453
H	-0.256493	-0.401741	1.031908
H	1.833402	0.578467	-1.386449
H	0.732053	1.222307	-0.465365
H	0.329664	2.444578	1.661146
H	-0.932736	2.595260	0.797515
H	-0.766621	-2.776041	-0.914967
H	-1.991582	-1.476692	-0.400731
H	-0.390833	-1.004763	-1.098086

Imaginary Frequency: 546.80i cm-1

TSb(B3,B5), H2O--CH2CH2--H--OH2+:

C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.084164
C	1.179705	0.000000	-0.730277
H	1.120276	-0.264217	-1.784217
H	1.228611	1.205846	-0.733375
H	2.094138	-0.276854	-0.208362
O	1.593752	2.788242	-0.813702
H	2.422069	3.077886	-1.238593
H	0.874807	3.280070	-1.250068
O	-0.742408	2.304737	0.383234
H	-0.183288	2.860944	0.953700
H	-1.656319	2.498316	0.657893
H	-0.969187	-0.000866	-0.486079

Imaginary Frequency: 225.55i cm-1

TS(B2,B5), H2O--CH2CH2--H--OH2+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.359426
O	2.265430	0.000000	-1.260945
O	-2.703122	-0.000000	0.922238
H	-0.033394	0.924993	-0.564107
H	-0.033394	-0.924993	-0.564107
H	0.099924	-0.927817	1.916653
H	0.099924	0.927817	1.916653
H	2.466127	-0.000000	-2.211073
H	3.138027	-0.000000	-0.835699
H	-3.136997	0.790598	1.304606
H	-1.402744	-0.000000	0.941084
H	-3.136997	-0.790598	1.304607

Imaginary Frequency: 839.19i cm-1

B6, (CH2CH2)H+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.381978
H	1.107393	0.000000	0.690989
H	-0.011106	-0.936068	1.936533
H	-0.011105	0.936068	1.936534
H	-0.011106	-0.936068	-0.554555
H	-0.011105	0.936068	-0.554555

B7, (CH2CH2)--HOH2+:

C	0.000017	0.000001	0.000013
C	-0.000022	0.000001	1.350301
O	2.875142	-0.000001	0.739667
H	1.818337	-0.000000	0.673253
H	-0.048142	-0.926615	-0.566267
H	-0.048140	0.926616	-0.566267
H	-0.032562	-0.926032	1.918208
H	-0.032561	0.926034	1.918208
H	3.270225	-0.807090	0.333675
H	3.270226	0.807087	0.333675

TS(B1,B7), (CH2CH2)--H--OH2+:

C	-0.011989	-0.000015	-0.001421
C	-0.000488	-0.000009	1.360759
O	2.733385	-0.000001	0.743205
H	1.232869	-0.000007	0.646378
H	-0.039972	-0.930668	-0.561950
H	-0.039980	0.930632	-0.561958
H	-0.000521	-0.930043	1.922926
H	-0.000529	0.930030	1.922918
H	3.290813	-0.783532	0.578908
H	3.290806	0.783534	0.578901

Imaginary Frequency: 119.36i cm⁻¹

C1, (CH3)2CHOH2+:

C	-0.000038	-0.115174	0.401687
C	1.277797	-0.715946	-0.111850
C	-1.278271	-0.715099	-0.111845
O	0.000450	1.357037	-0.170629
H	0.000013	0.028985	1.484391
H	2.162710	-0.183919	0.248497
H	1.339375	-1.739360	0.269853
H	1.282245	-0.753117	-1.202940
H	-1.340526	-1.738472	0.269855
H	-2.162832	-0.182487	0.248506
H	-1.282749	-0.752264	-1.202936
H	-0.800039	1.871091	0.090931
H	0.801282	1.870556	0.090925

C2, H2O--(CH3)2CHOH2+:

C	0.317258	-1.274868	0.688485
C	0.389704	-0.000001	-0.099217
O	1.862305	-0.000006	-0.707985
C	0.317262	1.274871	0.688477
O	-2.528222	0.000004	-0.373305
H	0.455426	2.160587	0.061647
H	1.042528	1.279209	1.504570
H	-0.690606	1.323584	1.107552
H	-0.690611	-1.323576	1.107560
H	1.042524	-1.279204	1.504577
H	0.455419	-2.160589	0.061661
H	-0.262235	-0.000003	-0.971202
H	2.039710	0.798287	-1.257986
H	2.039707	-0.798303	-1.257981
H	-3.124937	-0.763742	-0.438273
H	-3.124933	0.763753	-0.438277

C3, (CH3)2CHOH2--OH2+:

C	-2.135848	-0.541335	0.044386
C	-0.788938	0.054117	0.364810
C	-0.561093	1.453790	-0.144853
O	0.238706	-0.812974	-0.369577
O	2.606878	-0.026178	0.117558
H	-0.538142	-0.042254	1.424573
H	-2.224782	-1.573475	0.396913
H	-2.903913	0.044007	0.556454
H	-2.328935	-0.502564	-1.029801
H	-1.254634	2.124148	0.369445
H	0.454205	1.798396	0.063106
H	-0.757264	1.507680	-1.217810
H	1.226238	-0.545028	-0.158282

H	0.103328	-1.767425	-0.179763
H	3.186955	0.208558	-0.628821
H	3.187542	-0.338258	0.834083

C4, CH3CHCH2:

C	-0.460345	-0.009027	-0.135579
C	-0.493125	-0.008501	1.202164
H	0.418959	0.009692	1.792472
H	-1.429515	-0.026170	1.749792
H	-1.400170	-0.027715	-0.686433
C	0.794679	0.014554	-0.955330
H	1.680221	0.032523	-0.314202
H	0.858798	-0.865849	-1.603617
H	0.824452	0.895364	-1.605546

TS(C2,C2'), H2O--CH(CH3)2--OH2+:

C	0.000000	-1.281854	0.623077
C	0.000000	0.000000	-0.111326
C	0.000000	1.281854	0.623077
O	2.207592	0.000000	-0.461455
O	-2.207592	0.000000	-0.461455
H	0.000000	0.000000	-1.189891
H	-2.681901	0.773993	-0.815074
H	-2.681901	-0.773992	-0.815074
H	2.681901	-0.773993	-0.815074
H	2.681901	0.773992	-0.815074
H	0.000000	-2.147833	-0.037629
H	0.878021	-1.307749	1.274942
H	-0.878022	-1.307748	1.274942
H	0.878022	1.307748	1.274942
H	0.000000	2.147833	-0.037629
H	-0.878021	1.307749	1.274942

Imaginary Frequency: 296.17i cm-1

TS(C3,C3'), (CH3)2CH(OH)2+:

C	-1.774344	0.898395	-0.520007
C	-0.983468	-0.287510	-0.331265
C	-1.094597	-1.195739	0.781961
O	1.730194	-1.181480	-0.457148
O	1.322601	1.530732	0.425128
H	-1.489343	-2.120662	0.309069
H	-0.093516	-1.495723	1.112389
H	-1.766501	-0.879397	1.577886
H	-2.679919	0.953420	0.083262
H	-1.036724	1.635883	-0.120332
H	-1.921422	1.170436	-1.567269
H	1.732619	2.233117	-0.109480
H	1.566863	1.757584	1.339408
H	-0.193535	-0.523711	-1.046078
H	2.072995	-0.319160	-0.161611
H	2.500578	-1.696684	-0.745221

Imaginary Frequency: 70.79i cm-1

TS(C2,C3), H2O--(CH3)2CHOH2+:

C	0.210439	-0.217864	0.231078
H	-0.627171	0.396692	-0.100924
C	0.311882	-1.519459	-0.510509
C	1.484407	0.561882	0.384016
H	0.537214	-1.278934	-1.553492
H	-0.630771	-2.074351	-0.506008
H	1.114381	-2.144954	-0.114405
H	1.770339	0.909979	-0.612734
H	1.354858	1.450327	1.008839
H	2.289282	-0.059395	0.781934
O	-1.467801	1.535083	-1.647798
H	-2.092744	1.244098	-2.331575
H	-1.389963	2.491601	-1.795418
O	-0.168182	-0.642564	1.715539
H	-0.272482	0.139259	2.306763
H	-1.005448	-1.161825	1.747579

Imaginary Frequency: 54.70i cm-1

C5, CH3CHCH2--OH3--OH2+:

C	0.320387	1.528548	0.900346
C	-0.171596	1.708901	-0.344238
C	-0.495597	1.558083	2.155126
H	1.395156	1.386313	1.020136
H	0.484306	1.768465	-1.208529
H	-1.224480	1.929627	-0.507933
H	-1.561062	1.674309	1.941602
H	-0.344007	0.654967	2.754305
H	-0.178946	2.403186	2.774374
H	-0.237026	-0.244837	-0.074078
O	-0.391651	-1.255345	-0.134787
H	0.113572	-1.715643	-0.945226
H	-1.353399	-1.441224	-0.181349
H	1.338316	-3.200919	-1.793501
O	0.720177	-2.481151	-2.014105
H	1.020199	-2.095477	-2.856068

TS(C3,C5), CH3CHCH2--H--OH2--OH2+:

C	-0.741584	-0.303835	-1.633755
C	-1.028629	-0.414380	-0.266161
O	1.682724	-0.247857	0.052669
O	0.662906	2.141475	1.050166
C	-1.256115	-1.669491	0.447922
H	-0.961435	0.498263	0.329061
H	2.595132	-0.578906	0.091882
H	1.687187	0.652873	0.439982
H	0.693468	2.314205	2.006865
H	0.790311	3.016439	0.644872
H	-0.916939	-1.167911	-2.270433
H	-0.841032	0.674714	-2.099329
H	0.364188	-0.345778	-1.247806
H	-2.250613	-1.585033	0.913909
H	-1.224453	-2.548491	-0.194506
H	-0.542891	-1.753075	1.274797

Imaginary Frequency: 248.55i cm-1

TSb(C3,C5), H2O--(CH3)CHCH2--H--OH2+:

C	-0.000000	-0.000000	-0.000000
H	-0.000000	-0.000000	-1.087695
C	-1.236922	-0.000000	0.670699
H	-1.211120	0.265372	1.727645
H	-1.387740	-1.157879	0.646866
H	-2.088374	0.385743	0.110344
O	-1.791832	-2.844396	0.598062
H	-2.329532	-3.329284	1.247223
H	-0.968684	-3.348894	0.476642
O	0.302034	-2.508872	-1.104102
H	-0.414475	-2.771926	-1.708054
H	1.100568	-2.909778	-1.489232
C	1.299857	-0.015530	0.662374
H	2.012873	-0.654416	0.138880
H	1.241635	-0.246411	1.726214
H	1.676019	1.018803	0.553764

Imaginary Frequency: 144.12i cm-1

C6, CH3CHCH3+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.439013
H	1.097249	0.000000	1.651608
H	-0.431620	-0.888866	1.898376
H	-0.354458	0.941090	1.870774
C	-0.266240	-1.141628	-0.834602
H	0.220633	0.946065	-0.500874
H	-1.313397	-0.926841	-1.160912
H	0.308325	-1.138914	-1.766040
H	-0.265411	-2.099979	-0.315993

C7, CH3CHCH2--HOH2+:

C	0.000000	0.000000	0.000000
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C	0.000000	0.000000	1.355974
O	2.798236	0.000000	0.382838
H	1.706254	-0.011376	0.391882
H	-0.092217	-0.926419	-0.561652
H	-0.090297	0.929885	-0.558923
H	0.000111	-0.960800	1.873219
C	-0.029447	1.223183	2.212255
H	3.171111	-0.835609	0.017962
H	3.155004	0.764036	-0.126452
H	-0.965627	1.231636	2.780493
H	0.781534	1.217681	2.946671
H	0.018528	2.139442	1.619476

TS(C1,C7), CH3CHCH2--H--OH2+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.366037
O	2.701121	0.000000	0.279284
H	1.384716	-0.013465	0.287318
H	-0.142268	-0.926812	-0.550662
H	-0.131370	0.930749	-0.548989
H	0.037887	-0.963813	1.876578
C	0.021934	1.211795	2.220847
H	3.125215	-0.808059	-0.077058
H	3.115923	0.767093	-0.167006
H	-0.887120	1.204764	2.834825
H	0.865147	1.183146	2.918000
H	0.043445	2.134347	1.638494

Imaginary Frequency: 784.06i cm-1

D1, (CH3)3COH2+:

C	0.000019	0.145794	0.000000
C	1.470808	0.482093	0.000000
C	-0.731335	0.508741	1.267179
C	-0.731335	0.508741	-1.267179
O	-0.095677	-1.462672	0.000000
H	1.567260	1.572083	0.000000
H	1.976354	0.108212	0.894872
H	1.976354	0.108212	-0.894872
H	-0.762585	1.600089	-1.334740
H	-1.757463	0.136251	-1.254327
H	-0.213215	0.141890	-2.158360
H	-1.757463	0.136251	1.254327
H	-0.762585	1.600089	1.334740
H	-0.213215	0.141890	2.158360
H	0.331515	-1.857906	0.796713
H	0.331515	-1.857906	-0.796713

D2, H2O--(CH3)3COH2+:

C	0.122587	-0.292980	1.399942
C	0.548133	0.010784	-0.011682
C	0.155242	-1.024901	-1.029648
O	2.172281	-0.081967	-0.029846
C	0.304873	1.429907	-0.449852
O	-2.870952	-0.002969	0.024058
H	-0.969666	-0.221540	1.415274
H	0.404790	-1.305057	1.704362
H	0.521958	0.433655	2.113638
H	2.481040	-0.987069	0.209486
H	0.683940	2.155513	0.276014
H	0.738929	1.624554	-1.432440
H	-0.779334	1.553554	-0.513551
H	0.420310	-2.036998	-0.708756
H	-0.933480	-0.970166	-1.118757
H	0.600906	-0.814831	-2.004052
H	-3.451916	-0.775119	0.124596
H	-3.488989	0.738704	-0.084784
H	2.575867	0.547418	0.612723

TS(D2,D2'), H2O--(CH3)3C--OH2+, Shoulder TS(s):

C	0.159898	-0.016656	0.027217
C	0.077642	-0.869689	-1.156279

H	0.530639	1.806725	-1.031436
C	0.103233	1.441106	-0.099128
C	0.031915	-0.613689	1.365475
O	2.579665	0.008011	-0.032728
O	-2.813716	0.034920	-0.073011
H	-3.381634	-0.351846	0.614162
H	-3.444937	0.385537	-0.723754
H	3.162305	-0.713446	-0.326757
H	3.152241	0.794121	-0.012023
H	-0.982347	1.639217	-0.100850
H	0.522186	1.948518	0.771629
H	0.504434	-1.859333	-0.984685
H	-1.014223	-1.003442	-1.263510
H	0.472517	-0.402824	-2.056719
H	1.037038	-0.576641	1.805886
H	-0.301150	-1.651127	1.333491
H	-0.620795	-0.005343	1.996764

Imaginary Frequency: 95.86i cm⁻¹

TS(D2,D2'), H2O--(CH3)3C--OH2+, Intermediat(es):

C	0.001681	-0.000060	1.493001
C	-0.133189	-0.000001	0.030798
C	-0.090431	-1.271198	-0.690099
C	-0.090435	1.271255	-0.689996
O	2.804503	0.000004	-0.087223
O	-2.607803	0.000000	-0.026730
H	-3.192409	0.768856	-0.140888
H	-3.192410	-0.768852	-0.140914
H	3.371728	-0.000030	0.701811
H	3.436378	0.000034	-0.825904
H	-1.032976	-0.000071	1.866089
H	0.491728	-0.903210	1.860033
H	0.491733	0.903059	1.860104
H	0.995017	1.457238	-0.771627
H	-0.520767	1.215910	-1.688266
H	-0.510818	2.091645	-0.105381
H	0.995022	-1.457169	-0.771745
H	-0.510810	-2.091638	-0.105551
H	-0.520763	-1.215774	-1.688365

TS(D2,D2'), H2O--(CH3)3C--OH2+, Central TS :

C	0.070465	-0.441830	1.391591
C	0.010502	0.011556	0.002025
C	-0.101589	-0.968184	-1.075287
C	0.047067	1.448526	-0.292114
O	2.698912	-0.042341	-0.049047
O	-2.715616	0.003965	0.024778
H	-3.368310	0.666192	0.308842
H	-3.257245	-0.699113	-0.371427
H	3.284572	-0.539932	0.546183
H	3.310803	0.454457	-0.618323
H	-0.992274	-0.579687	1.652212
H	0.551377	-1.417944	1.479699
H	0.510499	0.291686	2.065901
H	0.930553	1.881683	0.185344
H	0.022202	1.671834	-1.357559
H	-0.827363	1.897012	0.196593
H	0.948588	-1.105116	-1.386103
H	-0.479621	-1.933021	-0.735820
H	-0.658824	-0.581454	-1.928689

Imaginary Frequency: 166.28i cm⁻¹

D3, (CH3)3COH2--OH2+:

C	0.532026	-1.121141	1.058094
C	0.735887	0.018187	0.082715
C	0.447937	1.380965	0.670532
C	2.044536	-0.048820	-0.670860
O	-0.340917	-0.128273	-1.027193
O	-2.697560	-0.002363	-0.024037
H	1.279625	-1.041292	1.851978
H	-0.456555	-1.074415	1.522157

H	0.666314	-2.094040	0.575228
H	2.863474	0.092699	0.039196
H	2.102477	0.737361	-1.426609
H	2.187988	-1.024606	-1.146397
H	0.523252	2.158687	-0.092521
H	1.189518	1.586289	1.446901
H	-0.541324	1.413072	1.134242
H	-1.308857	-0.121063	-0.648697
H	-0.201168	-0.956053	-1.538845
H	-3.295693	-0.755572	0.127700
H	-3.263550	0.748885	-0.277378

TS(D2,D3), H2O--(CH3)3COH2+:

C	1.563555	-0.093915	1.302052
C	0.641316	-0.012072	0.112925
C	-0.144446	1.268627	0.008286
C	-0.144281	-1.267648	-0.154398
O	1.688655	0.002964	-1.124914
O	-3.043407	0.013746	0.013982
H	-0.721117	-1.196514	-1.079975
H	-0.870684	-1.374800	0.654449
H	0.506796	-2.143904	-0.172995
H	-0.708794	1.324029	-0.925355
H	-0.880603	1.269156	0.815833
H	0.496812	2.147667	0.122108
H	2.189956	0.798081	1.397296
H	0.941795	-0.153996	2.200031
H	2.191895	-0.985516	1.258027
H	1.213593	0.010353	-1.989100
H	2.269362	0.799539	-1.099004
H	-3.657921	0.762475	0.083519
H	-3.629932	-0.760202	0.009425

Imaginary Frequency: 22.65i cm⁻¹

TS(D3,D3'), (CH3)3C(OH2)2+:

C	0.984492	-0.369307	0.034744
C	0.517259	-0.677079	1.388420
C	2.002950	0.655375	-0.194469
C	0.493464	-1.177345	-1.071270
O	-2.329974	-0.636527	-0.028361
O	-0.859760	1.787130	-0.098411
H	0.807607	0.067499	2.127532
H	-0.570036	-0.829907	1.355145
H	0.946420	-1.652712	1.666451
H	2.014205	1.432418	0.567958
H	2.953195	0.091999	-0.113111
H	1.970174	1.065856	-1.204517
H	-0.579930	-0.908210	-1.150400
H	1.014688	-1.010366	-2.012357
H	0.462680	-2.238900	-0.801110
H	-2.320571	0.336895	-0.040702
H	-3.261177	-0.906268	-0.080186
H	-0.963994	2.408124	0.643587
H	-0.944383	2.348884	-0.888664

Imaginary Frequency: 53.51i cm⁻¹

D4, CH2C(CH3)2:

C	-0.000055	0.000771	0.119450
C	-0.000670	0.009385	1.460243
H	0.923114	0.047189	2.029976
H	-0.924978	-0.021095	2.029567
C	-1.273152	-0.051421	-0.679793
C	1.273776	0.042684	-0.679229
H	2.152896	0.079342	-0.030807
H	1.357557	-0.839601	-1.324284
H	1.292537	0.920369	-1.335628
H	-2.152867	-0.079750	-0.031762
H	-1.356342	0.822497	-1.336215
H	-1.291309	-0.937472	-1.324871

D5, (CH3)2CCH2--OH3--OH2+:

C	0.377967	1.419895	-0.521825
C	-0.072869	1.324736	0.752774
C	0.855013	1.422259	1.930538
C	-1.531772	1.153110	1.067429
O	0.622098	-1.461552	-0.279084
O	-0.282048	-2.671680	-2.293410
H	-0.313595	1.448871	-1.361039
H	1.420743	1.644546	-0.735285
H	1.900671	1.511588	1.626389
H	0.596978	2.306831	2.522153
H	0.743700	0.558062	2.593855
H	-1.886382	2.024717	1.627433
H	-1.697180	0.279460	1.706419
H	-2.139703	1.058691	0.164590
H	0.485258	-0.435012	-0.249248
H	1.578821	-1.668649	-0.220955
H	0.209719	-1.910904	-1.137296
H	-0.929398	-3.386994	-2.161892
H	-0.460067	-2.285356	-3.168664

TS(D3,D5), (CH3)2CCH2--H--OH2--OH2+:

C	-0.762230	1.162236	0.751546
C	-0.367802	1.167561	-0.575514
C	-1.360064	1.219057	-1.679205
C	1.064945	1.005821	-0.940369
O	-0.744384	-1.560050	0.562629
O	1.802250	-1.956295	1.373253
H	-1.445116	-2.048012	1.031887
H	0.132139	-1.861851	0.925543
H	2.367706	-2.558913	0.860875
H	2.094999	-2.061529	2.294372
H	-1.777510	1.461103	1.002862
H	-0.008234	1.296927	1.525344
H	-0.800993	-0.111472	0.614264
H	1.454969	2.007015	-1.170075
H	1.183754	0.397362	-1.839801
H	1.655242	0.590627	-0.121089
H	-1.060903	2.003149	-2.384558
H	-2.373993	1.413201	-1.329181
H	-1.334086	0.275104	-2.236244

Imaginary Frequency: 398.98i cm⁻¹

D6, (CH3)3C+:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.462165
H	1.067748	0.000000	1.751820
H	-0.486137	-0.866670	1.907855
H	-0.397353	0.941167	1.858842
C	-0.285655	-1.225847	-0.740892
C	0.324975	1.226888	-0.720980
H	-0.488334	-1.061509	-1.799632
H	0.649420	-1.816121	-0.664909
H	-1.056509	-1.832655	-0.258332
H	0.835077	1.034057	-1.668836
H	-0.667593	1.638810	-0.994661
H	0.837524	1.974313	-0.114318