

Supplementary Information for: Proton Transfer from Pinene Stabilizes Water Clusters

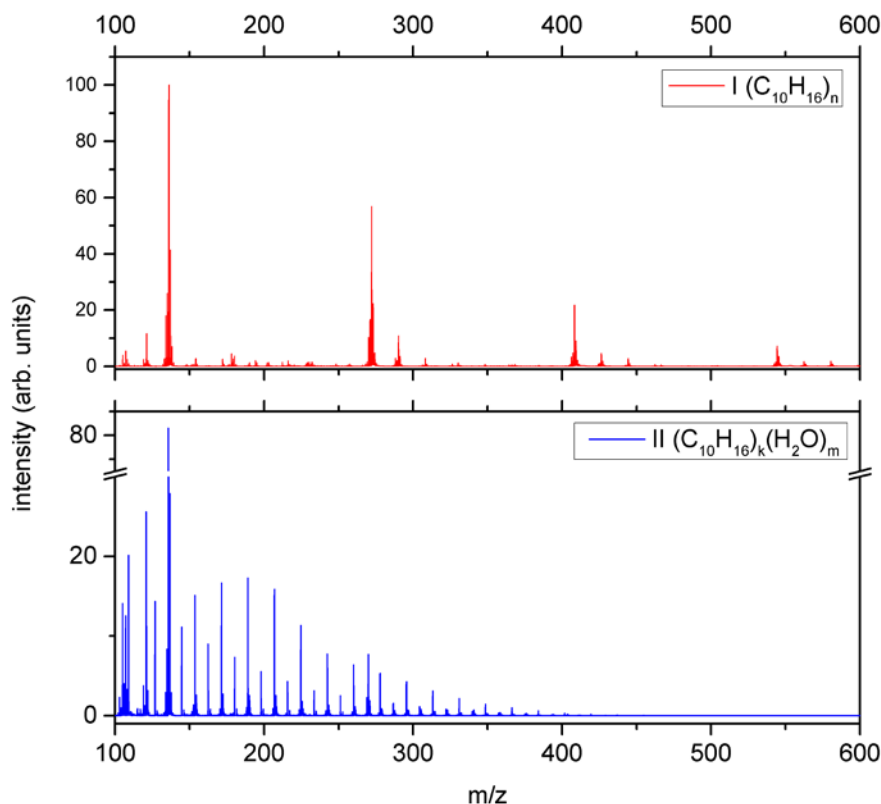
Jan Poštulka,^a Petr Slaviček,^{a,c} Alicja Domaracka,^b Andriy Pysanenko,^c Michal Fárník,^c Jaroslav Kočíšek,^c

^a Department of Physical Chemistry, University of Chemistry and Technology, Technická 5, Prague 6, Czech Republic. E-mail: petr.slavicek@vscht.cz

^b Normandie Univ, ENSICAEN, UNICAEN, CEA, CNRS, CIMAP, 14000 Caen, France

^c J. Heyrovský Institute of Physical Chemistry v.v.i., The Czech Academy of Sciences, Dolejškova 3, 18223 Prague, Czech Republic. E-mail: kocisek@jh-inst.cas.cz

1. $m/z=100$ to $m/z=600$ part of the mass spectra for pinene clusters (conditions I) and mixed pinene-water clusters (conditions II).



2. Binding energies E_b of the pinene molecule in the mixed (pinene(H_2O) $_n$) clusters with different number of water molecules n . calculated at the BMK/6-31++g** level.

n	1	2	3	4	5	6	7	8
E_b (eV)	0.2	0.35	0.3	0.32	0.39	0.39	0.34	0.3

3. Binding energies E_b of the n^{th} water molecule in the mixed (pinene(H_2O) $_n$) clusters calculated at the BMK/6-31++g level as presented in Fig. 2 of the main text and at B3LYP-D3 including dispersion correction.**

E_b (eV)			
neutral		ion	
BMK	B3LYP-D3	BMK	B3LYP-D3
0.20	0.24	0.44	0.45
0.40	0.43	0.56	0.60
0.51	0.53	0.61	0.61
0.58	0.69	0.64	0.73
0.47	0.48	0.51	0.60
0.49	0.60	0.47	0.51
0.54	0.60	0.67	0.71
0.62	0.75	0.47	0.53

4. Cartesian coordinates for neutral mixed cluster structures optimized at the BMK/6-31++g.**

Neutral pinene

E(BMK) = -390.434989 a.u.

C	0.387794	0.324622	0.185387
C	0.493695	1.043733	1.314913
C	1.554290	-0.125440	-0.658297
C	-0.760218	1.406554	2.098158
H	1.465518	1.358748	1.696684
C	-2.019920	0.903860	1.355069
H	-0.715301	0.967741	3.107922
H	-0.821089	2.497329	2.235174
C	-1.888167	1.259282	-0.157486
H	-2.940592	1.189272	1.881498
C	-1.023978	-0.041033	-0.266443
H	-2.837511	1.199002	-0.694408
H	-1.381225	2.198181	-0.405818
H	-1.033181	-0.611311	-1.204133
C	-1.865039	-0.604551	0.943932
C	-3.198401	-1.225526	0.482809
C	-1.200885	-1.579698	1.926250
H	-1.041539	-2.552362	1.439249
H	-0.233340	-1.223370	2.290259
H	-1.857605	-1.745037	2.792247
H	-3.013245	-2.188202	-0.013890
H	-3.843627	-1.414741	1.352069
H	-3.752856	-0.588745	-0.214146
H	1.469774	0.266750	-1.682629
H	2.508909	0.208473	-0.234942
H	1.571831	-1.222614	-0.736553

Neutral pinene(H₂O)₁

E(BMK) = -466.837512 a.u.

C	-0.344403	-0.656758	1.210293
C	0.014610	0.448441	2.270396
C	1.529942	0.755863	2.265757
C	2.016522	0.978843	0.840360
C	1.155306	0.846782	-0.186328
C	-0.293449	0.528070	0.168295
C	-0.708572	1.472712	1.344643
C	1.532182	0.984754	-1.640359
C	-1.776295	-1.197690	1.394041
C	0.595625	-1.858858	1.042206
H	3.073147	1.192040	0.667905
H	2.090471	-0.075945	2.721628
H	1.728797	1.644918	2.883729
H	-0.364153	0.306856	3.291282
H	-1.788281	1.499538	1.506250
H	-0.321341	2.496418	1.314176
H	-0.938188	0.464488	-0.717017
H	0.560752	-2.484811	1.945401
H	0.268485	-2.479495	0.196101
H	1.635548	-1.571809	0.865253
H	-1.819695	-1.849776	2.277594
H	-2.523463	-0.408362	1.522694
H	-2.066019	-1.797037	0.519721
H	2.598690	1.211438	-1.760254
H	1.312007	0.052381	-2.180549
H	0.945957	1.783822	-2.116799
O	1.189162	4.100119	0.052652
H	1.470628	3.184965	0.192840
H	1.985963	4.598137	-0.147261

Neutral pinene(H₂O)₂

E(BMK) = -543.247520 a.u.

C	-2.210854	0.362871	0.935573
C	-1.476253	-0.618783	1.898871
C	0.002627	-0.182878	2.020775
C	0.577356	0.122929	0.642657
C	-0.185530	-0.059112	-0.453148
C	-1.623190	-0.510277	-0.221012
C	-1.651462	-1.721503	0.793048
C	-3.039373	-2.389049	0.852472
C	-0.596845	-2.830643	0.671315
C	0.278744	0.134442	-1.874298
O	-0.362916	3.117269	-0.035346
H	1.625642	0.417303	0.559478
H	0.594476	-0.979422	2.499030
H	0.076742	0.698846	2.675762
H	-1.919908	-0.817663	2.883272
H	-3.298514	0.290412	1.011884
H	-1.909847	1.415257	0.968802

H	-2.184972	-0.600131	-1.157731
H	-0.797550	-3.442044	-0.219784
H	0.423870	-2.446780	0.593105
H	-0.649468	-3.493155	1.546965
H	-3.859735	-1.670359	0.944494
H	-3.212027	-2.981346	-0.056756
H	-3.090325	-3.070846	1.712777
H	-0.379436	0.850079	-2.387623
H	1.317229	0.485168	-1.919377
H	0.211447	-0.818191	-2.420651
H	0.356964	3.684983	-0.324140
H	0.012386	2.232097	0.107514
O	-2.342504	2.286573	-1.937041
H	-1.738726	2.693789	-1.294292
H	-3.142833	2.077963	-1.448615

Neutral pinene(H₂O)₃

E(BMK) = -619.661330 a.u.

C	-1.634158	-0.636087	0.749070
C	-2.287678	0.745811	1.108436
C	-1.803761	1.259064	2.484648
C	-0.286580	1.161026	2.581643
C	0.413462	0.635886	1.559187
C	-0.382288	0.225114	0.324419
C	-1.391908	1.381624	0.002603
C	1.904107	0.407513	1.564093
C	-2.312366	-1.301558	-0.464309
C	-1.479987	-1.692675	1.851367
O	1.163879	3.658474	0.777741
O	1.301490	2.438236	-1.735617
H	0.205599	1.468285	3.505750
H	-2.264526	0.672873	3.295241
H	-2.132915	2.299743	2.626907
H	-3.377825	0.826321	1.008342
H	-1.833742	1.308221	-0.994293
H	-1.042133	2.404550	0.176946
H	0.262282	-0.173723	-0.470750
H	-2.468848	-2.082501	2.131369
H	-0.880693	-2.537890	1.484753
H	-0.998335	-1.301308	2.751325
H	-2.452369	-0.617695	-1.307675
H	-1.709255	-2.151016	-0.813530
H	-3.300374	-1.686680	-0.176525
H	2.392227	0.937636	0.733292
H	2.360204	0.743740	2.502957
H	2.121285	-0.663299	1.435727
H	0.848916	3.011919	1.424252
H	2.128979	3.548495	0.728295
H	0.969646	2.896562	-0.938825
H	0.751712	1.658204	-1.848910
O	3.640436	2.809404	-0.288485
H	3.061012	2.572213	-1.034740
H	4.414892	3.244960	-0.652423

Neutral pinene(H₂O)₄

E(BMK) = -696.077987 a.u.

C	-2.076641	1.568318	-0.020798
C	-2.256714	1.173436	1.475846
C	-1.147298	1.862386	2.303665
C	0.203459	1.688750	1.622255
C	0.291579	0.968894	0.488082
C	-1.015853	0.418178	-0.075163
C	-1.841822	-0.287162	1.069539
C	-3.027430	-1.097381	0.509295
C	-1.106473	-1.163885	2.092505
C	1.579902	0.648576	-0.227131
O	1.280641	2.583287	-3.005685
O	-1.424747	2.254025	-3.160266
O	0.673442	4.030394	-0.710654
H	1.093973	2.103155	2.098039
H	-1.106891	1.432096	3.316971
H	-1.385816	2.929986	2.425698
H	-3.244574	1.306585	1.935655
H	-2.974461	1.365486	-0.611727
H	-1.725326	2.582782	-0.232079
H	-0.861382	-0.136571	-1.010867
H	-0.240400	-0.665035	2.535356
H	-1.793344	-1.447315	2.902465
H	-0.756621	-2.089558	1.613901
H	-3.693939	-1.400850	1.328453
H	-3.626464	-0.542374	-0.219935
H	-2.659624	-2.010143	0.020299
H	1.725690	-0.441485	-0.262769
H	1.559007	1.010094	-1.265585
H	2.440854	1.097711	0.282650
H	1.070415	3.582684	-1.483443
H	0.581543	3.346175	-0.031601
H	-1.733653	1.542013	-2.591099
H	-1.707090	3.086328	-2.726758
H	0.336864	2.399937	-3.204676
H	1.701181	2.864020	-3.821648
O	-1.785558	4.575363	-1.715192
H	-0.898292	4.539747	-1.290738
H	-1.923083	5.470568	-2.033069

Neutral pinene(H₂O)₅

E(BMK) = -772.490425 a.u.

C	0.015960	-0.611248	-0.286981
C	1.466631	-0.014662	-0.209256
C	2.417803	-0.719877	-1.205722
C	1.776143	-0.792995	-2.586407
C	0.529020	-0.318014	-2.764786
C	-0.145649	0.316091	-1.554642
C	0.897985	1.267458	-0.890077
C	-0.229836	-0.349432	-4.066998
C	-0.869069	-0.138814	0.882897

C	-0.156041	-2.129338	-0.433638
O	1.432194	4.638542	-1.315269
O	-0.127801	3.253742	-3.113725
O	2.216953	2.134848	-4.078364
O	3.836516	3.476864	-2.395187
H	2.325226	-1.268878	-3.400946
H	2.659964	-1.734369	-0.852073
H	3.372684	-0.172682	-1.259348
H	1.918106	0.061527	0.791295
H	0.448379	1.972720	-0.188216
H	1.564150	1.807193	-1.567581
H	-1.138950	0.715254	-1.787886
H	0.130530	-2.629791	0.502203
H	-1.210648	-2.369391	-0.629090
H	0.441902	-2.552865	-1.244990
H	-0.573163	-0.651432	1.808756
H	-0.807512	0.939557	1.059844
H	-1.920107	-0.387432	0.681755
H	0.360026	-0.803007	-4.872215
H	-1.163965	-0.917616	-3.949154
H	-0.510789	0.672912	-4.360322
H	2.264433	4.638933	-1.812883
H	1.689048	4.205073	-0.485286
H	1.342284	2.541915	-3.909714
H	2.116529	1.218646	-3.781599
H	3.330120	2.959745	-3.067732
H	4.669621	3.735853	-2.797028
H	-0.728896	3.862079	-3.551163
H	0.298475	3.757496	-2.385413
O	3.197517	3.076564	0.346933
H	2.973801	2.169538	0.577367
H	3.601381	3.039774	-0.537463

Neutral pinene(H₂O)₆

E(BMK) = -848.903771 a.u.

C	-0.025122	-0.113034	0.433736
C	-0.359997	-0.254901	1.951522
C	0.736281	0.463596	2.772325
C	2.117200	0.093299	2.246607
C	2.229826	-0.797454	1.242794
C	0.931910	-1.331627	0.645986
C	-0.041805	-1.786371	1.801404
C	-1.245538	-2.581009	1.258371
C	0.527882	-2.546516	3.006909
C	3.537770	-1.300836	0.686801
O	2.908131	1.686623	-0.557330
O	2.412420	-0.028281	-2.540012
O	5.601170	1.173024	-0.468604
O	5.259077	-0.547006	-2.512015
O	4.989695	-3.239865	-1.812682
H	3.000476	0.518933	2.725825
H	0.659786	0.185184	3.835666
H	0.583391	1.552812	2.722777

H	-1.366015	0.021008	2.294696
H	-0.875142	-0.346598	-0.211305
H	0.432033	0.826886	0.103325
H	1.108900	-2.026408	-0.182085
H	0.819555	-3.562659	2.706353
H	1.404084	-2.056208	3.439743
H	-0.240891	-2.637732	3.787455
H	-0.927005	-3.589759	0.961949
H	-2.011151	-2.685236	2.040040
H	-1.715446	-2.108907	0.389768
H	3.594457	-1.132776	-0.397280
H	4.399605	-0.808648	1.152117
H	3.609257	-2.387689	0.845361
H	3.887136	1.676041	-0.490218
H	2.597578	1.322925	0.284980
H	5.322268	-1.500519	-2.310583
H	4.334275	-0.388652	-2.758903
H	5.606450	0.516706	-1.205070
H	6.331521	1.776798	-0.623439
H	2.517548	0.606616	-1.782086
H	1.925205	0.442173	-3.222225
H	5.229601	-3.484248	-0.915204
H	4.013513	-3.228312	-1.854265
O	2.277204	-2.783076	-2.161070
H	2.207537	-1.817714	-2.301281
H	1.876241	-3.208108	-2.923913

Neutral pinene(H₂O)₇

E(BMK) = -925.318961 a.u.

C	-0.138143	-1.127173	1.610466
C	-0.417415	-0.764553	0.106271
C	-0.192664	0.740417	-0.164246
C	1.136805	1.187322	0.429201
C	1.894350	0.305998	1.109312
C	1.381379	-1.129627	1.181424
C	0.890448	-1.535328	-0.248216
C	3.172180	0.648294	1.833864
C	-0.642436	-2.537450	1.973125
C	-0.601541	-0.154521	2.703452
O	3.616306	0.320142	-1.599260
O	2.796999	-1.417579	-3.604537
O	5.110221	-1.320182	-0.147371
O	6.162232	-2.069099	-2.605571
O	3.831190	-3.763598	-2.836851
O	3.490010	-3.586594	-0.065727
H	1.420791	2.238950	0.358916
H	-1.010187	1.331802	0.277664
H	-0.221307	0.929284	-1.248338
H	-1.361106	-1.116681	-0.329696
H	0.704498	-2.607475	-0.362501
H	1.480400	-1.175291	-1.097262
H	2.070966	-1.788364	1.725422
H	-1.699187	-0.148785	2.758234

H	-0.220699	-0.477720	3.682428
H	-0.257633	0.868482	2.526562
H	-0.369751	-3.298535	1.234813
H	-0.231594	-2.846650	2.943854
H	-1.737863	-2.531647	2.057712
H	4.009816	0.034456	1.472836
H	3.429574	1.707305	1.712172
H	3.055967	0.440253	2.907996
H	4.154720	-0.250866	-0.984858
H	2.950567	0.756315	-1.048751
H	5.543808	-2.789046	-2.805004
H	5.914996	-1.325942	-3.179437
H	5.690771	-1.595947	-0.886193
H	4.582220	-2.116113	0.058273
H	2.924480	-0.840842	-2.823968
H	3.371008	-1.009759	-4.267116
H	3.606330	-4.516888	-3.389120
H	3.354477	-2.971341	-3.187246
H	2.570664	-3.334080	0.063218
H	3.581823	-3.790263	-1.016198
O	5.093552	0.296046	-3.892216
H	5.647509	0.999227	-4.240562
H	4.665046	0.626298	-3.078937

Neutral pinene(H₂O)₈

E(BMK) = -1001.737014 a.u.

C	-0.000593	-1.644077	0.345899
C	-1.367703	-0.965903	0.661764
C	-1.218734	0.568302	0.525810
C	0.052412	1.037749	1.225482
C	0.815404	0.142281	1.883947
C	0.374617	-1.317377	1.829836
C	-1.166412	-1.421046	2.153384
C	-1.613048	-2.877962	2.379316
C	-1.751099	-0.555344	3.275256
C	2.068762	0.479570	2.651975
O	2.555968	0.594032	-0.639161
O	4.317533	-0.081042	-3.950383
O	5.156411	1.095643	-1.600047
O	3.710434	-1.762734	0.325915
O	5.367943	-2.413363	-3.295859
O	2.846601	-2.917942	-2.059403
O	1.696533	-0.708835	-2.954838
H	0.304907	2.099849	1.214517
H	-2.092081	1.075095	0.964770
H	-1.198042	0.850982	-0.538444
H	-2.263151	-1.330696	0.142286
H	-0.089776	-2.714199	0.149489
H	0.619381	-1.189779	-0.433668
H	1.064988	-1.982552	2.362088
H	-2.849774	-0.592373	3.246932
H	-1.428838	-0.937757	4.253475
H	-1.440419	0.491763	3.204837

H	-1.211271	-3.568253	1.631208
H	-1.283221	-3.224439	3.368712
H	-2.709967	-2.942071	2.349524
H	2.327497	1.540873	2.560628
H	1.932400	0.243085	3.717591
H	2.910115	-0.132724	2.294057
H	2.198387	0.240196	-1.475529
H	1.784796	0.730710	-0.064794
H	5.002841	-1.554071	-3.649127
H	5.867697	-2.825323	-4.005939
H	3.309631	-0.892554	0.146374
H	4.652526	-1.668626	0.109302
H	3.353450	-0.143819	-3.862647
H	4.622196	0.484462	-3.209397
H	3.107446	-2.673365	-1.147817
H	3.682576	-3.006647	-2.545753
H	2.024841	-1.607086	-2.674871
H	0.797498	-0.805525	-3.280500
H	4.343898	1.137151	-1.071281
H	5.704497	0.393798	-1.216889
O	6.275076	-1.441532	-0.872703
H	6.094838	-1.894629	-1.719751
H	7.046621	-1.850573	-0.478559

5. Cartesian coordinates for ionized mixed cluster structures optimized at the BMK/6-31++g**.

Ionized pinene

E(BMK) = -390.145030 a.u.

C	0.321413	0.328159	0.119295
C	0.442624	1.110827	1.300546
C	1.501931	-0.273327	-0.558400
C	-0.779077	1.450732	2.085241
H	1.428986	1.417778	1.651650
C	-2.042012	0.918172	1.383164
H	-0.657381	1.062844	3.111266
H	-0.824720	2.549215	2.204101
C	-1.952388	1.327308	-0.110110
H	-2.949938	1.161173	1.944561
C	-1.043111	0.069423	-0.343554
H	-2.894103	1.225798	-0.649777
H	-1.502674	2.297885	-0.344389
H	-1.100783	-0.490011	-1.281620
C	-1.849095	-0.574636	0.950971
C	-3.138054	-1.241323	0.452401
C	-1.101913	-1.556375	1.861029
H	-0.850437	-2.470842	1.308134
H	-0.177249	-1.159918	2.293474
H	-1.760019	-1.846849	2.690066
H	-2.910608	-2.187151	-0.053682
H	-3.764705	-1.471857	1.325559
H	-3.728611	-0.618116	-0.223947
H	1.551429	0.098551	-1.594844
H	2.445968	-0.063940	-0.048386
H	1.358621	-1.362605	-0.639873

Ionized pinene(H₂O)₁

E(BMK) = -466.556499 a.u.

C	-3.018119	0.027265	1.112550
C	-3.199211	1.561543	1.359371
C	-2.091468	2.105293	2.281756
C	-0.753180	1.626576	1.833661
C	-0.651409	0.762500	0.707870
C	-1.911306	0.466452	0.008902
C	-2.742932	1.804355	-0.104411
C	0.641298	0.173844	0.277134
C	-4.226353	-0.611996	0.411411
C	-2.570515	-0.888576	2.259918
H	0.147533	1.913267	2.376199
H	-2.232510	1.825013	3.339555
H	-2.078379	3.210006	2.276037
H	-4.190325	1.909690	1.667608
H	-3.540944	1.691878	-0.839105
H	-2.168019	2.712454	-0.306118
H	-1.786840	-0.176400	-0.867406
H	-2.306438	-1.880519	1.871104

H	-1.708266	-0.512070	2.822234
H	-3.399613	-1.020152	2.966953
H	-4.595605	-0.034553	-0.441025
H	-3.973643	-1.620208	0.061296
H	-5.047184	-0.702545	1.135581
H	1.455457	0.363500	0.981993
H	0.528450	-0.906476	0.106230
H	0.904277	0.619295	-0.697139
O	0.330719	3.420179	-0.119658
H	0.058872	3.878879	-0.922127
H	1.113116	3.891791	0.186546

Ionized pinene(H₂O)₂

E(BMK) = -542.972126 a.u.

C	-1.754587	0.895230	-0.314640
C	-1.507955	0.170561	1.035888
C	-0.116358	0.591639	1.547503
C	0.895433	0.481326	0.459193
C	0.492275	0.061961	-0.837714
C	-0.934171	-0.281574	-0.996308
C	-1.428552	-1.177142	0.239979
C	-2.815557	-1.773794	-0.048564
C	-0.502038	-2.298830	0.730540
C	1.444012	-0.015116	-1.975870
O	0.918753	2.945148	-0.373920
H	1.945888	0.686432	0.657324
H	0.221733	-0.001775	2.412753
H	-0.128816	1.641898	1.892935
H	-2.267327	0.252536	1.820663
H	-2.792394	0.861930	-0.649568
H	-1.344042	1.900974	-0.441452
H	-1.195445	-0.605570	-2.008234
H	-0.428059	-3.087689	-0.029163
H	0.515469	-1.963408	0.962211
H	-0.918282	-2.751570	1.639708
H	-2.736772	-2.584963	-0.782942
H	-3.220898	-2.198516	0.879345
H	-3.536067	-1.040759	-0.423381
H	1.420031	-1.027425	-2.408271
H	1.096628	0.662043	-2.772625
H	2.467569	0.248132	-1.696076
H	1.478253	3.509323	-0.916436
H	0.613542	3.484414	0.378004
O	-0.173887	4.060810	1.945098
H	0.342586	4.461402	2.653049
H	-0.993418	4.564842	1.892692

Ionized pinene(H₂O)₃

E(BMK) = -619.389908 a.u.

C	-2.102467	-0.283087	0.485040
C	-1.929052	1.016625	1.340929
C	-0.547817	1.051511	2.020295
C	0.528998	0.721502	1.041082

C	0.172963	0.339265	-0.280199
C	-1.236035	0.529637	-0.646654
C	-1.809418	1.824944	0.022035
C	1.123032	-0.370985	-1.176951
C	-3.534876	-0.486151	-0.030783
C	-1.568934	-1.624541	1.003590
O	1.072594	3.693829	0.837082
O	1.104982	2.723606	-1.759842
H	1.581230	0.744168	1.325853
H	-0.470156	0.359618	2.876208
H	-0.331740	2.054970	2.425334
H	-2.733458	1.262038	2.042359
H	-2.771408	2.093163	-0.415681
H	-1.144235	2.692651	0.035639
H	-1.453652	0.303155	-1.694057
H	-0.556373	-1.575468	1.418763
H	-2.234820	-1.996798	1.792722
H	-1.566161	-2.370043	0.197413
H	-3.984777	0.420748	-0.444034
H	-3.554608	-1.265567	-0.802330
H	-4.163392	-0.823527	0.804849
H	1.086163	0.077046	-2.178012
H	2.146034	-0.360780	-0.791390
H	0.781723	-1.415409	-1.279711
H	1.978274	3.335441	0.844813
H	1.097822	4.558181	1.259299
H	0.879698	3.347837	-1.047751
H	1.002380	3.187992	-2.596245
O	3.137232	2.050416	0.000579
H	4.094941	2.100650	-0.075943
H	2.757425	2.206963	-0.881999

Ionized pinene(H₂O)₄

E(BMK) = -695.808774 a.u.

C	-1.851536	1.730893	0.829998
C	-0.773472	1.170672	1.796028
C	0.599620	1.466481	1.164644
C	0.622615	1.047815	-0.263633
C	-0.523623	0.421674	-0.825745
C	-1.726980	0.395868	0.019141
C	-1.262459	-0.274810	1.436615
C	-2.505694	-0.705803	2.229041
C	-0.267091	-1.442037	1.403477
C	-0.453499	-0.320217	-2.112490
O	2.632331	3.404083	-0.836282
O	1.784128	2.091841	-3.084515
O	0.116294	4.359436	-0.423737
H	1.516691	1.188512	-0.870323
H	1.437914	0.977723	1.688962
H	0.824735	2.547486	1.196248
H	-0.806533	1.460643	2.851584
H	-2.840925	1.816952	1.280560
H	-1.602813	2.648822	0.289759

H	-2.603173	-0.037772	-0.471912
H	-0.722970	-2.313325	0.914388
H	0.669639	-1.215618	0.881775
H	-0.014940	-1.735520	2.430499
H	-2.959746	-1.595883	1.775986
H	-2.196677	-0.969171	3.249903
H	-3.269222	0.073694	2.301207
H	-0.503616	-1.399855	-1.887558
H	-1.330318	-0.087661	-2.729749
H	0.469224	-0.107976	-2.659995
H	1.084290	4.238817	-0.513002
H	-0.050868	5.293731	-0.267718
H	2.123467	2.111907	-3.984424
H	0.846190	2.366545	-3.107189
H	2.582165	3.032212	-1.738649
H	3.510463	3.775702	-0.712341
O	-0.805184	2.754417	-2.420271
H	-0.612521	3.458721	-1.764052
H	-1.522186	3.070633	-2.978840

Ionized pinene(H₂O)₅

E(BMK) = -772.222640 a.u.

C	-1.241627	0.035101	0.921715
C	-0.782215	1.254060	1.792838
C	0.751846	1.382036	1.802718
C	1.300354	1.250583	0.425184
C	0.413812	1.003407	-0.660275
C	-1.021495	1.045029	-0.343816
C	-1.314722	2.194673	0.678086
C	0.913307	0.577803	-1.992473
C	-2.737332	-0.278376	1.071312
C	-0.450202	-1.278785	0.957030
O	1.557399	4.425344	0.843829
O	0.541019	3.782092	-1.620456
O	2.555221	3.068388	-3.240153
O	3.886784	2.966712	1.006509
H	2.374996	1.303748	0.249741
H	1.248968	0.644841	2.454874
H	1.063057	2.372639	2.181976
H	-1.204369	1.336837	2.799949
H	-2.386614	2.385007	0.745270
H	-0.772574	3.129612	0.514734
H	-1.668214	0.901017	-1.214472
H	-0.776584	-1.939874	0.143276
H	0.634567	-1.148546	0.868713
H	-0.648797	-1.797510	1.903801
H	-3.069269	-0.959179	0.277818
H	-2.898332	-0.780389	2.035154
H	-3.368782	0.614272	1.049093
H	0.538565	-0.438825	-2.198794
H	0.488134	1.231127	-2.767887
H	2.004690	0.596148	-2.052645
H	1.470694	5.346839	1.105780

H	1.191702	4.343694	-0.061765
H	2.999009	3.589732	-3.914584
H	3.240970	2.626304	-2.701092
H	3.159081	3.621212	1.010153
H	4.568779	3.280849	1.606782
H	1.255273	3.624085	-2.281531
H	-0.148508	4.286814	-2.062288
O	4.112205	1.717033	-1.417290
H	4.932567	1.249973	-1.601539
H	4.237727	2.219055	-0.585816

Ionized pinene(H₂O)₆

E(BMK) = -848.635293 a.u.

C	0.403767	-0.425293	-1.416840
C	0.214926	-0.063745	0.081353
C	1.618695	0.122164	0.686296
C	2.504836	-1.020708	0.330414
C	1.981139	-2.090860	-0.445182
C	0.608214	-1.912255	-0.958692
C	-0.314552	-1.518659	0.316897
C	-1.798597	-1.686367	-0.045728
C	-0.054104	-2.219713	1.657599
C	2.694407	-3.389265	-0.570199
O	3.476158	1.439845	-1.828517
O	3.523927	-1.217626	-2.469720
O	4.703253	1.297729	0.616852
O	5.750505	-2.484376	-1.532932
O	5.704589	-1.243371	0.861120
H	3.536358	-1.064622	0.685643
H	1.609471	0.229202	1.784107
H	2.098024	1.044672	0.315070
H	-0.453624	0.763061	0.343929
H	-0.511124	-0.324549	-2.002720
H	1.243113	0.046304	-1.936781
H	0.274269	-2.731586	-1.601427
H	-0.301830	-3.286859	1.580879
H	0.981616	-2.140069	2.006201
H	-0.701115	-1.784623	2.430070
H	-2.058865	-2.750953	-0.098736
H	-2.413542	-1.228059	0.740434
H	-2.068936	-1.219189	-0.996939
H	3.749910	-3.316724	-0.291921
H	2.190936	-4.116192	0.091118
H	2.599479	-3.774681	-1.592787
H	4.005568	1.516243	-1.007480
H	3.719269	2.176980	-2.395817
H	5.034321	-2.056972	-2.044985
H	6.500004	-2.615787	-2.120035
H	5.235517	0.488437	0.755229
H	5.130241	2.012491	1.097257
H	3.541853	-0.240936	-2.404600
H	2.886643	-1.472154	-3.159804
H	6.296695	-1.607855	1.524909

H	5.881899	-1.709606	0.013458
O	1.509514	-2.229539	-4.146421
H	0.878289	-1.667943	-4.608403
H	1.741547	-2.931363	-4.763964

Ionized pinene(H₂O)₇

E(BMK) = -925.055180 a.u.

C	-0.215549	-0.703370	1.060567
C	0.543074	-0.055440	-0.147841
C	1.759168	0.761746	0.333753
C	2.549468	-0.011770	1.331922
C	2.140400	-1.325602	1.685508
C	0.931584	-1.835771	1.010226
C	1.052322	-1.471875	-0.521396
C	2.862652	-2.137091	2.697776
C	-1.574667	-1.297312	0.657911
C	-0.392899	0.085423	2.365813
O	3.760681	-0.011491	-2.121815
O	6.086856	-2.276012	-3.212796
O	7.226680	-0.952798	-0.915750
O	6.336409	0.563110	-3.079248
O	4.711215	-1.129852	0.164630
O	3.515645	-3.612043	-0.252994
H	3.407410	0.435298	1.830198
H	1.481863	1.732448	0.776719
H	2.420472	0.995064	-0.521505
H	-0.049986	0.501336	-0.880901
H	0.341456	-2.059825	-1.103699
H	2.045657	-1.555012	-0.967376
H	0.668934	-2.856115	1.303568
H	-0.785752	-0.570995	3.153194
H	0.532458	0.537273	2.741471
H	-1.120615	0.893013	2.213202
H	-2.290082	-0.478066	0.505007
H	-1.539763	-1.884747	-0.264350
H	-1.963890	-1.938003	1.459000
H	3.170360	-3.079849	2.220039
H	3.737061	-1.625128	3.108093
H	2.169017	-2.411706	3.508038
H	4.539413	0.353628	-2.581188
H	3.483042	-0.793851	-2.626848
H	6.858423	0.307651	-2.296487
H	6.746286	1.336544	-3.477695
H	8.028396	-1.001093	-0.386762
H	6.455964	-1.010200	-0.312363
H	6.208344	-1.414929	-3.639999
H	6.608459	-2.198726	-2.398680
H	4.372791	-0.711908	-0.661880
H	4.431941	-2.065025	0.112255
H	3.884079	-4.495060	-0.152350
H	3.388321	-3.471696	-1.213647
O	3.482078	-2.742141	-2.879630
H	4.453935	-2.683611	-3.064804

H 3.072816 -3.190269 -3.626719

Ionized pinene(H₂O)₈

E(BMK) = -1001.467721 a.u.

C	0.586123	-0.705386	-0.321688
C	0.143649	-0.007685	0.993024
C	1.335800	0.839649	1.477468
C	2.590208	0.034183	1.476308
C	2.537159	-1.336797	1.108315
C	1.257685	-1.812268	0.562459
C	0.131972	-1.414112	1.685044
C	-1.152705	-2.212115	1.417260
C	0.498714	-1.549810	3.168555
C	3.650431	-2.272838	1.399849
O	3.522323	1.021295	-0.938141
O	3.421843	-1.376446	-2.270585
O	4.454482	0.844014	-3.629812
O	5.646063	0.231725	0.631085
O	5.925180	-1.858159	-1.143930
O	5.311886	-4.463295	-0.575198
O	2.759676	-3.939755	-1.525735
H	3.543474	0.465287	1.783424
H	1.186057	1.261867	2.484886
H	1.503398	1.704390	0.811325
H	-0.791739	0.561928	1.001965
H	-0.239747	-1.121823	-0.899037
H	1.250631	-0.138587	-0.979024
H	1.291886	-2.850027	0.219646
H	0.676822	-2.604302	3.418481
H	1.389570	-0.983002	3.461087
H	-0.340201	-1.201628	3.784786
H	-1.021747	-3.257224	1.723762
H	-1.965914	-1.782910	2.018859
H	-1.465683	-2.195050	0.369657
H	3.893484	-2.867958	0.507886
H	4.541787	-1.766316	1.777639
H	3.294922	-3.009625	2.141313
H	4.362283	0.943839	-0.442935
H	3.752684	1.391033	-1.806988
H	6.000696	-2.804466	-0.909626
H	5.067822	-1.788086	-1.608385
H	5.886344	-0.557098	0.100782
H	6.449832	0.751092	0.732531
H	3.294397	-0.603597	-1.679713
H	3.624327	-0.949559	-3.120114
H	5.746914	-5.318058	-0.632728
H	4.430455	-4.537907	-0.986935
H	2.854699	-3.065550	-1.950582
H	2.218457	-4.484197	-2.104849
H	5.403196	0.714626	-3.418295
H	4.404751	1.339201	-4.452688
O	6.923449	0.235135	-2.591940
H	6.849098	-0.636552	-2.161528

H 7.798098 0.297168 -2.985973