

Supporting Information

**On the Properties of Ammonium Ion-Water Clusters: Analyses
of Structure Evolution, Non-Covalent Interactions, and
Temperature and Humidity Effects**

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Table S1. Saturated water vapor pressures at different temperatures

Temperature / °C	Saturated water vapor pressure /KPa	Temperature / °C	Saturated water vapor pressure /KPa
0	0.611	25	3.169
1	0.657	26	3.363
2	0.706	27	3.567
3	0.758	28	3.782
4	0.814	29	4.008
5	0.873	30	4.246
6	0.935	31	4.495
7	1.002	32	4.758
8	1.073	33	5.034
9	1.148	34	5.323
10	1.228	35	5.627
11	1.313	36	5.945
12	1.403	37	6.280
13	1.498	38	6.630
14	1.599	39	6.997
15	1.706	40	7.381
16	1.819	41	7.784
17	1.938	42	8.205
18	2.064	43	8.646
19	2.198	44	9.108
20	2.339	45	9.590
21	2.488	46	10.094
22	2.645	47	10.620
23	2.810	48	11.171
24	2.985	49	11.745

PW91PW91/6-311++G(3df,3pd) Optimized Cartesian Coordinates (in Å) and Single Point

Energies (in kcal/mol) for Clusters Isomers

The E[DF-MP2-F12] line represents Second-order Møller–Plesset Perturbation Theory-explicitly

Correlated Methods with Density Fitting single point energies for each isomer.

Table S2: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for NH₄⁺ isomer

5			
NH ₄ ⁺	E[DF-MP2-F12]	-35623.56	
H	-0.317172000000	0.938016000000	-0.289898000000
H	0.608982000000	-0.398410000000	-0.731386000000
H	0.526930000000	0.073107000000	0.884032000000
H	-0.818716000000	-0.612685000000	0.137251000000
N	-0.000004000000	-0.000004000000	0.000000000000

Table S3: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for

H₂O isomer

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H ₂ O	E[DF-MP2-F12]	-47902.28	
O	0.000000000000	0.118861000000	0.000000000000
H	0.765442000000	-0.475446000000	0.000000000000
H	-0.765442000000	-0.475446000000	0.000000000000

Table S4: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for

NH₄⁺(H₂O) isomers

8			
1a.	E[DF-MP2-F12]	-83544.72	
H	1.679864000000	-0.521534000000	-0.813555000000
H	0.248959000000	0.001507000000	0.000200000000
H	1.680246000000	-0.441781000000	0.859502000000
H	1.683256000000	0.963655000000	-0.046290000000
N	1.328406000000	-0.000290000000	0.000115000000
O	-1.342904000000	0.000209000000	-0.000427000000
H	-1.922703000000	-0.779649000000	0.001363000000
H	-1.925237000000	0.778156000000	0.001395000000

Table S5: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for

NH₄⁺(H₂O)₂ isomers

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2a. E[DF-MP2-F12] -131462.33

H	-0.87703000000	0.43719700000	-0.00066100000
H	0.86675400000	0.45174000000	-0.00133700000
H	-0.01234200000	1.64705500000	-0.83610700000
H	-0.01351200000	1.64977300000	0.82985900000
N	-0.00968800000	1.04891400000	-0.00214500000
O	2.25043000000	-0.50375200000	-0.00049700000
H	2.70026800000	-0.87636300000	-0.77636900000
H	2.81632700000	-0.70894500000	0.76165700000
O	-2.24658200000	-0.52353800000	0.00305300000
H	-3.17103500000	-0.23337900000	-0.06266100000
H	-2.27239500000	-1.49116300000	0.08018800000

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2b. E[DF-MP2-F12] -131462.38

H	-2.81677100000	-0.18007700000	0.83540000000
H	-2.81688700000	-0.17981600000	-0.83525500000
H	-1.30371000000	0.14671000000	0.00000800000
H	-2.08559700000	-1.42460100000	-0.00017500000
N	-2.26741100000	-0.41383800000	-0.00000200000
O	2.28690100000	-0.43241300000	-0.00000500000
H	2.86518100000	-0.50654700000	-0.77635800000
H	2.86513400000	-0.50664400000	0.77637400000
O	-0.01575400000	0.84845700000	0.00000500000
H	0.88732900000	0.40961900000	0.00000500000
H	0.10801500000	1.80986900000	0.00001200000

Table S6: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for

NH₄⁺(H₂O)₃ isomers

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3a E[DF-MP2-F12] -179376.11

H	-1.43596400000	0.84507400000	-0.00038100000
H	-2.67371500000	-0.00046300000	-0.83663100000
H	-1.43639200000	-0.84522500000	0.00085500000
H	-2.67422000000	0.00089700000	0.83644700000
N	-2.08180800000	0.00007000000	0.00008700000
O	2.12198700000	-0.00001400000	0.00009900000
H	2.71392400000	-0.00170500000	-0.77283300000
H	2.71446400000	0.00159600000	0.77261600000
O	-0.08209500000	-1.79852400000	-0.00043600000

H	0.049066000000	-2.758807000000	0.001527000000
H	0.801443000000	-1.368370000000	0.001641000000
O	-0.081979000000	1.798454000000	0.000166000000
H	0.049104000000	2.758755000000	-0.001046000000
H	0.801635000000	1.368425000000	-0.001435000000
14			
3b.	E[DF-MP2-F12]	-179377.69	
H	0.745466000000	0.657171000000	0.351554000000
H	-0.000249000000	0.001657000000	1.718808000000
H	-0.941736000000	0.318781000000	0.351748000000
H	0.194665000000	-0.972689000000	0.351975000000
N	-0.000469000000	0.001355000000	0.693883000000
O	0.511705000000	-2.587384000000	-0.219826000000
H	0.170810000000	-3.421284000000	0.141729000000
H	1.127596000000	-2.837706000000	-0.927105000000
O	-2.498602000000	0.850033000000	-0.220529000000
H	-3.044141000000	1.572320000000	0.130261000000
H	-3.031619000000	0.428373000000	-0.913583000000
O	1.987214000000	1.736336000000	-0.220159000000
H	1.882318000000	2.435415000000	-0.885384000000
H	2.897632000000	1.816597000000	0.106925000000
14			
3c.	E[DF-MP2-F12]	-172.07522262	
H	0.238133000000	0.490209000000	-0.347420000000
H	0.886876000000	1.511258000000	0.875723000000
H	1.940098000000	0.437901000000	0.091756000000
H	1.302878000000	1.792315000000	-0.711574000000
N	1.096852000000	1.061967000000	-0.021960000000
O	-3.361580000000	-0.117601000000	0.511883000000
H	-3.734038000000	-0.819750000000	1.068887000000
H	-4.116825000000	0.407190000000	0.202099000000
O	3.301695000000	-0.576504000000	0.281134000000
H	4.236293000000	-0.315180000000	0.309197000000
H	3.289462000000	-1.539088000000	0.406246000000
O	-1.024834000000	-0.336761000000	-0.771660000000
H	-1.123500000000	-0.865517000000	-1.577665000000
H	-1.919596000000	-0.286174000000	-0.334379000000

Table S7: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for

$\text{NH}_4^+(\text{H}_2\text{O})_4$ isomer

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4a.	E[DF-MP2-F12]	-227289.26	
H	-2.180658000000	-0.844941000000	-0.293745000000
H	-3.083885000000	0.002289000000	-1.486436000000
H	-3.625718000000	0.001552000000	0.096085000000
H	-2.179551000000	0.846787000000	-0.292657000000
N	-2.795101000000	0.001447000000	-0.503524000000
O	-0.898553000000	-1.768583000000	0.133450000000
H	-0.756352000000	-2.721919000000	0.226881000000
H	-0.076797000000	-1.296400000000	0.419980000000
O	-0.896004000000	1.768400000000	0.134240000000
H	-0.075233000000	1.295130000000	0.421801000000
H	-0.753307000000	2.721526000000	0.228972000000
O	3.347354000000	0.000344000000	-0.623794000000
H	3.874460000000	0.776444000000	-0.870360000000
H	3.869868000000	-0.775804000000	-0.879793000000
O	1.100478000000	-0.001561000000	0.841289000000
H	1.385069000000	-0.002639000000	1.770505000000
H	1.941617000000	-0.000953000000	0.301951000000

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4b.	E[DF-MP2-F12]	-227290.65	
H	-0.529442000000	-0.847796000000	0.632598000000
H	-2.005093000000	-0.009782000000	0.282247000000
H	-1.375821000000	-0.022514000000	1.853155000000
H	-0.533062000000	0.826404000000	0.647545000000
N	-1.130871000000	-0.013979000000	0.858896000000
O	0.822439000000	-1.814861000000	0.174963000000
H	1.648395000000	-1.365243000000	-0.106269000000
H	0.975189000000	-2.770066000000	0.120699000000
O	0.807017000000	1.809800000000	0.190544000000
H	1.638871000000	1.368636000000	-0.087011000000
H	0.966305000000	2.765488000000	0.186301000000
O	-3.514936000000	0.007848000000	-0.621657000000
H	-3.929997000000	0.774433000000	-1.048067000000
H	-4.081709000000	-0.750924000000	-0.833369000000
O	2.910509000000	0.010083000000	-0.523306000000
H	3.224305000000	0.019867000000	-1.444415000000
H	3.717913000000	0.006401000000	0.019963000000

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4c.	E[DF-MP2-F12]	-227290.63	
H	2.841396000000	1.426278000000	-0.513203000000
H	2.076182000000	-0.048759000000	-0.049923000000

H	2.630674000000	1.105528000000	1.110584000000
H	1.270692000000	1.474786000000	0.148135000000
N	2.217776000000	0.999284000000	0.178846000000
O	1.621446000000	-1.495313000000	-0.434157000000
H	0.715546000000	-1.782519000000	-0.129175000000
H	2.145787000000	-2.285608000000	-0.630110000000
O	-0.296389000000	2.059672000000	0.059937000000
H	-1.106597000000	1.512183000000	-0.052706000000
H	-0.578418000000	2.986975000000	0.072196000000
O	-0.853848000000	-1.904033000000	0.460186000000
H	-1.545591000000	-1.267032000000	0.183217000000
H	-1.301199000000	-2.731298000000	0.694180000000
O	-2.529895000000	0.318528000000	-0.250716000000
H	-3.265776000000	0.473008000000	0.367464000000
H	-2.937634000000	0.310639000000	-1.134581000000

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4d.	E[DF-MP2-F12]	-227290.65	
H	-1.516794000000	-0.769417000000	-0.342561000000
H	-1.228299000000	0.920892000000	-0.317120000000
H	0.075238000000	-0.173921000000	-0.011896000000
H	-0.613358000000	-0.035057000000	-1.561018000000
N	-0.824573000000	-0.014329000000	-0.558767000000
O	1.488754000000	-0.393127000000	0.795166000000
H	1.601715000000	-0.741853000000	1.691791000000
H	2.397359000000	-0.280285000000	0.410305000000
O	3.903281000000	-0.044143000000	-0.369148000000
H	4.486962000000	0.711674000000	-0.197509000000
H	4.480086000000	-0.762290000000	-0.674056000000
O	-1.903194000000	2.499452000000	0.105766000000
H	-1.580080000000	3.079404000000	0.813631000000
H	-2.595190000000	3.002540000000	-0.352288000000
O	-2.687523000000	-2.050057000000	-0.004226000000
H	-3.593520000000	-1.941543000000	0.326144000000
H	-2.552646000000	-3.006843000000	-0.094510000000

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4e.	E[DF-MP2-F12]	-227289.73	
H	-0.016735000000	1.007513000000	0.183161000000
H	0.958779000000	-0.258831000000	-0.430828000000
H	-0.146272000000	-0.560613000000	0.846034000000
H	-0.731090000000	-0.252896000000	-0.734070000000
N	0.016942000000	-0.017634000000	-0.037111000000
O	-2.108410000000	-0.698606000000	-1.896149000000

H	-2.151902000000	-1.473283000000	-2.501371000000
H	-2.858637000000	-0.124227000000	-2.171155000000
O	-0.473327000000	-1.400420000000	2.456210000000
H	-1.352609000000	-1.685687000000	2.794306000000
H	0.179808000000	-1.834430000000	3.050965000000
O	-0.028997000000	2.802275000000	0.624837000000
H	0.021879000000	3.158441000000	1.540774000000
H	-0.255490000000	3.578187000000	0.063831000000
O	2.642368000000	-0.678536000000	-1.063014000000
H	3.363516000000	-0.037437000000	-1.256942000000
H	2.940178000000	-1.523818000000	-1.469479000000

Table S8: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for

$\text{NH}_4^+(\text{H}_2\text{O})_5$ isomers

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5a.	E[DF-MP2-F12]	-275200.29	
H	1.374355000000	-1.172169000000	-0.737548000000
H	0.725470000000	-2.180296000000	0.462886000000
H	-0.283101000000	-1.686954000000	-0.770322000000
H	0.967269000000	-2.822601000000	-1.078913000000
N	0.700414000000	-1.988445000000	-0.548066000000
O	-1.220560000000	1.639949000000	-1.106558000000
H	-0.612465000000	1.941606000000	-0.392324000000
H	-1.760276000000	2.399714000000	-1.373444000000
O	0.657974000000	1.654907000000	0.944653000000
H	0.940685000000	2.341895000000	1.570192000000
H	0.282862000000	0.907298000000	1.482479000000
O	-1.838787000000	-0.839797000000	-0.516874000000
H	-2.706004000000	-1.165903000000	-0.806554000000
H	-1.759735000000	0.118382000000	-0.825168000000
O	2.283190000000	0.151380000000	-0.687449000000
H	1.866508000000	0.867586000000	-0.146388000000
H	2.798731000000	0.569819000000	-1.393646000000
O	-0.469885000000	-0.679617000000	1.845957000000
H	-1.259090000000	-0.757493000000	1.256152000000
H	-0.773561000000	-0.856347000000	2.751229000000

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5b.	E[DF-MP2-F12]	-275201.48	
H	0.034439000000	1.043161000000	1.455512000000
H	0.874364000000	1.774636000000	0.191727000000
H	-0.845202000000	1.795961000000	0.224063000000

H	0.047025000000	2.739270000000	1.352341000000
N	0.026098000000	1.865897000000	0.819412000000
O	-1.460364000000	-1.536389000000	-0.483361000000
H	-1.274328000000	-1.492286000000	0.483051000000
H	-2.095492000000	-2.260779000000	-0.611218000000
O	-2.103304000000	1.179524000000	-0.713381000000
H	-2.077027000000	0.205217000000	-0.848360000000
H	-2.772308000000	1.551730000000	-1.306722000000
O	1.340186000000	-1.565688000000	-0.619435000000
H	1.870845000000	-2.324813000000	-0.912539000000
H	0.419188000000	-1.724489000000	-0.934563000000
O	2.122004000000	1.114067000000	-0.726638000000
H	2.014639000000	0.151543000000	-0.902180000000
H	2.692811000000	1.482710000000	-1.417327000000
O	0.090426000000	-0.878578000000	1.751014000000
H	0.814746000000	-1.244132000000	1.188288000000
H	0.202025000000	-1.262495000000	2.636451000000

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5c.	E[DF-MP2-F12]	-275203.04	
H	-1.294396000000	0.877137000000	0.561001000000
H	-2.806944000000	0.040628000000	0.403816000000
H	-1.308932000000	-0.798202000000	0.630594000000
H	-2.009684000000	0.098282000000	1.894021000000
N	-1.876530000000	0.056129000000	0.879914000000
O	4.296774000000	0.003142000000	0.371484000000
H	4.765680000000	0.792965000000	0.682800000000
H	4.880780000000	-0.749555000000	0.553061000000
O	-4.413861000000	-0.022336000000	-0.346966000000
H	-4.736877000000	-0.706358000000	-0.954694000000
H	-5.127177000000	0.632468000000	-0.284015000000
O	-0.053900000000	-1.784509000000	0.039194000000
H	0.746150000000	-1.319397000000	-0.308387000000
H	0.146196000000	-2.730759000000	0.084025000000
O	0.021489000000	1.798872000000	-0.005592000000
H	0.116514000000	2.720452000000	-0.287262000000
H	0.781398000000	1.287896000000	-0.377614000000
O	1.909366000000	-0.048098000000	-0.873271000000
H	2.110530000000	-0.082915000000	-1.823057000000
H	2.793518000000	-0.032119000000	-0.412478000000

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5d.	E[DF-MP2-F12]	-275203.12	
H	2.741274000000	0.000101000000	-0.043434000000

H	1.432384000000	-0.846750000000	0.715813000000
H	2.595997000000	-0.018653000000	1.640139000000
H	1.431997000000	0.828960000000	0.734529000000
N	2.072893000000	-0.009158000000	0.760242000000
O	-3.820536000000	0.016501000000	-1.379396000000
H	-4.228352000000	0.796530000000	-1.786603000000
H	-4.203570000000	-0.754965000000	-1.825144000000
O	0.018870000000	-1.795343000000	0.650828000000
H	-0.171454000000	-2.742894000000	0.708090000000
H	-0.841862000000	-1.309628000000	0.660134000000
O	-2.107421000000	-0.008469000000	0.700070000000
H	-2.668467000000	-0.018848000000	1.493164000000
H	-2.737423000000	0.000841000000	-0.072563000000
O	3.954263000000	0.017089000000	-1.338598000000
H	4.338761000000	-0.751514000000	-1.789060000000
H	4.302458000000	0.795427000000	-1.801672000000
O	0.018784000000	1.778636000000	0.691211000000
H	-0.842068000000	1.293008000000	0.689003000000
H	-0.171599000000	2.725178000000	0.762985000000

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5e.	E[DF-MP2-F12]	-275202.15	
H	-0.519366000000	-0.000540000000	1.679873000000
H	-1.078336000000	-0.001164000000	0.071549000000
H	0.382421000000	0.835342000000	0.517791000000
H	0.383201000000	-0.836204000000	0.518161000000
N	-0.223829000000	-0.000648000000	0.699744000000
O	1.794166000000	1.814838000000	0.160040000000
H	1.941734000000	2.768822000000	0.079140000000
H	2.643048000000	1.366980000000	-0.042398000000
O	-4.950582000000	0.000886000000	0.224447000000
H	-5.532819000000	-0.774081000000	0.264328000000
H	-5.534157000000	0.774968000000	0.262078000000
O	1.795596000000	-1.814019000000	0.160163000000
H	2.644427000000	-1.364974000000	-0.040231000000
H	1.945394000000	-2.767909000000	0.082273000000
O	3.959927000000	0.000408000000	-0.328326000000
H	4.379454000000	-0.001779000000	-1.206118000000
H	4.697685000000	0.002615000000	0.306010000000
O	-2.459233000000	-0.001350000000	-0.849880000000
H	-3.389135000000	-0.000344000000	-0.505575000000
H	-2.515747000000	-0.003298000000	-1.816640000000

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5f.	E[DF-MP2-F12]	-275201.28	
H	1.809268000000	0.084868000000	1.794239000000
H	0.959019000000	-0.791407000000	0.625202000000
H	1.092904000000	0.914088000000	0.487346000000
H	2.490008000000	-0.095455000000	0.261919000000
N	1.599121000000	0.024189000000	0.793854000000
O	-2.455265000000	1.532775000000	-0.186005000000
H	-2.738018000000	0.594307000000	-0.187829000000
H	-3.185715000000	2.048451000000	0.188112000000
O	-0.255710000000	-1.994508000000	0.309088000000
H	-1.195577000000	-1.823477000000	0.077805000000
H	-0.145604000000	-2.956896000000	0.338646000000
O	0.138109000000	2.172321000000	0.102932000000
H	0.363816000000	2.925991000000	-0.462262000000
H	-0.835930000000	1.998831000000	-0.012251000000
O	4.032615000000	-0.302441000000	-0.617483000000
H	4.922779000000	-0.066857000000	-0.311132000000
H	4.143213000000	-0.613748000000	-1.529776000000
O	-2.958525000000	-1.304825000000	-0.337871000000
H	-3.635743000000	-1.686261000000	0.247614000000
H	-3.248054000000	-1.528330000000	-1.239890000000

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5g.	E[DF-MP2-F12]	-275201.10	
H	0.000081000000	0.525892000000	1.007181000000
H	-0.869984000000	1.770960000000	0.285732000000
H	0.000564000000	2.097851000000	1.714208000000
H	0.869532000000	1.770868000000	0.284886000000
N	0.000029000000	1.575538000000	0.834664000000
O	-2.396981000000	1.365912000000	-0.503159000000
H	-3.101363000000	1.880208000000	-0.924818000000
H	-2.662750000000	0.421944000000	-0.531705000000
O	2.397502000000	1.365999000000	-0.502200000000
H	2.662182000000	0.421800000000	-0.532765000000
H	3.099906000000	1.879798000000	-0.927748000000
O	0.000065000000	-1.146074000000	0.876047000000
H	-0.792034000000	-1.491090000000	0.414468000000
H	0.792015000000	-1.491089000000	0.414190000000
O	2.643170000000	-1.489988000000	-0.288250000000
H	2.833929000000	-2.015878000000	-1.083981000000
H	3.267830000000	-1.817065000000	0.382519000000
O	-2.643474000000	-1.489697000000	-0.287800000000
H	-2.834767000000	-2.013793000000	-1.084591000000
H	-3.267598000000	-1.818388000000	0.382680000000

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5h.	E[DF-MP2-F12]	-275203.38	
H	-1.481901000000	-0.848157000000	0.078525000000
H	-1.478351000000	0.849409000000	-0.081287000000
H	-0.249128000000	0.077177000000	0.827907000000
H	-0.248909000000	-0.080742000000	-0.829961000000
N	-0.881435000000	-0.000585000000	-0.001241000000
O	1.229628000000	0.230178000000	1.811488000000
H	2.095745000000	0.144942000000	1.359290000000
H	1.399898000000	0.198918000000	2.764656000000
O	-2.568325000000	2.290815000000	-0.172772000000
H	-3.307884000000	2.429400000000	-0.785259000000
H	-2.468837000000	3.126145000000	0.310557000000
O	-2.573976000000	-2.286733000000	0.172469000000
H	-2.442767000000	-3.146373000000	-0.257734000000
H	-3.356981000000	-2.392570000000	0.735476000000
O	3.447581000000	0.002768000000	0.000771000000
H	4.042328000000	-0.764205000000	0.067326000000
H	4.035316000000	0.775161000000	-0.065469000000
O	1.231533000000	-0.237320000000	-1.811022000000
H	1.402777000000	-0.213578000000	-2.764230000000
H	2.097209000000	-0.149099000000	-1.358588000000

Table S9: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for

$\text{NH}_4^+(\text{H}_2\text{O})_6$ isomers

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6a.	E[DF-MP2-F12]	-323114.52	
H	-1.280105000000	1.093347000000	1.121942000000
H	-1.042621000000	2.041236000000	-0.252731000000
H	-2.167209000000	0.714262000000	-0.256534000000
H	-2.514970000000	2.147557000000	0.624092000000
N	-1.770852000000	1.519650000000	0.309028000000
O	-0.357346000000	-2.208872000000	0.223293000000
H	-0.405743000000	-3.136295000000	0.508303000000
H	0.485920000000	-2.116801000000	-0.326119000000
O	0.417526000000	2.523100000000	-0.952962000000
H	1.218949000000	2.066628000000	-0.603838000000
H	0.706118000000	3.294274000000	-1.462940000000
O	0.038147000000	-0.102775000000	1.872745000000
H	-0.131665000000	-0.985485000000	1.430110000000
H	0.076651000000	-0.274409000000	2.828172000000

O	-2.493531000000	-0.822152000000	-0.830710000000
H	-1.808179000000	-1.493309000000	-0.592711000000
H	-2.978228000000	-1.146571000000	-1.604000000000
O	1.894115000000	-1.659458000000	-0.992566000000
H	2.177801000000	-1.777066000000	-1.911623000000
H	2.177944000000	-0.762023000000	-0.700439000000
O	2.166840000000	0.789247000000	0.332418000000
H	3.008511000000	1.022922000000	0.757758000000
H	1.546780000000	0.521462000000	1.059623000000

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6b.	E[DF-MP2-F12]	-323113.66	
H	-0.105672000000	-1.544481000000	-2.586555000000
H	-1.227525000000	-0.721020000000	-1.568805000000
H	0.074939000000	-1.560077000000	-0.890997000000
H	0.390133000000	-0.139928000000	-1.744675000000
N	-0.213080000000	-1.000060000000	-1.726435000000
O	1.390806000000	1.253057000000	-1.162584000000
H	1.775690000000	1.886160000000	-1.790401000000
H	0.803329000000	1.782141000000	-0.534663000000
O	-0.296685000000	2.321793000000	0.549743000000
H	-0.731432000000	1.626098000000	1.100024000000
H	-0.181101000000	3.104656000000	1.109241000000
O	-1.448901000000	0.044163000000	1.645550000000
H	-1.848729000000	-0.033116000000	2.527188000000
H	-0.763349000000	-0.674551000000	1.577406000000
O	-2.672553000000	-0.384488000000	-0.819597000000
H	-2.513698000000	-0.150148000000	0.124665000000
H	-3.457539000000	0.098625000000	-1.118906000000
O	0.470347000000	-1.773517000000	0.923217000000
H	1.395375000000	-1.369109000000	0.916505000000
H	0.551970000000	-2.660760000000	1.309900000000
O	2.723227000000	-0.533783000000	0.459724000000
H	3.506967000000	-0.310111000000	0.983652000000
H	2.492283000000	0.248234000000	-0.096966000000

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6c.	E[DF-MP2-F12]	-323114.11	
H	-1.001182000000	0.169708000000	1.663443000000
H	-1.004988000000	1.650457000000	0.817160000000
H	-2.251411000000	0.494154000000	0.582618000000
H	-2.150178000000	1.357007000000	2.065974000000
N	-1.614138000000	0.933062000000	1.304376000000
O	1.563123000000	0.493987000000	-1.437008000000

H	2.162624000000	0.206720000000	-0.678064000000
H	2.130742000000	0.630272000000	-2.213359000000
O	0.110942000000	2.457697000000	-0.137004000000
H	0.183525000000	3.383022000000	-0.413757000000
H	0.680432000000	1.913910000000	-0.735119000000
O	2.722928000000	-0.461810000000	0.710513000000
H	1.969172000000	-0.768380000000	1.263829000000
H	3.401539000000	-0.106098000000	1.304114000000
O	0.169307000000	-1.327564000000	1.504635000000
H	-0.005927000000	-1.633949000000	0.574483000000
H	0.051259000000	-2.104423000000	2.076243000000
O	-2.782823000000	-0.528892000000	-0.658235000000
H	-3.511714000000	-0.477544000000	-1.294458000000
H	-2.016586000000	-0.956159000000	-1.105818000000
O	-0.246457000000	-1.526717000000	-1.209644000000
H	0.414462000000	-0.828327000000	-1.482525000000
H	-0.048963000000	-2.315401000000	-1.741451000000

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6d.	E[DF-MP2-F12]	-323111.06	
H	1.632974000000	-0.463414000000	1.553119000000
H	0.382239000000	0.658897000000	1.954272000000
H	2.008560000000	0.895335000000	2.493005000000
H	1.644587000000	1.021070000000	0.827130000000
N	1.426825000000	0.534886000000	1.731456000000
O	-0.927229000000	-2.311219000000	-0.334158000000
H	0.052858000000	-2.192022000000	-0.363898000000
H	-1.131491000000	-3.148807000000	-0.776362000000
O	1.795825000000	1.018708000000	-0.995289000000
H	0.903001000000	1.277181000000	-1.401180000000
H	2.472799000000	1.533519000000	-1.463395000000
O	-0.617138000000	1.599089000000	-1.806728000000
H	-1.323875000000	1.052620000000	-1.378871000000
H	-0.914051000000	1.810163000000	-2.704478000000
O	-1.200718000000	0.878709000000	2.034058000000
H	-1.773243000000	0.855899000000	2.815405000000
H	-1.735424000000	0.572325000000	1.253571000000
O	-2.250888000000	-0.035079000000	-0.308618000000
H	-3.206346000000	-0.117540000000	-0.460920000000
H	-1.858494000000	-0.960570000000	-0.380444000000
O	1.761026000000	-1.590866000000	-0.201436000000
H	1.918091000000	-0.782728000000	-0.755052000000
H	2.453013000000	-2.230864000000	-0.434737000000

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6e.	E[DF-MP2-F12]	-323113.62	
H	-1.990293000000	0.280928000000	-0.946742000000
H	-1.997768000000	-0.949553000000	0.234523000000
H	-1.990623000000	0.690045000000	0.708745000000
H	-3.389022000000	0.013950000000	-0.003473000000
N	-2.366092000000	0.008853000000	-0.001571000000
O	1.711100000000	1.169325000000	1.095808000000
H	2.411912000000	1.712682000000	1.493056000000
H	1.819797000000	1.245913000000	0.116742000000
O	-1.016166000000	-2.301357000000	0.626044000000
H	-0.037087000000	-2.198895000000	0.603201000000
H	-1.211553000000	-3.249818000000	0.641984000000
O	-0.993863000000	0.610534000000	-2.308501000000
H	-0.015674000000	0.580346000000	-2.203061000000
H	-1.184092000000	1.049617000000	-3.150574000000
O	-0.998139000000	1.705079000000	1.672950000000
H	-0.020175000000	1.616706000000	1.600015000000
H	-1.185874000000	2.203095000000	2.482187000000
O	1.716236000000	0.353347000000	-1.562201000000
H	2.418057000000	0.418671000000	-2.230996000000
H	1.813479000000	-0.535453000000	-1.142064000000
O	1.696117000000	-1.542782000000	0.478399000000
H	1.805718000000	-0.732879000000	1.033413000000
H	2.393569000000	-2.160491000000	0.754055000000

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6f.	E[DF-MP2-F12]	-323113.92	
H	1.045801000000	-0.852786000000	-0.623277000000
H	1.157087000000	-0.248923000000	0.904668000000
H	2.518775000000	-0.107316000000	-0.139184000000
H	1.074469000000	0.841440000000	-0.370706000000
N	1.475958000000	-0.094359000000	-0.068186000000
O	-0.583180000000	-0.684702000000	1.871866000000
H	-0.708747000000	-0.882097000000	2.813637000000
H	-1.226703000000	0.039619000000	1.639503000000
O	4.287072000000	-0.085010000000	-0.233715000000
H	4.861465000000	0.645393000000	0.046387000000
H	4.877854000000	-0.752444000000	-0.617195000000
O	-0.609184000000	-2.129641000000	-0.447761000000
H	-0.621915000000	-3.096691000000	-0.532153000000
H	-0.715844000000	-1.921220000000	0.514182000000
O	-2.126562000000	1.211165000000	0.655476000000
H	-2.869549000000	1.706710000000	1.036033000000

H	-2.486980000000	0.664463000000	-0.109460000000
O	-2.563820000000	-0.385263000000	-1.382837000000
H	-3.351408000000	-0.693089000000	-1.856024000000
H	-1.982374000000	-1.167076000000	-1.228742000000
O	0.183640000000	2.255811000000	-0.434809000000
H	-0.730228000000	2.106040000000	-0.087959000000
H	0.122862000000	2.919615000000	-1.138167000000

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6g. E[DF-MP2-F12] -323114.20

H	2.549265000000	0.664477000000	0.181893000000
H	1.353881000000	1.784920000000	-0.286979000000
H	2.927197000000	1.884349000000	-0.963791000000
H	1.890189000000	0.579832000000	-1.367400000000
N	2.201413000000	1.252056000000	-0.618773000000
O	0.237190000000	-1.879053000000	0.360899000000
H	-0.523499000000	-1.302063000000	0.644204000000
H	-0.040124000000	-2.796041000000	0.518040000000
O	2.489427000000	-0.580209000000	1.393737000000
H	1.788379000000	-1.238579000000	1.179749000000
H	3.161116000000	-1.027670000000	1.929324000000
O	1.054320000000	-0.764522000000	-2.068276000000
H	1.194040000000	-1.289585000000	-2.870117000000
H	0.730030000000	-1.372473000000	-1.363724000000
O	-0.202531000000	2.242098000000	0.277123000000
H	-0.779682000000	1.518300000000	0.619056000000
H	-0.461630000000	3.055740000000	0.734941000000
O	-1.678533000000	-0.032940000000	1.053914000000
H	-1.962656000000	-0.035732000000	1.983273000000
H	-2.517617000000	-0.075452000000	0.513748000000
O	-3.892712000000	-0.107861000000	-0.465694000000
H	-4.122921000000	0.573424000000	-1.116682000000
H	-4.653150000000	-0.707946000000	-0.417739000000

23

6h. E[DF-MP2-F12] -323113.47

H	-0.070675000000	0.102340000000	-1.430950000000
H	1.386096000000	0.964546000000	-1.482488000000
H	1.375361000000	-0.753222000000	-1.577419000000
H	0.799067000000	0.186380000000	-2.897305000000
N	0.875413000000	0.129039000000	-1.878875000000
O	-1.288392000000	-0.023425000000	-0.046543000000
H	-1.096325000000	-0.840749000000	0.460554000000
H	-2.267491000000	-0.006893000000	-0.219146000000

O	0.327005000000	1.292496000000	1.715792000000
H	-0.460710000000	1.087434000000	1.147412000000
H	0.015239000000	1.867737000000	2.433507000000
O	0.442582000000	-1.503335000000	1.663122000000
H	0.616829000000	-0.589856000000	1.992220000000
H	0.362423000000	-2.071245000000	2.446404000000
O	1.891969000000	2.178830000000	-0.408608000000
H	2.687633000000	2.724300000000	-0.322034000000
H	1.514083000000	2.041931000000	0.491251000000
O	-3.950362000000	0.036047000000	-0.540234000000
H	-4.598117000000	0.651848000000	-0.163531000000
H	-4.452230000000	-0.569142000000	-1.108193000000
O	1.822086000000	-2.104605000000	-0.661811000000
H	2.620311000000	-2.653377000000	-0.654877000000
H	1.481508000000	-2.053369000000	0.262971000000

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6i.	E[DF-MP2-F12]	-323113.00	
H	1.221725000000	-1.578016000000	-0.865269000000
H	-0.472855000000	-1.384645000000	-0.727021000000
H	0.218750000000	-2.924684000000	-0.498437000000
H	0.485622000000	-1.680920000000	0.657067000000
N	0.350732000000	-1.918913000000	-0.367070000000
O	2.077876000000	1.247840000000	0.675350000000
H	2.663812000000	1.933191000000	1.034541000000
H	1.266384000000	1.717613000000	0.314252000000
O	-0.211769000000	2.167561000000	-0.312735000000
H	-0.319603000000	2.948935000000	-0.876073000000
H	-0.761298000000	1.450456000000	-0.709074000000
O	0.850783000000	-0.798470000000	2.046008000000
H	1.096240000000	-1.056050000000	2.946933000000
H	1.394795000000	-0.010502000000	1.795378000000
O	-1.690275000000	-0.080052000000	-1.180151000000
H	-2.510592000000	-0.097102000000	-0.609555000000
H	-2.005665000000	-0.056427000000	-2.098839000000
O	2.493674000000	-0.576739000000	-1.338633000000
H	3.355804000000	-0.746209000000	-1.746410000000
H	2.605527000000	0.151729000000	-0.678641000000
O	-3.787389000000	-0.118188000000	0.494409000000
H	-4.653161000000	-0.543591000000	0.391094000000
H	-3.903818000000	0.573004000000	1.165560000000

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6j.	E[DF-MP2-F12]	-323112.70	
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H	2.341964000000	1.143288000000	0.422662000000
H	0.763868000000	1.896200000000	0.353148000000
H	1.021066000000	0.553684000000	1.317616000000
H	1.721695000000	2.033849000000	1.763414000000
N	1.471933000000	1.428497000000	0.977173000000
O	-1.885756000000	-0.335852000000	-0.678533000000
H	-1.841426000000	-0.803661000000	-1.529304000000
H	-2.842366000000	-0.377831000000	-0.394488000000
O	2.171385000000	-1.971706000000	-0.603797000000
H	2.520124000000	-2.873804000000	-0.536325000000
H	1.435941000000	-1.899990000000	0.045289000000
O	3.529989000000	0.328265000000	-0.328030000000
H	4.118229000000	0.603437000000	-1.046733000000
H	3.191035000000	-0.583999000000	-0.539729000000
O	-4.438564000000	-0.415865000000	0.155607000000
H	-4.986720000000	-1.204613000000	0.291852000000
H	-5.049949000000	0.337141000000	0.132634000000
O	0.077206000000	-1.096823000000	1.087652000000
H	-0.710567000000	-0.917376000000	0.505083000000
H	-0.253926000000	-1.603924000000	1.846633000000
O	-0.659845000000	2.176635000000	-0.568676000000
H	-1.208025000000	1.377158000000	-0.750051000000
H	-0.879783000000	2.843734000000	-1.235694000000

23

6k.	E[DF-MP2-F12]	-323113.30	
H	-2.393096000000	-0.667745000000	-1.909868000000
H	-3.022641000000	-0.555426000000	-0.350372000000
H	-1.387878000000	-1.056733000000	-0.602364000000
H	-1.834898000000	0.580040000000	-0.884119000000
N	-2.168988000000	-0.433830000000	-0.938890000000
O	-1.236610000000	2.073690000000	-0.623378000000
H	-1.258754000000	2.815592000000	-1.246094000000
H	-0.356754000000	2.118119000000	-0.149948000000
O	-4.524577000000	-0.646347000000	0.615161000000
H	-4.930209000000	0.105347000000	1.075545000000
H	-5.076495000000	-1.415395000000	0.827324000000
O	2.205068000000	-0.528122000000	0.904800000000
H	2.481929000000	-0.791924000000	1.797919000000
H	3.034260000000	-0.557599000000	0.350252000000
O	1.121738000000	2.040933000000	0.629670000000
H	1.291756000000	2.594302000000	1.406897000000
H	1.530851000000	1.160623000000	0.809857000000
O	0.010799000000	-1.895463000000	-0.094954000000

H	0.133983000000	-2.852232000000	-0.008755000000
H	0.826836000000	-1.465146000000	0.265222000000
O	4.467787000000	-0.540258000000	-0.547493000000
H	4.915769000000	0.265561000000	-0.848905000000
H	4.874613000000	-1.276035000000	-1.030808000000
23			
6l.	E[DF-MP2-F12]	-323112.99	
H	1.313576000000	0.324496000000	0.980127000000
H	2.735560000000	-0.331950000000	1.659657000000
H	2.006345000000	-1.060035000000	0.307799000000
H	2.850145000000	0.441108000000	0.163510000000
N	2.247052000000	-0.146534000000	0.779375000000
O	-1.476868000000	-1.759083000000	0.347479000000
H	-2.107539000000	-1.317916000000	-0.291447000000
H	-2.008829000000	-2.359518000000	0.893939000000
O	-0.306423000000	0.603983000000	1.290777000000
H	-0.881025000000	1.314218000000	0.941455000000
H	-0.792438000000	-0.235447000000	1.101500000000
O	-2.951085000000	-0.181395000000	-1.196163000000
H	-2.957146000000	0.734346000000	-0.843659000000
H	-3.724664000000	-0.283383000000	-1.770039000000
O	3.924246000000	1.418410000000	-0.889755000000
H	4.169579000000	1.203228000000	-1.803583000000
H	4.491337000000	2.163159000000	-0.634274000000
O	-2.428271000000	2.290303000000	0.118955000000
H	-2.221025000000	3.062581000000	-0.434486000000
H	-3.043134000000	2.622414000000	0.795685000000
O	1.112119000000	-2.342514000000	-0.361264000000
H	1.316167000000	-3.189158000000	-0.783892000000
H	0.133982000000	-2.300038000000	-0.218152000000

Table S10: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for $\text{NH}_4^+(\text{H}_2\text{O})_7$ isomers

26			
7a.	E[DF-MP2-F12]	-371026.07	
H	-0.927977000000	-1.416760000000	1.131619000000
H	-1.944274000000	-1.531809000000	-0.209097000000
H	-0.335671000000	-2.177429000000	-0.285221000000
H	-1.531568000000	-2.936790000000	0.677525000000
N	-1.190839000000	-2.036131000000	0.331028000000
O	0.595593000000	2.060039000000	-1.508160000000

H	-0.207575000000	2.053158000000	-0.932212000000
H	0.305592000000	2.318195000000	-2.396094000000
O	-0.493673000000	0.113472000000	2.097483000000
H	-0.743765000000	0.141139000000	3.035686000000
H	0.520945000000	0.186702000000	2.068737000000
O	1.085742000000	-2.202863000000	-1.132977000000
H	1.333499000000	-2.760578000000	-1.885115000000
H	1.644381000000	-1.384169000000	-1.168600000000
O	-1.555449000000	1.832088000000	0.266470000000
H	-1.198448000000	1.327006000000	1.049963000000
H	-1.910937000000	2.666267000000	0.614714000000
O	2.376478000000	0.208797000000	-0.929924000000
H	1.746174000000	0.935161000000	-1.236169000000
H	3.236385000000	0.390919000000	-1.342600000000
O	2.086903000000	0.177660000000	1.790890000000
H	2.343889000000	0.231591000000	0.833229000000
H	2.728901000000	0.700681000000	2.294168000000
O	-2.882551000000	-0.294272000000	-0.923773000000
H	-2.638418000000	0.599780000000	-0.587058000000
H	-3.789597000000	-0.249502000000	-1.260743000000

26

7b.	E[DF-MP2-F12]	-371026.33	
H	-1.770750000000	-2.923474000000	-0.552986000000
H	-1.799946000000	-1.555074000000	0.479898000000
H	-0.307830000000	-2.257478000000	0.006488000000
H	-1.233507000000	-1.367702000000	-1.108205000000
N	-1.286053000000	-2.062284000000	-0.288922000000
O	1.487800000000	-0.050207000000	2.111612000000
H	1.905126000000	0.053629000000	2.979749000000
H	1.451680000000	0.837638000000	1.685785000000
O	1.564468000000	-1.866674000000	0.216379000000
H	2.211125000000	-2.582492000000	0.328646000000
H	1.630744000000	-1.285211000000	1.036877000000
O	-1.016528000000	-0.074587000000	-2.080997000000
H	-1.337385000000	0.722864000000	-1.601724000000
H	-0.055600000000	0.081342000000	-2.206644000000
O	-2.421587000000	-0.242066000000	1.387897000000
H	-2.243710000000	0.644934000000	0.995037000000
H	-3.122961000000	-0.140117000000	2.047641000000
O	1.205079000000	2.054085000000	0.287919000000
H	1.718987000000	2.878353000000	0.298078000000
H	1.547885000000	1.513829000000	-0.475976000000
O	1.793128000000	0.172288000000	-1.603690000000

H	1.878901000000	-0.656022000000	-1.056940000000
H	2.522870000000	0.169066000000	-2.244459000000
O	-1.536807000000	1.929196000000	-0.122641000000
H	-2.001455000000	2.771221000000	-0.256683000000
H	-0.596228000000	2.154405000000	0.096054000000

26

7c.	E[DF-MP2-F12]	-371025.74	
H	0.615979000000	-0.982034000000	-1.371276000000
H	0.281636000000	-1.980736000000	-0.030776000000
H	0.912992000000	-2.687322000000	-1.445599000000
H	1.892232000000	-1.665135000000	-0.470289000000
N	0.924393000000	-1.862360000000	-0.841022000000
O	0.329156000000	0.542986000000	-1.904118000000
H	-0.555326000000	0.926255000000	-1.714194000000
H	0.961532000000	1.132177000000	-1.437199000000
O	-0.406638000000	1.254084000000	1.603732000000
H	-0.566716000000	1.610877000000	2.493160000000
H	-0.533700000000	0.265591000000	1.674073000000
O	-0.894183000000	-1.434979000000	1.364184000000
H	-1.020882000000	-2.011638000000	2.135321000000
H	-1.771800000000	-1.404732000000	0.866038000000
O	1.940457000000	1.691247000000	0.157033000000
H	2.354125000000	2.566125000000	0.235100000000
H	1.194375000000	1.667057000000	0.807445000000
O	-2.898773000000	-1.059049000000	-0.266784000000
H	-3.829983000000	-1.326580000000	-0.289152000000
H	-2.854480000000	-0.100438000000	-0.500117000000
O	3.155354000000	-0.802502000000	0.305628000000
H	2.969231000000	0.166126000000	0.303096000000
H	4.116892000000	-0.918655000000	0.327868000000
O	-2.041289000000	1.527958000000	-0.642017000000
H	-1.583362000000	1.680802000000	0.221143000000
H	-2.526167000000	2.340821000000	-0.858739000000

26

7d.	E[DF-MP2-F12]	-371025.46	
H	0.594167000000	-0.937065000000	-1.394849000000
H	0.251879000000	-1.961431000000	-0.070059000000
H	0.845629000000	-2.650336000000	-1.508496000000
H	1.858924000000	-1.673961000000	-0.518711000000
N	0.883786000000	-1.839550000000	-0.886044000000
O	0.341023000000	0.590335000000	-1.898770000000
H	-0.539509000000	0.969592000000	-1.677763000000

H	0.987947000000	1.160806000000	-1.428914000000
O	-0.813910000000	-1.439415000000	1.448901000000
H	-0.619597000000	-0.488660000000	1.662895000000
H	-0.747364000000	-1.928455000000	2.285348000000
O	-2.941502000000	-1.022582000000	-0.285723000000
H	-2.407712000000	-1.369161000000	0.465399000000
H	-3.831107000000	-1.401081000000	-0.214166000000
O	1.979941000000	1.678466000000	0.177674000000
H	2.418207000000	2.541360000000	0.255287000000
H	1.217177000000	1.687038000000	0.808839000000
O	-2.042432000000	1.439786000000	-0.612527000000
H	-2.562148000000	0.582267000000	-0.554374000000
H	-2.654557000000	2.134712000000	-0.903548000000
O	3.127452000000	-0.849403000000	0.294181000000
H	2.957150000000	0.122288000000	0.310283000000
H	4.087240000000	-0.980226000000	0.312427000000
O	-0.431317000000	1.317140000000	1.531554000000
H	-0.697002000000	1.825832000000	2.315743000000
H	-1.099859000000	1.528719000000	0.814634000000

26

7e.	E[DF-MP2-F12]	-371025.43	
H	0.526525000000	-2.945489000000	0.782563000000
H	0.787347000000	-1.759759000000	-0.407913000000
H	-0.820680000000	-2.032599000000	0.211835000000
H	0.416335000000	-1.300829000000	1.167838000000
N	0.230598000000	-2.027251000000	0.439589000000
O	0.906797000000	0.338579000000	1.935816000000
H	1.002937000000	0.396409000000	2.900742000000
H	1.837414000000	0.393122000000	1.541937000000
O	3.137725000000	0.174117000000	0.596135000000
H	2.863363000000	-0.096902000000	-0.314872000000
H	3.902657000000	0.763430000000	0.513157000000
O	0.176238000000	1.289491000000	-1.994136000000
H	-0.506217000000	1.398146000000	-2.673846000000
H	-0.190612000000	1.659245000000	-1.153847000000
O	-0.713477000000	2.033079000000	0.538605000000
H	-0.641968000000	2.965310000000	0.801699000000
H	-0.126480000000	1.516499000000	1.157527000000
O	-3.114811000000	0.706648000000	0.049201000000
H	-3.910040000000	1.029307000000	0.500158000000
H	-2.370390000000	1.291153000000	0.325568000000
O	1.754289000000	-0.766282000000	-1.583943000000
H	1.161538000000	0.001255000000	-1.868317000000

H	2.160533000000	-1.125426000000	-2.389357000000
O	-2.392556000000	-1.856124000000	0.002961000000
H	-2.983551000000	-2.395228000000	-0.543366000000
H	-2.756526000000	-0.922953000000	0.014259000000

26

7f.	E[DF-MP2-F12]	-371025.43	
H	1.401880000000	-0.872280000000	-0.604727000000
H	1.399170000000	0.848039000000	-0.626852000000
H	1.229166000000	0.003149000000	0.809506000000
H	2.753336000000	-0.000831000000	0.032063000000
N	1.720126000000	-0.004295000000	-0.102143000000
O	-1.745175000000	1.991534000000	0.486903000000
H	-1.329285000000	1.384372000000	1.155459000000
H	-2.109698000000	2.743135000000	0.982170000000
O	0.531898000000	-2.303106000000	-1.043749000000
H	0.506382000000	-2.805448000000	-1.871617000000
H	-0.374018000000	-2.332924000000	-0.653502000000
O	-0.492559000000	-0.041197000000	1.858997000000
H	-0.480366000000	-0.144817000000	2.824439000000
H	-0.992853000000	-0.826363000000	1.494811000000
O	0.527951000000	2.268664000000	-1.122222000000
H	-0.352741000000	2.347208000000	-0.686797000000
H	0.470875000000	2.725246000000	-1.974710000000
O	-1.811049000000	-1.910063000000	0.400721000000
H	-2.339983000000	-2.644267000000	0.752477000000
H	-2.442725000000	-1.299221000000	-0.093556000000
O	-3.136669000000	-0.012856000000	-0.845293000000
H	-2.850452000000	0.841867000000	-0.444559000000
H	-4.060631000000	0.085199000000	-1.119933000000
O	4.536598000000	0.003745000000	0.279222000000
H	5.126460000000	0.773891000000	0.262396000000
H	5.116633000000	-0.769658000000	0.361310000000

26

7g.	E[DF-MP2-F12]	-371024.54	
H	-2.458201000000	-0.181879000000	-0.170778000000
H	-0.972353000000	0.381568000000	-0.834598000000
H	-1.049661000000	0.000357000000	0.794345000000
H	-1.097084000000	-1.248306000000	-0.321433000000
N	-1.418174000000	-0.258280000000	-0.142570000000
O	-0.220819000000	-2.715318000000	-0.195407000000
H	-0.150118000000	-3.467507000000	-0.802130000000
H	0.689521000000	-2.512406000000	0.127505000000

O	0.411506000000	0.306201000000	2.046148000000
H	0.307566000000	0.171852000000	3.001968000000
H	1.102804000000	-0.345483000000	1.738230000000
O	0.323269000000	1.558727000000	-1.559643000000
H	0.115113000000	2.120713000000	-2.323415000000
H	0.458154000000	2.169295000000	-0.770992000000
O	2.462117000000	-0.180334000000	-1.492769000000
H	1.775378000000	0.514577000000	-1.654326000000
H	3.277822000000	0.108188000000	-1.928400000000
O	2.053900000000	-1.448128000000	0.771320000000
H	2.357037000000	-0.972356000000	-0.065476000000
H	2.838487000000	-1.865357000000	1.162137000000
O	0.545500000000	2.747838000000	0.775868000000
H	0.631776000000	1.999395000000	1.414464000000
H	1.103715000000	3.472731000000	1.094990000000
O	-4.243579000000	-0.073730000000	-0.224811000000
H	-4.862143000000	-0.816304000000	-0.311977000000
H	-4.795752000000	0.716830000000	-0.117775000000

26

7h.	E[DF-MP2-F12]	-371027.22	
H	1.075684000000	-0.206475000000	-0.792261000000
H	2.620551000000	-0.356824000000	-0.062479000000
H	1.580001000000	0.978548000000	0.283378000000
H	1.168997000000	-0.565656000000	0.855382000000
N	1.635120000000	-0.046521000000	0.069244000000
O	0.029247000000	-1.277569000000	1.974440000000
H	0.170730000000	-1.522676000000	2.901165000000
H	-0.894341000000	-0.937823000000	1.903514000000
O	-2.274059000000	-1.829698000000	-1.074227000000
H	-2.496901000000	-1.487301000000	-0.177096000000
H	-2.256706000000	-2.797196000000	-1.019263000000
O	-1.643341000000	1.802871000000	-0.409538000000
H	-2.284985000000	2.391866000000	-0.839881000000
H	-1.273277000000	1.215935000000	-1.128784000000
O	-0.478332000000	-0.123788000000	-1.933843000000
H	-1.116228000000	-0.879722000000	-1.729468000000
H	-0.393239000000	-0.083969000000	-2.900372000000
O	0.913705000000	2.597531000000	0.433765000000
H	1.111976000000	3.387527000000	0.957745000000
H	-0.052163000000	2.594447000000	0.248721000000
O	-2.458175000000	-0.262754000000	1.225764000000
H	-3.241511000000	-0.132606000000	1.784408000000
H	-2.297303000000	0.597002000000	0.752506000000

O	4.329716000000	-0.880409000000	-0.314285000000
H	4.710683000000	-1.755948000000	-0.142187000000
H	5.072101000000	-0.322951000000	-0.596347000000

26

7i. E[DF-MP2-F12] -371027.22

H	-1.140490000000	-0.575771000000	0.866646000000
H	-1.066234000000	-0.242991000000	-0.789743000000
H	-2.601810000000	-0.378553000000	-0.041767000000
H	-1.554170000000	0.958645000000	0.274919000000
N	-1.613889000000	-0.070766000000	0.075240000000
O	2.083725000000	-1.974649000000	-0.960430000000
H	2.468415000000	-1.530933000000	-0.168516000000
H	2.774202000000	-2.534918000000	-1.345759000000
O	-4.316970000000	-0.886724000000	-0.295691000000
H	-5.062455000000	-0.305675000000	-0.514954000000
H	-4.705916000000	-1.760510000000	-0.132927000000
O	-0.019155000000	-1.083151000000	2.096997000000
H	-0.031308000000	-1.865883000000	2.667623000000
H	0.926600000000	-0.863992000000	1.927240000000
O	0.494941000000	-0.132292000000	-1.964871000000
H	1.103222000000	-0.907199000000	-1.753699000000
H	0.374213000000	-0.119785000000	-2.928059000000
O	-0.925862000000	2.591670000000	0.380303000000
H	-1.101063000000	3.310048000000	1.006402000000
H	0.042959000000	2.577634000000	0.211841000000
O	2.504605000000	-0.249509000000	1.172982000000
H	3.263241000000	-0.094491000000	1.758669000000
H	2.330971000000	0.606249000000	0.697706000000
O	1.645667000000	1.807612000000	-0.454385000000
H	1.280996000000	1.217580000000	-1.173398000000
H	2.260249000000	2.422261000000	-0.888142000000

26

7j. E[DF-MP2-F12] -371025.43

H	0.114388000000	-1.537340000000	0.095327000000
H	1.424274000000	-1.506767000000	-1.020812000000
H	-0.033502000000	-2.383806000000	-1.368846000000
H	-0.051601000000	-0.681697000000	-1.341071000000
N	0.355912000000	-1.550570000000	-0.919938000000
O	0.464074000000	1.678990000000	0.906431000000
H	0.145467000000	2.506170000000	1.304179000000
H	0.072091000000	1.636159000000	-0.012384000000

O	-0.619335000000	1.052867000000	-1.496567000000
H	-0.430544000000	1.549885000000	-2.309326000000
H	-1.628563000000	1.084096000000	-1.347829000000
O	-2.872023000000	-1.229534000000	0.749686000000
H	-3.574571000000	-1.641075000000	1.276549000000
H	-2.102528000000	-1.102896000000	1.351351000000
O	3.154798000000	0.863498000000	0.770398000000
H	3.857093000000	1.526801000000	0.851129000000
H	2.298471000000	1.340760000000	0.858623000000
O	-3.091053000000	0.982531000000	-0.768478000000
H	-3.908635000000	1.100353000000	-1.274784000000
H	-3.192255000000	0.164645000000	-0.208869000000
O	2.974415000000	-1.079936000000	-1.062045000000
H	3.757007000000	-1.643696000000	-1.152867000000
H	3.190284000000	-0.360218000000	-0.403877000000
O	-0.318111000000	-0.798173000000	1.761815000000
H	0.068410000000	-1.111435000000	2.595875000000
H	-0.038793000000	0.152101000000	1.657274000000

26

7k.	E[DF-MP2-F12]	-371023.97	
H	0.247383000000	3.127450000000	0.182546000000
H	-0.117634000000	1.793561000000	-0.823058000000
H	1.371234000000	1.855877000000	0.049651000000
H	-0.098278000000	1.620205000000	0.885536000000
N	0.351702000000	2.115096000000	0.074320000000
O	0.141939000000	-1.753163000000	0.474334000000
H	-0.024731000000	-1.091396000000	1.183450000000
H	1.101902000000	-1.739823000000	0.284270000000
O	3.012693000000	-1.635772000000	-0.084350000000
H	3.523802000000	-2.142112000000	0.570825000000
H	3.250152000000	-2.022886000000	-0.944735000000
O	-0.787734000000	1.038805000000	-2.158325000000
H	-1.239213000000	1.456930000000	-2.906798000000
H	-1.247650000000	0.177144000000	-1.981131000000
O	-0.819504000000	0.428986000000	1.989720000000
H	-0.827343000000	0.521179000000	2.955850000000
H	-1.775688000000	0.287089000000	1.695835000000
O	-1.824640000000	-1.308103000000	-1.213963000000
H	-2.123688000000	-2.073721000000	-1.729882000000
H	-1.041007000000	-1.611115000000	-0.653962000000
O	2.960047000000	1.184344000000	0.132340000000
H	3.814641000000	1.625026000000	0.012105000000
H	3.115597000000	0.218997000000	0.028897000000

O	-3.122965000000	0.043575000000	0.796918000000
H	-2.893974000000	-0.540857000000	0.031665000000
H	-3.976102000000	-0.256598000000	1.145305000000
26			
7l.	E[DF-MP2-F12]	-371026.96	
H	0.766252000000	-1.728372000000	-2.133525000000
H	1.718962000000	-1.438446000000	-0.722430000000
H	0.629676000000	-0.256573000000	-1.305989000000
H	-0.006246000000	-1.681679000000	-0.624319000000
N	0.771074000000	-1.289517000000	-1.208754000000
O	3.009420000000	1.333561000000	0.349758000000
H	3.226246000000	1.920206000000	1.089786000000
H	2.137962000000	1.619580000000	-0.003846000000
O	0.558458000000	1.571755000000	-1.046919000000
H	0.634460000000	2.160129000000	-1.816294000000
H	-0.310285000000	1.799470000000	-0.610100000000
O	-1.443898000000	-1.970190000000	0.433682000000
H	-1.654210000000	-2.847030000000	0.793388000000
H	-1.298229000000	-1.353332000000	1.216545000000
O	3.053442000000	-1.328646000000	0.166107000000
H	3.201096000000	-0.357424000000	0.341651000000
H	3.919488000000	-1.733283000000	0.007297000000
O	-1.836204000000	1.811769000000	0.208560000000
H	-2.338785000000	2.635806000000	0.312495000000
H	-2.420450000000	1.162745000000	-0.292120000000
O	-2.961384000000	-0.214590000000	-1.052731000000
H	-3.878900000000	-0.376503000000	-1.320844000000
H	-2.652155000000	-1.013161000000	-0.560128000000
O	-0.960191000000	-0.001427000000	2.110491000000
H	-1.100748000000	0.093888000000	3.064776000000
H	-1.328789000000	0.802741000000	1.673350000000

Table S11: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for $\text{NH}_4^+(\text{H}_2\text{O})_8$ isomers

29			
8a.	E[DF-MP2-F12]	-418936.18	
H	0.202700000000	-1.429018000000	-3.026537000000
H	0.259457000000	-0.005197000000	-2.099298000000
H	-0.779909000000	-1.283020000000	-1.642085000000
H	0.915701000000	-1.443415000000	-1.429154000000
N	0.139478000000	-1.041473000000	-2.081461000000

O	-2.034284000000	-1.630604000000	-0.342474000000
H	-2.713405000000	-2.302435000000	-0.518246000000
H	-2.524378000000	-0.750201000000	-0.223715000000
O	-0.856743000000	2.282021000000	0.509219000000
H	-0.961042000000	3.172806000000	0.882594000000
H	-0.333326000000	1.727083000000	1.201097000000
O	0.570790000000	0.787302000000	2.040201000000
H	0.289747000000	-0.158113000000	2.060222000000
H	1.470503000000	0.785471000000	1.644267000000
O	-0.137226000000	-1.910147000000	1.646530000000
H	-0.311578000000	-2.524024000000	2.378513000000
H	-0.932501000000	-1.932570000000	1.052404000000
O	1.914703000000	-1.871668000000	-0.296199000000
H	1.374397000000	-2.081813000000	0.499708000000
H	2.444974000000	-1.078650000000	-0.050932000000
O	2.757746000000	0.753771000000	0.228031000000
H	3.645921000000	1.139161000000	0.301644000000
H	2.282353000000	1.245394000000	-0.485191000000
O	-3.029761000000	0.773285000000	-0.155694000000
H	-3.875445000000	1.038447000000	0.236415000000
H	-2.344440000000	1.426802000000	0.145363000000
O	0.797038000000	1.721599000000	-1.540549000000
H	0.148502000000	2.079295000000	-0.862439000000
H	0.907327000000	2.419824000000	-2.206916000000

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8b.	E[DF-MP2-F12]	-418934.86	
H	-3.983035000000	-0.063633000000	0.026066000000
H	-2.602184000000	0.392704000000	-0.872545000000
H	-2.561761000000	0.484496000000	0.815436000000
H	-2.565144000000	-1.044569000000	0.050957000000
N	-2.959907000000	-0.058049000000	0.004296000000
O	0.194610000000	2.284332000000	-0.155370000000
H	0.456311000000	3.218587000000	-0.114976000000
H	-0.333344000000	2.096195000000	0.671046000000
O	1.897642000000	-0.038953000000	-0.000160000000
H	2.890856000000	-0.062253000000	-0.017117000000
H	1.621823000000	0.898160000000	-0.092777000000
O	0.164828000000	-0.866146000000	1.983744000000
H	-0.324873000000	-1.595947000000	1.543499000000
H	0.934831000000	-0.676953000000	1.388323000000
O	-1.304167000000	1.217428000000	1.845903000000
H	-0.704056000000	0.386981000000	2.017533000000
H	-1.494525000000	1.622590000000	2.707797000000

O	0.165257000000	-1.384320000000	-1.681060000000
H	0.922256000000	-0.973682000000	-1.189935000000
H	-0.287670000000	-0.628331000000	-2.107666000000
O	-1.443364000000	-2.324925000000	0.114701000000
H	-1.647965000000	-3.271788000000	0.052777000000
H	-0.800737000000	-2.091287000000	-0.647040000000
O	4.611668000000	-0.072496000000	-0.053218000000
H	5.123149000000	-0.413775000000	-0.803716000000
H	5.157925000000	-0.229421000000	0.733113000000
O	-1.376498000000	1.077609000000	-2.033224000000
H	-0.782772000000	1.674498000000	-1.500907000000
H	-1.579542000000	1.543530000000	-2.860464000000

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8c.	E[DF-MP2-F12]	-418936.48	
H	-0.770644000000	-1.144216000000	1.237413000000
H	0.750852000000	-0.779057000000	1.926735000000
H	-0.181190000000	0.429573000000	1.143124000000
H	-0.704364000000	-0.196615000000	2.650026000000
N	-0.233951000000	-0.422639000000	1.769780000000
O	2.511415000000	2.146748000000	-0.149039000000
H	3.037435000000	2.889306000000	-0.482707000000
H	2.910741000000	1.320880000000	-0.502482000000
O	-2.660196000000	1.860611000000	0.562346000000
H	-1.763652000000	2.044220000000	0.192233000000
H	-3.116258000000	2.710776000000	0.654647000000
O	0.302196000000	-0.718252000000	-1.912893000000
H	-0.347984000000	-1.310596000000	-1.436724000000
H	0.112599000000	-0.805393000000	-2.861255000000
O	-1.476604000000	-1.949154000000	-0.290397000000
H	-1.665854000000	-2.901543000000	-0.279841000000
H	-2.371224000000	-1.468167000000	-0.374831000000
O	-0.075362000000	1.520356000000	-0.216513000000
H	0.823472000000	1.958714000000	-0.195396000000
H	-0.035378000000	0.926950000000	-1.002020000000
O	2.873445000000	-0.544665000000	-0.913303000000
H	2.013856000000	-0.714508000000	-1.382170000000
H	3.564692000000	-0.967814000000	-1.448205000000
O	2.308651000000	-1.379922000000	1.681674000000
H	3.042255000000	-1.461416000000	2.309482000000
H	2.693674000000	-1.131879000000	0.805906000000
O	-3.609072000000	-0.489297000000	-0.309469000000
H	-4.353319000000	-0.457916000000	-0.928159000000
H	-3.397830000000	0.445780000000	-0.033480000000

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8d.	E[DF-MP2-F12]	-418936.88	
H	2.652573000000	-0.120105000000	-0.515570000000
H	3.555513000000	-1.455514000000	0.058336000000
H	2.209320000000	-0.916700000000	0.941334000000
H	1.985807000000	-1.717661000000	-0.543311000000
N	2.615579000000	-1.058840000000	-0.018063000000
O	-2.508379000000	0.396231000000	-1.644974000000
H	-2.335789000000	0.736831000000	-2.535669000000
H	-2.280614000000	1.109987000000	-1.001370000000
O	0.728780000000	-2.686420000000	-1.210027000000
H	-0.221292000000	-2.478586000000	-1.034209000000
H	0.754684000000	-3.309660000000	-1.950869000000
O	2.559239000000	1.396434000000	-1.149937000000
H	1.865724000000	2.040705000000	-0.833314000000
H	2.893527000000	1.729692000000	-1.995334000000
O	-1.485823000000	-0.546498000000	1.828426000000
H	-2.101145000000	-0.828839000000	2.525288000000
H	-1.658069000000	-1.148382000000	1.045687000000
O	-1.775646000000	1.901034000000	0.568967000000
H	-2.443521000000	2.485465000000	0.963949000000
H	-1.702376000000	1.112662000000	1.169801000000
O	1.266595000000	-0.587920000000	2.355062000000
H	0.282007000000	-0.603975000000	2.298925000000
H	1.503615000000	-0.705616000000	3.286855000000
O	0.644194000000	3.058150000000	-0.282786000000
H	0.885228000000	3.825868000000	0.257384000000
H	-0.193749000000	2.701284000000	0.092810000000
O	-1.839824000000	-1.865172000000	-0.518476000000
H	-2.113696000000	-1.060548000000	-1.068739000000
H	-2.559885000000	-2.511746000000	-0.605573000000

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8e.	E[DF-MP2-F12]	-418936.65	
H	-0.998271000000	0.886370000000	-1.562852000000
H	0.407072000000	1.864810000000	-1.555761000000
H	0.538847000000	0.197851000000	-1.257391000000
H	0.142423000000	0.741001000000	-2.827727000000
N	0.022020000000	0.918024000000	-1.827318000000
O	-2.365429000000	-2.018350000000	-0.919720000000
H	-3.123513000000	-2.583523000000	-1.133482000000
H	-2.685556000000	-1.082243000000	-0.934093000000
O	1.333703000000	-0.691817000000	0.082011000000

H	2.161364000000	-1.192719000000	-0.136150000000
H	0.695594000000	-1.336946000000	0.493038000000
O	-1.567169000000	0.613029000000	1.704573000000
H	-0.716964000000	1.088752000000	1.840461000000
H	-1.342965000000	-0.339086000000	1.808297000000
O	0.925107000000	3.143727000000	-0.583865000000
H	1.123702000000	2.814218000000	0.325633000000
H	1.343715000000	4.009546000000	-0.695166000000
O	-2.523956000000	0.709046000000	-0.703726000000
H	-2.231181000000	0.771667000000	0.274612000000
H	-3.279088000000	1.308173000000	-0.818578000000
O	-0.747415000000	-2.055015000000	1.181666000000
H	-1.401481000000	-2.222442000000	0.438185000000
H	-0.743475000000	-2.842956000000	1.747732000000
O	3.638547000000	-2.000252000000	-0.584316000000
H	4.490222000000	-1.919040000000	-0.127069000000
H	3.712521000000	-2.788569000000	-1.144647000000
O	1.138675000000	1.534879000000	1.629210000000
H	1.679079000000	1.627115000000	2.430119000000
H	1.417315000000	0.689881000000	1.179391000000

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8f.	E[DF-MP2-F12]	-418937.90	
H	-1.475351000000	0.973863000000	-0.470497000000
H	-2.813537000000	0.064906000000	0.131983000000
H	-1.503737000000	-0.704287000000	-0.680288000000
H	-1.273097000000	-0.052540000000	0.870744000000
N	-1.785446000000	0.071259000000	-0.027640000000
O	-4.606924000000	0.040830000000	0.441635000000
H	-5.217641000000	0.792883000000	0.388621000000
H	-5.167807000000	-0.741422000000	0.563256000000
O	-0.613274000000	2.199396000000	-1.350766000000
H	0.367141000000	2.080446000000	-1.325046000000
H	-0.778257000000	3.153883000000	-1.374246000000
O	1.652694000000	-2.146779000000	1.214405000000
H	1.515062000000	-3.105729000000	1.248941000000
H	1.862943000000	-1.922863000000	0.274197000000
O	1.996131000000	-1.205136000000	-1.384359000000
H	2.727289000000	-1.527063000000	-1.936164000000
H	2.106896000000	-0.212524000000	-1.318270000000
O	2.061898000000	1.479465000000	-0.984671000000
H	2.768044000000	2.024118000000	-1.369172000000
H	2.100882000000	1.616116000000	0.019203000000
O	-0.687211000000	-1.871993000000	-1.694094000000

H	0.280707000000	-1.693860000000	-1.771610000000
H	-0.990389000000	-2.150689000000	-2.571528000000
O	1.848616000000	1.738173000000	1.609096000000
H	1.216677000000	1.054095000000	1.951978000000
H	2.576735000000	1.792523000000	2.246733000000
O	0.067661000000	-0.286941000000	2.185659000000
H	-0.187181000000	-0.435095000000	3.110837000000
H	0.626017000000	-1.081695000000	1.908569000000

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8g.	E[DF-MP2-F12]	-418937.96	
H	-0.694507000000	-1.120918000000	-1.499612000000
H	1.038251000000	-1.397199000000	-1.364368000000
H	0.434555000000	0.151519000000	-1.679666000000
H	0.183070000000	-0.547494000000	-0.178976000000
N	0.229157000000	-0.743830000000	-1.216074000000
O	2.680858000000	-1.885335000000	-1.044747000000
H	3.236200000000	-2.673252000000	-1.136578000000
H	3.034776000000	-1.345908000000	-0.302119000000
O	-1.846814000000	-2.015219000000	1.515588000000
H	-2.318254000000	-2.332170000000	2.300118000000
H	-1.118978000000	-1.424997000000	1.819289000000
O	1.572178000000	1.908775000000	-0.746685000000
H	0.829989000000	2.316405000000	-0.227987000000
H	1.953853000000	2.616796000000	-1.289891000000
O	2.893715000000	0.141307000000	0.886511000000
H	2.632089000000	0.905405000000	0.307926000000
H	3.673986000000	0.424302000000	1.390070000000
O	0.180196000000	-0.159076000000	1.531105000000
H	-0.116834000000	0.785501000000	1.536287000000
H	1.153871000000	-0.139891000000	1.681281000000
O	-0.637485000000	2.365857000000	0.794949000000
H	-1.425420000000	2.132201000000	0.214654000000
H	-0.895156000000	3.126080000000	1.340412000000
O	-2.562763000000	-1.254236000000	-0.913998000000
H	-3.245732000000	-1.789965000000	-1.347912000000
H	-2.456096000000	-1.615691000000	0.017593000000
O	-2.474066000000	1.481454000000	-0.892321000000
H	-2.694701000000	0.513799000000	-0.895065000000
H	-3.255612000000	1.954069000000	-1.216168000000

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8h.	E[DF-MP2-F12]	-418936.67	
H	-0.277039000000	-0.979628000000	-2.665921000000

H	-0.202874000000	-0.964106000000	-0.943248000000
H	0.266302000000	0.421601000000	-1.844527000000
H	-1.363213000000	-0.031641000000	-1.750322000000
N	-0.392695000000	-0.397336000000	-1.832211000000
O	-0.736937000000	2.312940000000	0.635180000000
H	-0.868680000000	3.229744000000	0.928832000000
H	-0.015644000000	2.336189000000	-0.063219000000
O	0.586453000000	0.414006000000	2.218119000000
H	0.048832000000	1.174914000000	1.887029000000
H	0.555840000000	0.442508000000	3.188127000000
O	-2.692747000000	0.801619000000	-0.623768000000
H	-3.463797000000	1.291482000000	-0.952920000000
H	-2.150355000000	1.449762000000	-0.102147000000
O	-0.098425000000	-1.701946000000	0.555173000000
H	-1.048440000000	-1.964317000000	0.684950000000
H	0.103654000000	-1.053370000000	1.275322000000
O	1.170094000000	1.824809000000	-1.191224000000
H	1.629617000000	2.478481000000	-1.743271000000
H	1.892021000000	1.334781000000	-0.621091000000
O	2.368029000000	-2.069563000000	-0.573149000000
H	3.003469000000	-2.802342000000	-0.570255000000
H	1.578372000000	-2.368267000000	-0.071142000000
O	-2.764580000000	-1.830255000000	0.424299000000
H	-3.524500000000	-2.265619000000	0.838728000000
H	-3.028284000000	-0.910809000000	0.204578000000
O	2.737026000000	0.492110000000	0.302118000000
H	2.284688000000	0.466588000000	1.171118000000
H	2.777594000000	-0.454349000000	0.000873000000

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8i.	E[DF-MP2-F12]	-418935.44	
H	-0.390983000000	-1.538842000000	1.739294000000
H	-0.291232000000	0.090618000000	2.199504000000
H	0.544413000000	-1.102977000000	3.088405000000
H	1.074906000000	-0.725731000000	1.478662000000
N	0.234429000000	-0.815991000000	2.156668000000
O	-1.328890000000	0.761007000000	-2.065252000000
H	-2.037681000000	0.496173000000	-1.377897000000
H	-1.796101000000	0.997729000000	-2.883003000000
O	-2.863275000000	0.022659000000	-0.103382000000
H	-2.599801000000	-0.898657000000	0.113051000000
H	-2.570806000000	0.558184000000	0.668665000000
O	2.083688000000	-0.818383000000	0.278388000000
H	1.628780000000	-0.972265000000	-0.578336000000

H	2.905992000000	-0.298399000000	0.106968000000
O	-1.333044000000	1.498442000000	1.789711000000
H	-0.890079000000	2.043948000000	1.067673000000
H	-1.687808000000	2.122758000000	2.442780000000
O	-0.150641000000	2.557777000000	-0.327037000000
H	-0.514594000000	2.064607000000	-1.105413000000
H	-0.096115000000	3.490278000000	-0.586240000000
O	-1.341674000000	-2.351446000000	0.338788000000
H	-1.660471000000	-3.268426000000	0.336394000000
H	-0.792576000000	-2.232714000000	-0.483041000000
O	0.201338000000	-1.441290000000	-1.740046000000
H	0.444583000000	-1.928128000000	-2.544119000000
H	-0.308855000000	-0.632226000000	-2.035942000000
O	4.420887000000	0.510812000000	-0.213770000000
H	5.282692000000	0.067407000000	-0.177916000000
H	4.607613000000	1.461983000000	-0.225352000000

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8j.	E[DF-MP2-F12]	-418934.82	
H	-2.069438000000	1.474860000000	-0.557474000000
H	-0.399480000000	1.757137000000	-0.108370000000
H	-0.843908000000	0.378565000000	-1.010291000000
H	-0.876981000000	1.911204000000	-1.721593000000
N	-1.042263000000	1.395531000000	-0.852610000000
O	1.311200000000	-2.091626000000	0.540645000000
H	1.475159000000	-3.020342000000	0.772248000000
H	2.104159000000	-1.774708000000	-0.014020000000
O	-0.796519000000	-1.453801000000	-1.022047000000
H	-0.045695000000	-1.787327000000	-0.447810000000
H	-0.670427000000	-1.877573000000	-1.887283000000
O	2.448261000000	1.554119000000	-1.146735000000
H	3.053195000000	2.229084000000	-1.491820000000
H	2.095991000000	1.897606000000	-0.288896000000
O	3.122041000000	-1.061217000000	-1.000866000000
H	2.984291000000	-0.077945000000	-1.088782000000
H	4.077950000000	-1.218322000000	-0.983675000000
O	-3.373305000000	-1.434891000000	0.149382000000
H	-3.992020000000	-2.155231000000	-0.044184000000
H	-2.516369000000	-1.668356000000	-0.273191000000
O	0.926494000000	2.099677000000	1.072334000000
H	0.936906000000	2.892089000000	1.632703000000
H	0.953061000000	1.301578000000	1.692083000000
O	0.844848000000	-0.143350000000	2.424362000000
H	1.137243000000	-0.326205000000	3.329716000000

H	1.061160000000	-0.939401000000	1.875467000000
O	-3.632546000000	1.197691000000	-0.232579000000
H	-4.243165000000	1.677817000000	0.346087000000
H	-3.729591000000	0.223935000000	-0.038606000000

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8k.	E[DF-MP2-F12]	-418934.69	
H	-0.165834000000	2.436506000000	-0.329662000000
H	-0.532351000000	1.170315000000	-1.433874000000
H	-1.819108000000	1.910842000000	-0.578269000000
H	-0.968934000000	2.755740000000	-1.803047000000
N	-0.872421000000	2.073430000000	-1.046144000000
O	1.308624000000	-2.703538000000	1.005604000000
H	1.947201000000	-2.100215000000	0.556756000000
H	1.540880000000	-2.732386000000	1.946108000000
O	-3.161323000000	1.512225000000	0.252097000000
H	-4.066540000000	1.822435000000	0.101601000000
H	-3.221880000000	0.567338000000	0.572044000000
O	0.989776000000	2.946472000000	0.691124000000
H	1.799704000000	2.378200000000	0.832310000000
H	0.801509000000	3.386487000000	1.533681000000
O	-0.994377000000	-2.398481000000	-0.196976000000
H	-0.171889000000	-2.580559000000	0.363362000000
H	-1.279299000000	-3.261332000000	-0.542052000000
O	2.602386000000	-0.920169000000	-0.697522000000
H	3.283148000000	-1.282358000000	-1.288303000000
H	1.798180000000	-0.761719000000	-1.259108000000
O	-3.142006000000	-1.050157000000	0.986215000000
H	-2.384195000000	-1.592902000000	0.664227000000
H	-3.369376000000	-1.373178000000	1.870887000000
O	0.107377000000	-0.588081000000	-1.875437000000
H	-0.008469000000	-0.833745000000	-2.808606000000
H	-0.386805000000	-1.285584000000	-1.346612000000
O	3.074245000000	1.291309000000	0.957093000000
H	3.985617000000	1.621754000000	0.953858000000
H	3.047776000000	0.523698000000	0.340099000000

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8l.	E[DF-MP2-F12]	-418936.62	
H	1.452416000000	0.426987000000	3.132833000000
H	2.198268000000	0.903824000000	1.664054000000
H	1.839117000000	-0.770485000000	1.970102000000
H	0.607142000000	0.341851000000	1.647921000000
N	1.533927000000	0.227452000000	2.133051000000

O	1.893035000000	-2.374922000000	1.396834000000
H	1.328655000000	-2.472616000000	0.591485000000
H	2.624518000000	-3.005321000000	1.320077000000
O	1.687297000000	-0.680839000000	-2.539872000000
H	1.820362000000	-1.005311000000	-3.442835000000
H	1.129913000000	-1.342418000000	-2.062840000000
O	-0.571802000000	0.361697000000	0.295640000000
H	-0.184802000000	0.975863000000	-0.378189000000
H	-1.523707000000	0.643326000000	0.449560000000
O	0.118601000000	-2.036040000000	-0.707046000000
H	-0.312152000000	-1.206094000000	-0.340510000000
H	-0.597095000000	-2.665746000000	-0.890176000000
O	-5.268500000000	-0.284567000000	-0.180033000000
H	-5.855156000000	-0.798428000000	0.397015000000
H	-5.822212000000	0.019624000000	-0.916309000000
O	-3.078677000000	1.086540000000	0.708440000000
H	-3.374387000000	1.838759000000	1.241183000000
H	-3.890820000000	0.611416000000	0.402202000000
O	2.830077000000	2.044876000000	0.582329000000
H	3.741064000000	2.316108000000	0.396213000000
H	2.339045000000	2.033720000000	-0.277278000000
O	1.085407000000	1.674028000000	-1.511672000000
H	1.338887000000	0.865089000000	-2.052651000000
H	0.839950000000	2.371499000000	-2.140167000000

Table S12: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for $\text{NH}_4^+(\text{H}_2\text{O})_9$ isomers

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9a.	E[DF-MP2-F12]	-466849.66	
H	-1.612264000000	-3.009613000000	-1.406828000000
H	-0.764177000000	-1.488224000000	-1.384315000000
H	-1.935833000000	-1.882352000000	-0.164466000000
H	-0.437233000000	-2.675405000000	-0.218953000000
N	-1.209366000000	-2.289658000000	-0.801966000000
O	-2.714978000000	-0.785467000000	1.026297000000
H	-2.994633000000	0.028917000000	0.500459000000
H	-3.461918000000	-1.027698000000	1.596869000000
O	-3.133276000000	1.263317000000	-0.558166000000
H	-2.302649000000	1.752599000000	-0.785507000000
H	-3.868198000000	1.892025000000	-0.611277000000
O	2.611914000000	-0.941036000000	-0.931449000000
H	3.336427000000	-1.259720000000	-1.493723000000
H	2.933500000000	-0.084201000000	-0.499849000000

O	-0.609548000000	2.201595000000	-1.089883000000
H	-0.403333000000	2.984762000000	-1.625724000000
H	-0.103324000000	2.296692000000	-0.231460000000
O	3.170959000000	1.362818000000	0.183310000000
H	3.954597000000	1.593545000000	0.704484000000
H	2.379402000000	1.717837000000	0.664538000000
O	1.141121000000	-2.398251000000	0.794328000000
H	1.819443000000	-1.966660000000	0.198825000000
H	1.611531000000	-3.067073000000	1.317575000000
O	-0.166114000000	-0.215504000000	2.086975000000
H	0.342805000000	-0.997435000000	1.772264000000
H	-1.107484000000	-0.398304000000	1.856597000000
O	0.097345000000	-0.351202000000	-2.066279000000
H	-0.130151000000	0.582852000000	-1.842974000000
H	1.047874000000	-0.467374000000	-1.829126000000
O	0.743225000000	2.061801000000	1.245023000000
H	0.380871000000	1.186285000000	1.632370000000
H	0.655130000000	2.731593000000	1.942727000000

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9b.	E[DF-MP2-F12]	-466850.55	
H	-3.142688000000	-0.161396000000	-0.102215000000
H	-2.014171000000	1.112971000000	0.177103000000
H	-1.756334000000	-0.415719000000	0.873276000000
H	-1.549551000000	-0.223222000000	-0.778903000000
N	-2.142119000000	0.079395000000	0.045800000000
O	-0.354850000000	-1.311699000000	1.883116000000
H	-0.529490000000	-1.648631000000	2.776908000000
H	0.392456000000	-0.624077000000	1.977194000000
O	1.658174000000	0.345284000000	1.887333000000
H	2.352742000000	-0.091264000000	1.348131000000
H	1.531781000000	1.225039000000	1.463277000000
O	-1.401533000000	2.726888000000	0.384702000000
H	-0.427074000000	2.848557000000	0.283338000000
H	-1.816394000000	3.592445000000	0.256902000000
O	1.358000000000	2.587447000000	0.168099000000
H	1.946720000000	3.353016000000	0.267867000000
H	1.656787000000	2.102235000000	-0.647118000000
O	0.868665000000	-2.684028000000	-0.098701000000
H	0.372064000000	-2.365570000000	0.710271000000
H	0.811862000000	-3.652886000000	-0.110815000000
O	-4.879158000000	-0.634707000000	-0.396407000000
H	-5.646229000000	-0.477891000000	0.176330000000
H	-5.241396000000	-0.961699000000	-1.234967000000

O	-0.355292000000	-0.786496000000	-1.865398000000
H	0.056551000000	-1.588242000000	-1.476244000000
H	0.396642000000	-0.174981000000	-2.023111000000
O	2.058298000000	0.822169000000	-1.807156000000
H	2.528534000000	1.021233000000	-2.633145000000
H	2.595334000000	0.133872000000	-1.327986000000
O	3.063960000000	-1.093244000000	-0.156332000000
H	3.946786000000	-1.495783000000	-0.128108000000
H	2.399795000000	-1.836683000000	-0.162627000000

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9c.	E[DF-MP2-F12]	-466847.49	
H	-2.144561000000	-2.772661000000	-1.507136000000
H	-1.270661000000	-2.314950000000	-0.116214000000
H	-0.935159000000	-1.530109000000	-1.603590000000
H	-2.385930000000	-1.221185000000	-0.772030000000
N	-1.695690000000	-1.999431000000	-1.010782000000
O	-1.130427000000	1.967678000000	-1.516440000000
H	-0.664411000000	2.287750000000	-0.705063000000
H	-1.284966000000	2.744406000000	-2.078244000000
O	-0.403268000000	-2.013919000000	1.582646000000
H	-0.437353000000	-2.718311000000	2.250981000000
H	0.588712000000	-1.860087000000	1.388855000000
O	2.088613000000	-1.519418000000	1.053531000000
H	2.332743000000	-0.582194000000	1.226505000000
H	2.372168000000	-1.638618000000	0.123985000000
O	0.076826000000	2.328056000000	0.984834000000
H	-0.019005000000	3.176405000000	1.449100000000
H	-0.472872000000	1.667729000000	1.501288000000
O	-3.051385000000	0.241490000000	-0.297248000000
H	-2.785931000000	0.406302000000	0.631841000000
H	-2.603570000000	0.953591000000	-0.807147000000
O	-1.468965000000	0.413813000000	2.127615000000
H	-1.077443000000	-0.506470000000	2.044675000000
H	-1.794330000000	0.494964000000	3.039083000000
O	0.071388000000	-0.476670000000	-2.335959000000
H	-0.249241000000	0.444947000000	-2.214880000000
H	1.042049000000	-0.460813000000	-2.158366000000
O	2.733796000000	-0.423771000000	-1.513175000000
H	3.479443000000	-0.437429000000	-2.134476000000
H	2.872788000000	0.345116000000	-0.911285000000
O	2.612247000000	1.234653000000	0.721026000000
H	3.312124000000	1.764801000000	1.134931000000
H	1.764627000000	1.737530000000	0.838026000000

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9d.	E[DF-MP2-F12]	-466848.38	
H	-2.458779000000	2.125821000000	2.083628000000
H	-2.516742000000	0.542055000000	1.477965000000
H	-1.842898000000	1.752876000000	0.501587000000
H	-1.008452000000	1.195587000000	1.910614000000
N	-1.975860000000	1.425086000000	1.516104000000
O	0.621898000000	-1.047021000000	-1.402307000000
H	0.842188000000	-0.083507000000	-1.494516000000
H	-0.245338000000	-1.140815000000	-1.860218000000
O	-2.112094000000	-0.702957000000	-1.953184000000
H	-2.710744000000	-0.979127000000	-2.665981000000
H	-2.512150000000	-1.017886000000	-1.102756000000
O	-0.088885000000	-1.919004000000	1.053303000000
H	0.264392000000	-1.644112000000	0.154700000000
H	0.340846000000	-2.760168000000	1.278945000000
O	-1.519096000000	1.957564000000	-1.081128000000
H	-1.803404000000	1.159945000000	-1.581509000000
H	-0.552717000000	2.035376000000	-1.250027000000
O	1.266832000000	1.651833000000	-1.432630000000
H	1.733010000000	2.071298000000	-2.174065000000
H	1.899203000000	1.647201000000	-0.661998000000
O	-2.693114000000	-1.308150000000	0.697983000000
H	-1.815631000000	-1.723595000000	0.930452000000
H	-3.381193000000	-1.922416000000	1.001717000000
O	0.455843000000	0.540017000000	2.312169000000
H	0.394442000000	-0.414373000000	2.080150000000
H	1.300434000000	0.836164000000	1.904374000000
O	2.787730000000	1.041513000000	0.716169000000
H	3.079232000000	0.134779000000	0.411736000000
H	3.572288000000	1.484779000000	1.077687000000
O	3.139748000000	-1.440880000000	-0.291545000000
H	3.942088000000	-1.873921000000	-0.621946000000
H	2.440047000000	-1.584866000000	-0.963909000000

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9e.	E[DF-MP2-F12]	-466848.62	
H	-0.076477000000	-0.112368000000	-1.953912000000
H	-0.803641000000	-1.557798000000	-1.268949000000
H	-0.105525000000	-1.524535000000	-2.886183000000
H	0.897852000000	-1.443166000000	-1.520699000000
N	-0.012868000000	-1.151013000000	-1.937996000000
O	2.136280000000	-1.935056000000	-0.194006000000

H	2.808518000000	-1.180677000000	-0.151819000000
H	2.646057000000	-2.749749000000	-0.334158000000
O	1.798609000000	2.199340000000	0.201263000000
H	2.065110000000	3.126189000000	0.315987000000
H	1.139295000000	2.184306000000	-0.542836000000
O	-0.266496000000	1.770194000000	-1.578348000000
H	-1.041526000000	1.897519000000	-0.947551000000
H	-0.442105000000	2.341003000000	-2.344797000000
O	-0.173266000000	1.032369000000	1.939607000000
H	-0.020315000000	0.058096000000	1.993934000000
H	0.648912000000	1.421541000000	1.571708000000
O	0.233510000000	-1.741444000000	1.785646000000
H	1.016267000000	-1.919811000000	1.199744000000
H	0.369519000000	-2.254103000000	2.599019000000
O	-1.729895000000	-2.109094000000	-0.234510000000
H	-1.263731000000	-2.102874000000	0.630440000000
H	-2.548047000000	-1.542258000000	-0.138690000000
O	3.640820000000	0.204465000000	-0.216773000000
H	4.520243000000	0.342773000000	0.165843000000
H	3.103646000000	1.015629000000	-0.032421000000
O	-3.693501000000	-0.320521000000	-0.200216000000
H	-4.591502000000	-0.376079000000	0.159315000000
H	-3.308981000000	0.541881000000	0.085534000000
O	-2.079615000000	1.858285000000	0.390941000000
H	-2.451942000000	2.688728000000	0.730239000000
H	-1.403110000000	1.534540000000	1.087397000000

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9f.	E[DF-MP2-F12]	-466846.82	
H	-1.684200000000	2.316976000000	-0.796116000000
H	-2.433514000000	0.736755000000	-0.767344000000
H	-2.834679000000	1.870243000000	-2.001293000000
H	-1.319864000000	1.118014000000	-1.972090000000
N	-2.082385000000	1.525517000000	-1.399876000000
O	-1.115170000000	-0.798741000000	2.424273000000
H	-0.464087000000	-1.480476000000	2.125479000000
H	-1.404002000000	-1.055310000000	3.314931000000
O	-0.840898000000	3.271545000000	0.189729000000
H	-0.356253000000	2.703740000000	0.866102000000
H	-1.059096000000	4.118544000000	0.604958000000
O	4.427165000000	0.548807000000	-0.417923000000
H	5.211127000000	-0.013202000000	-0.518993000000
H	4.748338000000	1.394295000000	-0.066371000000
O	-0.962741000000	-2.487108000000	-1.166861000000

H	-0.345839000000	-2.652704000000	-0.402760000000
H	-1.173938000000	-3.351061000000	-1.556030000000
O	0.412464000000	1.530508000000	1.714451000000
H	-0.155906000000	0.853937000000	2.141927000000
H	1.008822000000	1.011749000000	1.127651000000
O	-2.734489000000	-0.617111000000	0.123628000000
H	-2.335280000000	-0.639095000000	1.025194000000
H	-2.360630000000	-1.405232000000	-0.325127000000
O	0.712484000000	-2.320169000000	0.974871000000
H	1.306921000000	-3.007547000000	1.316518000000
H	1.292915000000	-1.572704000000	0.625666000000
O	1.828901000000	-0.160914000000	-0.080716000000
H	1.386045000000	-0.066834000000	-0.958197000000
H	2.790651000000	0.052642000000	-0.207496000000
O	0.095018000000	-0.237199000000	-2.320298000000
H	-0.286037000000	-1.127649000000	-2.091632000000
H	0.463326000000	-0.320655000000	-3.215077000000

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9g.	E[DF-MP2-F12]	-466848.01	
H	0.104381000000	1.034667000000	0.982689000000
H	-0.901023000000	2.239831000000	0.337394000000
H	0.845705000000	2.253611000000	0.058114000000
H	-0.187299000000	1.104185000000	-0.675679000000
N	-0.032721000000	1.679821000000	0.175356000000
O	2.153151000000	-1.806221000000	0.628523000000
H	2.658037000000	-2.555155000000	0.986173000000
H	1.458080000000	-2.197195000000	0.024177000000
O	-3.237973000000	-0.068292000000	-0.595458000000
H	-2.548806000000	-0.099066000000	-1.306060000000
H	-4.072015000000	-0.354768000000	-1.002198000000
O	-1.730054000000	-1.896818000000	0.975827000000
H	-1.203600000000	-1.369020000000	1.616542000000
H	-2.414601000000	-1.291136000000	0.608999000000
O	-0.845284000000	-0.164199000000	-1.984837000000
H	-0.656221000000	0.003562000000	-2.922507000000
H	-0.463531000000	-1.061022000000	-1.771583000000
O	0.361113000000	-0.386198000000	2.161129000000
H	0.545926000000	-0.220511000000	3.099951000000
H	1.126285000000	-0.910102000000	1.804003000000
O	-2.653003000000	2.440170000000	0.509787000000
H	-3.295165000000	3.148769000000	0.661459000000
H	-3.138695000000	1.661553000000	0.155974000000
O	3.445062000000	0.227664000000	-0.853843000000

H	3.138084000000	-0.538416000000	-0.316387000000
H	4.325502000000	-0.002758000000	-1.186614000000
O	2.490758000000	2.629673000000	-0.042697000000
H	3.003068000000	3.426498000000	-0.241300000000
H	3.006894000000	1.843642000000	-0.360079000000
O	-0.012172000000	-2.491994000000	-0.848401000000
H	-0.134311000000	-3.367688000000	-1.250644000000
H	-0.740431000000	-2.378515000000	-0.130158000000

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9h.	E[DF-MP2-F12]	-466848.85	
H	-2.530921000000	-0.355564000000	1.331366000000
H	-4.184678000000	-0.625527000000	1.021318000000
H	-3.332093000000	0.649833000000	0.242811000000
H	-3.009026000000	-0.990135000000	-0.175192000000
N	-3.290033000000	-0.343622000000	0.613215000000
O	-0.816929000000	0.019410000000	1.997286000000
H	-0.502795000000	0.632133000000	1.251315000000
H	-0.754192000000	0.535527000000	2.817885000000
O	0.227404000000	-0.663588000000	-1.935625000000
H	1.011119000000	-1.122148000000	-1.509096000000
H	0.497151000000	-0.435796000000	-2.840490000000
O	2.224064000000	-1.756365000000	-0.493565000000
H	2.626533000000	-2.590308000000	-0.786708000000
H	1.756615000000	-1.961893000000	0.381560000000
O	-2.245566000000	-1.783099000000	-1.453715000000
H	-2.443319000000	-2.613621000000	-1.910429000000
H	-1.341580000000	-1.492157000000	-1.732346000000
O	-0.217412000000	1.447080000000	-0.145478000000
H	0.638073000000	1.989421000000	-0.119546000000
H	-0.070921000000	0.785117000000	-0.867263000000
O	0.850542000000	-2.163146000000	1.709196000000
H	0.259191000000	-1.398769000000	1.933090000000
H	1.256815000000	-2.456504000000	2.539068000000
O	2.121924000000	2.605888000000	-0.203186000000
H	2.825374000000	1.912721000000	-0.069447000000
H	2.425797000000	3.416723000000	0.230500000000
O	3.785279000000	0.511976000000	0.115637000000
H	4.702301000000	0.478605000000	-0.195893000000
H	3.367419000000	-0.342719000000	-0.142186000000
O	-2.823213000000	2.198986000000	-0.171428000000
H	-1.838153000000	2.169956000000	-0.287584000000
H	-3.177223000000	2.883316000000	-0.758216000000

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9i.	E[DF-MP2-F12]	-466847.35	
H	-1.781223000000	-0.201975000000	1.795767000000
H	-0.271578000000	-0.970915000000	2.083406000000
H	-0.410138000000	0.746301000000	2.178914000000
H	-1.171702000000	-0.195783000000	3.378820000000
N	-0.926735000000	-0.141883000000	2.386929000000
O	-1.181398000000	-2.563193000000	-0.654780000000
H	-1.376696000000	-3.386504000000	-1.130376000000
H	-0.673580000000	-1.943826000000	-1.295529000000
O	1.966905000000	-0.124147000000	-0.095535000000
H	1.728551000000	0.702399000000	0.386789000000
H	2.934674000000	-0.075265000000	-0.309027000000
O	0.717680000000	1.935277000000	1.381160000000
H	0.156179000000	2.497549000000	0.758262000000
H	1.222874000000	2.557251000000	1.929531000000
O	0.650230000000	-2.017036000000	1.420859000000
H	0.108561000000	-2.495307000000	0.751340000000
H	1.298671000000	-1.484987000000	0.890613000000
O	4.630571000000	0.020366000000	-0.665668000000
H	4.968397000000	0.161592000000	-1.564166000000
H	5.290176000000	-0.534779000000	-0.220559000000
O	0.079404000000	-0.765146000000	-2.014548000000
H	0.829547000000	-0.453970000000	-1.445698000000
H	-0.534215000000	-0.005160000000	-2.102133000000
O	-0.948610000000	3.156816000000	-0.240846000000
H	-1.401448000000	2.525008000000	-0.854952000000
H	-0.824684000000	3.988959000000	-0.721356000000
O	-2.847016000000	-0.713526000000	0.269085000000
H	-2.373322000000	-1.533378000000	-0.079915000000
H	-3.775832000000	-0.963908000000	0.403641000000
O	-2.091192000000	1.107031000000	-1.668536000000
H	-2.734202000000	1.261768000000	-2.379638000000
H	-2.534465000000	0.506565000000	-1.011770000000

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9j.	E[DF-MP2-F12]	-466847.64	
H	1.063314000000	-2.360014000000	0.734183000000
H	0.767582000000	-2.787506000000	2.356986000000
H	0.346440000000	-1.200226000000	1.769007000000
H	-0.519738000000	-2.608467000000	1.242958000000
N	0.423520000000	-2.261813000000	1.550170000000
O	-4.077507000000	1.588798000000	0.068875000000
H	-4.609549000000	2.257138000000	-0.390726000000

H	-4.511446000000	1.448285000000	0.925111000000
O	0.164278000000	0.361265000000	1.876370000000
H	0.959937000000	0.924512000000	1.724778000000
H	-0.494159000000	0.682546000000	1.208037000000
O	-1.960589000000	-2.740556000000	0.262298000000
H	-1.805979000000	-2.300454000000	-0.605965000000
H	-2.629890000000	-3.427890000000	0.129313000000
O	3.367703000000	-0.031850000000	-0.579086000000
H	3.044378000000	0.748311000000	-0.049814000000
H	3.974813000000	0.318078000000	-1.248417000000
O	0.536826000000	2.997019000000	-0.791348000000
H	0.266207000000	3.910963000000	-0.963108000000
H	-0.288796000000	2.455075000000	-0.680157000000
O	-1.397021000000	1.156321000000	-0.277452000000
H	-2.365485000000	1.330152000000	-0.159668000000
H	-1.314562000000	0.387181000000	-0.891143000000
O	2.262075000000	1.958688000000	0.887884000000
H	1.677345000000	2.512486000000	0.280089000000
H	2.790587000000	2.572458000000	1.422374000000
O	-0.880075000000	-1.181474000000	-1.770560000000
H	-1.039366000000	-1.187863000000	-2.728126000000
H	0.079644000000	-1.426162000000	-1.642645000000
O	1.638770000000	-1.932407000000	-1.030503000000
H	2.323614000000	-1.187321000000	-0.925130000000
H	2.084787000000	-2.635016000000	-1.530957000000

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9k.	E[DF-MP2-F12]	-466848.66	
H	-1.244661000000	-1.133972000000	-1.948404000000
H	-0.584192000000	0.368997000000	-1.458091000000
H	0.460179000000	-0.826120000000	-2.109439000000
H	-0.653624000000	-0.018108000000	-3.108487000000
N	-0.507218000000	-0.399233000000	-2.170236000000
O	-0.607054000000	1.500595000000	-0.063044000000
H	-0.671807000000	0.991478000000	0.790093000000
H	-1.354898000000	2.150202000000	-0.064922000000
O	-2.462463000000	-2.002319000000	1.321040000000
H	-1.794936000000	-1.382458000000	1.705182000000
H	-2.477237000000	-2.780838000000	1.898203000000
O	-2.691851000000	3.280027000000	-0.128197000000
H	-3.635724000000	3.061059000000	-0.086144000000
H	-2.642011000000	4.248599000000	-0.130555000000
O	-2.287005000000	-2.255015000000	-1.336239000000
H	-3.113913000000	-2.586854000000	-1.715524000000

H	-2.405470000000	-2.227454000000	-0.343469000000
O	3.287654000000	0.025035000000	0.106458000000
H	2.892042000000	0.942456000000	-0.042504000000
H	4.252293000000	0.132322000000	0.087924000000
O	1.987554000000	2.262942000000	-0.359228000000
H	2.213279000000	3.150806000000	-0.044515000000
H	1.012468000000	2.132849000000	-0.211813000000
O	1.840107000000	-1.072494000000	2.155616000000
H	2.354899000000	-1.402701000000	2.906512000000
H	2.480207000000	-0.695363000000	1.497838000000
O	-0.606831000000	-0.106393000000	2.170395000000
H	0.332908000000	-0.469767000000	2.241485000000
H	-0.799038000000	0.315233000000	3.023730000000
O	2.041355000000	-1.372672000000	-1.926355000000
H	2.319500000000	-2.298111000000	-1.997560000000
H	2.598546000000	-0.955263000000	-1.221452000000

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9I.	E[DF-MP2-F12]	-466846.63	
H	1.474094000000	3.253742000000	-1.166685000000
H	0.513854000000	2.390109000000	-0.015807000000
H	1.250581000000	1.560137000000	-1.325087000000
H	2.219327000000	2.163761000000	-0.085607000000
N	1.369585000000	2.371537000000	-0.660729000000
O	2.815961000000	-1.391907000000	-0.073586000000
H	2.073230000000	-1.830914000000	0.411309000000
H	3.484013000000	-2.076667000000	-0.238772000000
O	-3.003935000000	1.920911000000	-0.580795000000
H	-3.824784000000	2.435457000000	-0.608084000000
H	-3.258339000000	0.974898000000	-0.521955000000
O	-3.043966000000	-0.873562000000	-0.101547000000
H	-3.845493000000	-1.421821000000	-0.097109000000
H	-2.402691000000	-1.316188000000	-0.722979000000
O	0.425816000000	-2.410180000000	0.947622000000
H	0.412496000000	-3.227663000000	1.472390000000
H	-0.123347000000	-1.745716000000	1.458571000000
O	3.358692000000	1.188974000000	0.859855000000
H	4.197465000000	1.381479000000	1.303862000000
H	3.356373000000	0.231014000000	0.632501000000
O	-1.271929000000	-0.559653000000	1.963099000000
H	-1.604796000000	-0.569722000000	2.875642000000
H	-2.061175000000	-0.680383000000	1.368198000000
O	-0.782955000000	2.211057000000	0.956525000000
H	-1.638705000000	2.229470000000	0.452858000000

H	-0.810422000000	1.370368000000	1.455442000000
O	1.210794000000	-0.032054000000	-2.011047000000
H	0.392675000000	-0.568957000000	-2.012822000000
H	1.867523000000	-0.581222000000	-1.528853000000
O	-0.937089000000	-1.992367000000	-1.426329000000
H	-1.002809000000	-2.697369000000	-2.091332000000
H	-0.427267000000	-2.364323000000	-0.660956000000

Table S13: PW91PW91/6-311++G(3df,3pd) optimized Cartesian coordinates for $\text{NH}_4^+(\text{H}_2\text{O})_{10}$ isomers

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10a.	E[DF-MP2-F12]	-514756.32	
H	-1.164239000000	2.168638000000	-0.125327000000
H	-0.724353000000	1.440927000000	-1.628572000000
H	-0.859201000000	3.131518000000	-1.500575000000
H	0.441697000000	2.329757000000	-0.755130000000
N	-0.578896000000	2.280144000000	-1.005253000000
O	2.460661000000	-1.819117000000	0.223982000000
H	2.373206000000	-1.391181000000	-0.690284000000
H	3.139145000000	-2.510465000000	0.158699000000
O	-1.911462000000	-1.837432000000	-0.894853000000
H	-1.206177000000	-2.068796000000	-0.145757000000
H	-2.248052000000	-2.682920000000	-1.234431000000
O	2.536966000000	0.441202000000	1.671286000000
H	2.648152000000	-0.462555000000	1.248676000000
H	3.240912000000	0.530797000000	2.334252000000
O	-2.038799000000	1.723904000000	1.261167000000
H	-2.501019000000	2.378095000000	1.810144000000
H	-2.734921000000	1.045860000000	0.961492000000
O	2.169027000000	2.053723000000	-0.448048000000
H	2.389633000000	1.561815000000	0.398394000000
H	2.838401000000	2.750098000000	-0.547343000000
O	-3.635146000000	-0.073398000000	0.253275000000
H	-3.109337000000	-0.816995000000	-0.150821000000
H	-4.381317000000	-0.476716000000	0.722857000000
O	-0.701255000000	-0.104586000000	-2.478766000000
H	-1.197938000000	-0.822433000000	-1.962600000000
H	-1.007671000000	-0.165431000000	-3.398535000000
O	-0.180638000000	-0.079516000000	2.507736000000
H	-0.791457000000	0.633419000000	2.223160000000
H	0.728185000000	0.271953000000	2.405273000000
O	2.085359000000	-0.420812000000	-1.962574000000
H	2.264874000000	0.498368000000	-1.673329000000

H	1.149665000000	-0.411814000000	-2.267981000000
O	-0.242063000000	-2.267549000000	0.939406000000
H	0.705239000000	-2.309377000000	0.674811000000
H	-0.282363000000	-1.514925000000	1.598800000000

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10b.	E[DF-MP2-F12]	-514758.78	
H	-2.793610000000	-0.525777000000	-1.256488000000
H	-3.289923000000	-2.184006000000	-1.413296000000
H	-1.611636000000	-1.768824000000	-1.269470000000
H	-2.679630000000	-1.595809000000	0.059396000000
N	-2.620010000000	-1.548677000000	-0.973315000000
O	0.423579000000	1.564549000000	0.710755000000
H	0.509056000000	0.725959000000	1.229544000000
H	-0.460434000000	1.920601000000	0.966909000000
O	-2.709176000000	1.082025000000	-1.536546000000
H	-1.806098000000	1.254306000000	-1.891353000000
H	-2.734604000000	1.561247000000	-0.680376000000
O	3.013116000000	2.125657000000	0.011172000000
H	3.550706000000	2.821007000000	0.420313000000
H	2.114942000000	2.182778000000	0.412873000000
O	-0.053507000000	-1.719234000000	-1.740408000000
H	0.144626000000	-0.783597000000	-1.983791000000
H	0.680133000000	-1.997987000000	-1.145590000000
O	-2.232563000000	-0.907341000000	1.877385000000
H	-2.675085000000	-1.310332000000	2.642354000000
H	-1.253900000000	-1.025194000000	2.029611000000
O	0.079009000000	1.068555000000	-1.965693000000
H	0.645932000000	1.602123000000	-2.546134000000
H	0.321655000000	1.308817000000	-1.030325000000
O	3.840375000000	-0.430553000000	-0.182355000000
H	3.598794000000	0.536254000000	-0.113634000000
H	4.495815000000	-0.507240000000	-0.891916000000
O	0.492382000000	-0.906795000000	2.040783000000
H	1.048780000000	-1.481204000000	1.422402000000
H	0.938361000000	-0.928407000000	2.903567000000
O	1.944790000000	-2.159926000000	0.216748000000
H	2.724490000000	-1.531156000000	0.023056000000
H	2.327420000000	-3.040814000000	0.360393000000
O	-2.320028000000	1.814921000000	1.217440000000
H	-2.825058000000	2.438219000000	1.764440000000
H	-2.454477000000	0.914919000000	1.606465000000

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10c.	E[DF-MP2-F12]	-514760.15	
H	-3.257724000000	-1.233542000000	0.239175000000
H	-2.867684000000	-2.722196000000	1.001085000000
H	-2.097571000000	-2.319531000000	-0.467312000000
H	-1.713880000000	-1.473686000000	0.941088000000
N	-2.497070000000	-1.954855000000	0.435101000000
O	0.922634000000	-0.790727000000	-1.185317000000
H	1.843189000000	-1.080784000000	-0.960926000000
H	0.477929000000	-0.720288000000	-0.289432000000
O	-4.277811000000	0.036347000000	0.044320000000
H	-5.014976000000	0.072467000000	-0.583162000000
H	-3.877212000000	0.950765000000	0.072690000000
O	1.178138000000	1.849386000000	-1.442294000000
H	1.050987000000	0.851651000000	-1.526395000000
H	0.932829000000	2.241583000000	-2.296176000000
O	-1.055365000000	-2.609348000000	-1.819031000000
H	-0.248298000000	-2.038829000000	-1.834471000000
H	-1.158496000000	-3.005656000000	-2.696274000000
O	-3.064759000000	2.432085000000	0.117137000000
H	-3.501421000000	3.203102000000	0.509755000000
H	-2.119510000000	2.471216000000	0.397402000000
O	-0.254078000000	-0.490957000000	1.251187000000
H	-0.311623000000	0.492949000000	1.319166000000
H	0.519377000000	-0.787164000000	1.816518000000
O	3.444594000000	-1.070815000000	-0.040659000000
H	4.190012000000	-1.629861000000	-0.311873000000
H	3.728622000000	-0.117338000000	-0.164088000000
O	3.729797000000	1.556282000000	-0.352821000000
H	4.479316000000	2.102368000000	-0.634040000000
H	2.937246000000	1.866922000000	-0.850775000000
O	1.988856000000	-1.419588000000	2.290358000000
H	2.679012000000	-1.336780000000	1.588094000000
H	2.436862000000	-1.397459000000	3.148512000000
O	-0.348369000000	2.270195000000	0.786358000000
H	0.050807000000	2.926173000000	1.380880000000
H	0.212590000000	2.265028000000	-0.039051000000

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10d.	E[DF-MP2-F12]	-514758.55	
H	0.383849000000	0.721574000000	2.252311000000
H	-0.995828000000	-0.357927000000	2.324642000000
H	0.559976000000	-1.001396000000	2.381150000000
H	-0.009539000000	-0.139749000000	3.718085000000
N	-0.009843000000	-0.198385000000	2.696804000000

O	-2.886019000000	1.032682000000	-0.666716000000
H	-2.433877000000	0.489102000000	-1.366953000000
H	-3.783142000000	1.215503000000	-0.989877000000
O	2.872426000000	-1.171799000000	-0.664758000000
H	2.331337000000	-1.708236000000	-0.026036000000
H	3.562136000000	-1.758345000000	-1.014192000000
O	-1.341495000000	-0.603089000000	-2.240724000000
H	-0.402171000000	-0.195052000000	-2.251196000000
H	-1.564499000000	-0.775131000000	-3.170640000000
O	0.866549000000	2.006107000000	1.557533000000
H	1.664004000000	1.926446000000	0.980245000000
H	0.174962000000	2.449501000000	0.997144000000
O	1.075486000000	0.306996000000	-2.218151000000
H	1.313920000000	1.185376000000	-1.868905000000
H	1.733332000000	-0.300896000000	-1.805031000000
O	1.098179000000	-2.434199000000	1.021702000000
H	0.272002000000	-2.591856000000	0.482129000000
H	1.342831000000	-3.298269000000	1.392210000000
O	-2.388256000000	-0.736623000000	1.483827000000
H	-2.209322000000	-1.517354000000	0.917830000000
H	-2.710137000000	-0.050990000000	0.853383000000
O	-1.231787000000	-2.586990000000	-0.397600000000
H	-1.608960000000	-3.428351000000	-0.702027000000
H	-1.276080000000	-1.955514000000	-1.174079000000
O	-1.003824000000	3.020908000000	-0.119196000000
H	-1.329950000000	3.932799000000	-0.082968000000
H	-1.781553000000	2.446106000000	-0.312732000000
O	2.925639000000	1.583250000000	-0.241220000000
H	3.208247000000	0.641476000000	-0.269443000000
H	3.732175000000	2.121939000000	-0.260243000000

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10e.	E[DF-MP2-F12]	-514759.16	
H	4.022446000000	-0.602093000000	0.832283000000
H	2.368651000000	-0.487719000000	1.210260000000
H	2.931323000000	-0.019456000000	-0.342552000000
H	2.884784000000	-1.680869000000	0.126866000000
N	3.073200000000	-0.689900000000	0.460094000000
O	-0.328863000000	1.837185000000	0.900336000000
H	-1.307689000000	2.002539000000	1.025983000000
H	-0.053579000000	1.164031000000	1.566639000000
O	2.085198000000	-3.054261000000	-0.377914000000
H	1.113721000000	-2.947709000000	-0.202157000000
H	2.285101000000	-3.998429000000	-0.453652000000

O	-0.381592000000	0.296351000000	-1.305258000000
H	0.440666000000	0.485946000000	-1.805651000000
H	-0.346577000000	0.935266000000	-0.530075000000
O	2.379173000000	1.089312000000	-1.597131000000
H	2.262164000000	1.969898000000	-1.118631000000
H	2.914072000000	1.264771000000	-2.387866000000
O	-0.313951000000	-1.981331000000	0.209838000000
H	-0.322888000000	-1.246319000000	-0.463772000000
H	-1.272586000000	-2.265461000000	0.251647000000
O	0.757531000000	-0.449279000000	2.098591000000
H	0.244425000000	-1.121923000000	1.547606000000
H	0.663285000000	-0.711191000000	3.028817000000
O	1.889080000000	3.089279000000	0.023466000000
H	1.961359000000	4.053467000000	-0.034750000000
H	1.008675000000	2.875271000000	0.428182000000
O	-3.108418000000	0.164294000000	-1.349324000000
H	-3.632790000000	0.313816000000	-2.152377000000
H	-2.155512000000	0.241580000000	-1.617283000000
O	-2.980212000000	1.876889000000	0.891960000000
H	-3.256019000000	1.360786000000	0.099744000000
H	-3.669790000000	2.533605000000	1.068741000000
O	-2.970942000000	-2.225893000000	0.151434000000
H	-3.240941000000	-1.470317000000	-0.419861000000
H	-3.570734000000	-2.960550000000	-0.046793000000

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10f.	E[DF-MP2-F12]	-514757.88	
H	-0.224995000000	2.786235000000	-1.494640000000
H	-0.163560000000	1.888311000000	-0.059568000000
H	-0.641855000000	1.112345000000	-1.515961000000
H	1.008389000000	1.640465000000	-1.296110000000
N	0.006591000000	1.873345000000	-1.093546000000
O	1.339710000000	-0.118113000000	2.135207000000
H	1.276329000000	-0.987188000000	1.678804000000
H	2.187171000000	0.311625000000	1.832499000000
O	-0.614368000000	1.430377000000	1.663293000000
H	0.184241000000	0.805260000000	1.911274000000
H	-0.621722000000	2.140683000000	2.326073000000
O	-1.662056000000	0.005624000000	-2.016273000000
H	-1.590443000000	-0.852411000000	-1.546367000000
H	-2.565597000000	0.339712000000	-1.772313000000
O	2.681998000000	0.996708000000	-1.545468000000
H	3.226359000000	1.312988000000	-2.284352000000
H	2.606637000000	-0.001580000000	-1.653175000000

O	0.908315000000	-2.479303000000	0.602847000000
H	1.101806000000	-3.321957000000	1.044941000000
H	-0.070832000000	-2.472478000000	0.411148000000
O	-1.707502000000	-2.116732000000	-0.023665000000
H	-2.167384000000	-1.494434000000	0.609342000000
H	-2.317722000000	-2.856437000000	-0.176553000000
O	-3.848972000000	1.052740000000	-0.826943000000
H	-4.793560000000	1.131817000000	-1.028162000000
H	-3.770717000000	0.688910000000	0.082725000000
O	2.342843000000	-1.613536000000	-1.582231000000
H	2.437849000000	-2.268616000000	-2.288667000000
H	1.858668000000	-2.042089000000	-0.832895000000
O	3.401548000000	1.264966000000	1.123862000000
H	4.332840000000	1.238210000000	1.390502000000
H	3.376009000000	1.219774000000	0.139235000000
O	-2.781277000000	-0.127805000000	1.490471000000
H	-2.006422000000	0.496520000000	1.651575000000
H	-3.189552000000	-0.288488000000	2.356677000000

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10g.	E[DF-MP2-F12]	-514756.39	
H	1.617826000000	-3.164759000000	-1.663789000000
H	1.967122000000	-1.795872000000	-0.674840000000
H	0.723676000000	-1.720306000000	-1.886786000000
H	0.490273000000	-2.658493000000	-0.495138000000
N	1.208060000000	-2.354290000000	-1.192153000000
O	-0.285604000000	-0.513667000000	-2.631244000000
H	0.017470000000	0.432200000000	-2.328661000000
H	-0.402975000000	-0.471893000000	-3.594245000000
O	3.004428000000	-0.903273000000	0.192005000000
H	3.203292000000	-0.019069000000	-0.184054000000
H	2.657294000000	-0.666899000000	1.081705000000
O	-2.786865000000	0.881826000000	0.973745000000
H	-2.175389000000	0.474536000000	1.638241000000
H	-3.643432000000	0.989756000000	1.418364000000
O	-0.884936000000	-0.559806000000	2.461524000000
H	-1.124286000000	-0.845156000000	3.359190000000
H	-0.885621000000	-1.393271000000	1.899108000000
O	1.709444000000	0.488605000000	2.291902000000
H	0.771367000000	0.188987000000	2.409893000000
H	2.058601000000	0.640817000000	3.184872000000
O	-0.967227000000	-2.570423000000	0.656699000000
H	-1.396344000000	-3.408719000000	0.895524000000
H	-1.609367000000	-2.074924000000	0.007195000000

O	-2.374482000000	-1.168730000000	-0.941955000000
H	-2.674213000000	-0.372689000000	-0.447570000000
H	-1.765897000000	-0.852960000000	-1.658276000000
O	0.415451000000	1.785484000000	-1.792535000000
H	1.219769000000	1.865683000000	-1.229827000000
H	-0.298097000000	2.284187000000	-1.311539000000
O	2.579009000000	1.872755000000	-0.000156000000
H	3.100048000000	2.689931000000	0.054867000000
H	2.223914000000	1.698276000000	0.902275000000
O	-1.467002000000	3.003170000000	-0.291269000000
H	-2.009668000000	3.759233000000	-0.561097000000
H	-2.059515000000	2.373920000000	0.179929000000

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10h.	E[DF-MP2-F12]	-514759.29	
H	-1.882699000000	0.252927000000	-2.293416000000
H	-0.476973000000	-0.732612000000	-2.399012000000
H	-1.946693000000	-1.397445000000	-1.819776000000
H	-1.802605000000	-0.981274000000	-3.462306000000
N	-1.539361000000	-0.715472000000	-2.510313000000
O	-1.092584000000	2.572310000000	0.728849000000
H	-0.114465000000	2.353352000000	0.778671000000
H	-1.177194000000	3.489911000000	1.035983000000
O	3.788782000000	-1.105913000000	0.818107000000
H	4.477048000000	-1.783252000000	0.738683000000
H	3.880464000000	-0.509221000000	0.041478000000
O	1.458649000000	1.703558000000	0.905312000000
H	1.307001000000	0.705219000000	1.006642000000
H	1.922790000000	1.981872000000	1.712776000000
O	-2.408449000000	-2.410845000000	-0.497503000000
H	-2.015660000000	-2.310456000000	0.405348000000
H	-2.862984000000	-3.265725000000	-0.517389000000
O	1.156112000000	-0.905306000000	0.867983000000
H	0.448309000000	-1.373673000000	1.379689000000
H	2.062469000000	-1.269576000000	1.056779000000
O	1.081716000000	-0.871476000000	-1.907536000000
H	1.815835000000	-0.234265000000	-2.026877000000
H	1.082336000000	-1.032866000000	-0.931649000000
O	-2.243000000000	1.848558000000	-1.708262000000
H	-1.841724000000	2.203377000000	-0.878063000000
H	-2.638308000000	2.598105000000	-2.177070000000
O	3.226936000000	0.886461000000	-1.126992000000
H	3.831526000000	1.488292000000	-1.589728000000
H	2.699054000000	1.441002000000	-0.503082000000

O	-2.249843000000	0.620566000000	2.358379000000
H	-3.206715000000	0.749401000000	2.444209000000
H	-1.914203000000	1.359589000000	1.792738000000
O	-1.210001000000	-1.776200000000	1.925638000000
H	-1.640385000000	-0.891366000000	2.145163000000
H	-1.297234000000	-2.326717000000	2.720600000000

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10i.	E[DF-MP2-F12]	-514756.85	
H	-0.934094000000	-2.090373000000	1.142279000000
H	-2.147619000000	-3.202717000000	0.525831000000
H	-2.261511000000	-1.525086000000	0.203609000000
H	-1.050275000000	-2.440751000000	-0.536030000000
N	-1.624551000000	-2.345941000000	0.330127000000
O	-0.821210000000	0.666998000000	-2.026339000000
H	-0.420925000000	-0.240912000000	-2.135012000000
H	-0.967406000000	1.019352000000	-2.919082000000
O	-2.672958000000	0.265139000000	0.000825000000
H	-3.605928000000	0.585380000000	-0.102334000000
H	-2.185255000000	0.524215000000	-0.821616000000
O	-5.233134000000	1.169019000000	-0.289347000000
H	-5.567977000000	2.032030000000	0.000329000000
H	-6.011245000000	0.660731000000	-0.566564000000
O	4.464273000000	-0.502772000000	-0.206259000000
H	5.178158000000	-0.779645000000	0.387867000000
H	4.407615000000	0.486735000000	-0.141273000000
O	0.125701000000	-1.513518000000	2.123662000000
H	0.951414000000	-1.412053000000	1.583251000000
H	-0.142386000000	-0.594026000000	2.345197000000
O	-0.924408000000	1.148443000000	1.925469000000
H	-1.706395000000	0.940046000000	1.346233000000
H	-1.235271000000	1.749449000000	2.621455000000
O	1.901841000000	-0.978092000000	0.086760000000
H	1.655789000000	-0.012444000000	0.059381000000
H	2.911747000000	-0.967895000000	0.018395000000
O	1.005450000000	1.612297000000	-0.046590000000
H	0.390275000000	1.671338000000	0.724342000000
H	0.419614000000	1.550462000000	-0.834383000000
O	0.261644000000	-1.820461000000	-1.741306000000
H	0.636751000000	-2.359727000000	-2.456303000000
H	1.031400000000	-1.584138000000	-1.109001000000
O	3.777166000000	2.115164000000	0.018405000000
H	4.150565000000	2.923406000000	-0.362839000000
H	2.799893000000	2.190470000000	-0.046851000000

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10j.	E[DF-MP2-F12]	-514757.88	
H	0.221376000000	-2.681248000000	-2.753396000000
H	0.617526000000	-2.439524000000	-1.121479000000
H	0.029857000000	-1.115041000000	-2.013256000000
H	-1.019065000000	-2.452705000000	-1.601818000000
N	-0.039143000000	-2.196056000000	-1.891604000000
O	0.252782000000	0.439197000000	-1.960113000000
H	1.097628000000	0.575127000000	-1.465057000000
H	-0.431842000000	0.910485000000	-1.419882000000
O	-1.493737000000	1.550568000000	-0.108810000000
H	-2.066103000000	2.342240000000	-0.274538000000
H	-2.068307000000	0.852177000000	0.279783000000
O	2.349376000000	0.384865000000	-0.114238000000
H	1.843608000000	0.905024000000	0.590101000000
H	3.269873000000	0.744957000000	-0.173941000000
O	-0.151058000000	-1.247397000000	2.364429000000
H	-0.061432000000	-1.717712000000	3.208795000000
H	0.509090000000	-1.659900000000	1.739045000000
O	4.929340000000	1.294644000000	-0.338685000000
H	5.446759000000	1.648033000000	0.401978000000
H	5.231562000000	1.779115000000	-1.123040000000
O	1.643897000000	-2.059638000000	0.450512000000
H	2.067098000000	-1.153624000000	0.240998000000
H	2.369520000000	-2.651963000000	0.706405000000
O	-3.097700000000	3.728619000000	-0.535791000000
H	-3.018052000000	4.538463000000	-0.007485000000
H	-3.369436000000	4.017943000000	-1.421039000000
O	-2.553149000000	-0.757862000000	1.178928000000
H	-3.277907000000	-0.681248000000	1.820540000000
H	-1.737877000000	-0.991738000000	1.705915000000
O	-2.526176000000	-2.653294000000	-0.822601000000
H	-2.717795000000	-2.007257000000	-0.098097000000
H	-3.372173000000	-3.008242000000	-1.132342000000
O	0.695823000000	1.473496000000	1.623810000000
H	0.418413000000	0.714949000000	2.175545000000
H	-0.103498000000	1.678510000000	1.077966000000

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10k.	E[DF-MP2-F12]	-514757.66	
H	1.969634000000	2.486690000000	0.537787000000
H	2.889356000000	2.074947000000	1.923539000000
H	1.285124000000	1.548502000000	1.748519000000

H	2.499103000000	0.844016000000	0.764700000000
N	2.182244000000	1.748025000000	1.261018000000
O	-1.781472000000	-1.290558000000	2.017247000000
H	-1.342018000000	-0.395400000000	2.048872000000
H	-1.763139000000	-1.646461000000	2.919625000000
O	-3.730213000000	-1.369088000000	0.066886000000
H	-3.256065000000	-1.317831000000	0.934422000000
H	-4.597657000000	-1.765185000000	0.247096000000
O	-3.348414000000	1.069071000000	-1.176230000000
H	-3.971194000000	1.300385000000	-1.880951000000
H	-3.633805000000	0.199383000000	-0.800330000000
O	2.696000000000	-0.513355000000	-0.015922000000
H	3.496747000000	-1.078072000000	-0.123223000000
H	2.026128000000	-0.771236000000	-0.693201000000
O	1.063346000000	3.400014000000	-0.601331000000
H	1.295353000000	4.029641000000	-1.299478000000
H	0.332984000000	2.823215000000	-0.940641000000
O	-0.732076000000	1.384225000000	-0.901990000000
H	-1.703385000000	1.332541000000	-1.145398000000
H	-0.295880000000	0.589295000000	-1.313578000000
O	-0.625455000000	1.171046000000	1.739540000000
H	-0.723967000000	1.270320000000	0.733211000000
H	-1.163826000000	1.883361000000	2.123801000000
O	0.521994000000	-0.922961000000	-1.694742000000
H	0.650003000000	-1.176788000000	-2.622780000000
H	-0.099839000000	-1.614017000000	-1.285391000000
O	-1.128829000000	-2.538794000000	-0.458838000000
H	-2.071425000000	-2.400475000000	-0.682757000000
H	-1.107485000000	-2.305473000000	0.495424000000
O	4.968163000000	-2.049354000000	-0.209521000000
H	5.703066000000	-1.946960000000	-0.833649000000
H	5.082130000000	-2.922542000000	0.196474000000

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10L.	E[DF-MP2-F12]	-514756.32	
H	0.713693000000	-2.266883000000	-1.177710000000
H	1.007769000000	-2.027118000000	-2.865782000000
H	0.833632000000	-0.667411000000	-1.819956000000
H	2.214455000000	-1.597569000000	-1.779417000000
N	1.196996000000	-1.659180000000	-1.929591000000
O	0.720317000000	0.917660000000	-1.199471000000
H	0.657002000000	0.848691000000	-0.196574000000
H	-0.001021000000	1.550615000000	-1.439094000000
O	-3.023702000000	0.164180000000	-1.378541000000

H	-2.583585000000	1.049517000000	-1.286699000000
H	-3.907675000000	0.336995000000	-1.736555000000
O	-0.739934000000	-1.420045000000	2.307311000000
H	-1.592074000000	-1.466250000000	1.802637000000
H	-0.959363000000	-1.542012000000	3.244599000000
O	3.364978000000	0.303440000000	-1.315247000000
H	4.072539000000	0.728828000000	-1.825264000000
H	2.553742000000	0.858055000000	-1.431911000000
O	-0.158393000000	-3.004390000000	-0.061519000000
H	-1.109720000000	-2.731839000000	-0.076831000000
H	0.095554000000	-2.821370000000	0.864531000000
O	-2.628166000000	-1.802524000000	0.366661000000
H	-3.457187000000	-2.293761000000	0.481351000000
H	-2.831145000000	-1.040010000000	-0.258935000000
O	-1.561095000000	2.483879000000	-1.160748000000
H	-1.788586000000	3.278324000000	-1.669270000000
H	-1.436673000000	2.773815000000	-0.202060000000
O	0.672758000000	0.772602000000	1.482844000000
H	0.190086000000	-0.010458000000	1.860574000000
H	1.643231000000	0.627784000000	1.662856000000
O	-1.055607000000	2.857193000000	1.392005000000
H	-0.327243000000	2.222820000000	1.617732000000
H	-0.933758000000	3.651724000000	1.932069000000
O	3.280397000000	0.164415000000	1.474453000000
H	3.554994000000	0.232380000000	0.529730000000
H	4.039942000000	0.428114000000	2.015120000000

Table S14: The relative energies with ZPE corrections and without ZPE corrections at DF-MP2-F12/VDZ level.

Isomers	ΔE	$\Delta E+ZPE$	ΔG
2a	0	0.05	0
2b	0	0	1.20
3a	0	1.58	4.82
3b	0.02	0	0
4a	1.19	1.39	3.18
4b	0	0	1.39
4d	0	0	1.44
4e	1.38	0.92	0
5a	0.81	3.09	8.85
5b	0	1.9	6.99
5c	0.46	0.34	1.20

5d	0.5	0.26	1.81
5e	1.09	1.23	2.35
5f	1.85	2.1	3.77
5g	1.24	2.28	5.83
5h	0.48	0	0

6a	0	0	3.74
6b	0.61	0.86	5.35
6c	0.33	0.41	4.53
6d	2.41	3.46	8.75
6e	0.88	0.9	4.33
6f	1.2	0.6	2.87
6g	1.56	0.32	1.53
6h	1.81	1.05	3.21
6i	2.6	1.52	2.93
6j	2.78	1.82	3.24
6k	3.49	1.22	0
6l	2.91	1.53	2.20

7a	0.61	1.15	2.71
7b	0.61	0.89	2.76
7c	0.22	1.48	3.89
7d	0.14	1.76	4.66
7e	0.21	1.79	4.67
7f	0.21	1.79	4.67
7g	1.91	2.68	4.31
7h	0	0	0
7i	0	0	0
7k	2	3.25	6.09
7l	0.34	0.26	0.27

8a	0	1.78	5.84
8b	1.74	3.1	6.12
8c	0.77	1.48	3.47
8d	1.42	1.08	0.96
8e	0.93	1.31	2.33
8f	0.48	0.06	0.12
8g	-0.7	0	1.82
8i	2.14	2.52	3.57
8j	3.07	3.15	3.42
8k	3.38	3.27	3.38
8l	2.05	1.34	0

9a	0	0.89	3.13
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9b	0	0	0
9c	1.97	3.06	5.49
9d	0.85	2.17	4.77
9f	4.12	3.73	3.87
9g	2.37	2.54	3.03
9h	1.63	1.7	1.85
9i	3.64	3.2	3.00
9l	3.8	3.92	4.77

10a	2.45	3.83	7.68
10b	0.08	1.37	3.91
10c	0	0	0
10d	0.94	1.6	3.06
10e	0.3	0.99	3.01
10f	2.04	2.27	4.68
10g	2.9	3.76	6.52
10h	1.18	0.86	0.95
10i	2.89	3.3	4.22
10j	2.78	2.27	1.81
10k	3.05	2.49	1.82
10l	3.56	3.83	4.83
