Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Structural Evolution and Solvation of OH radical in Ionized Water Radical Cations $(H_2O)_n^+$, n = 5 ~ 8

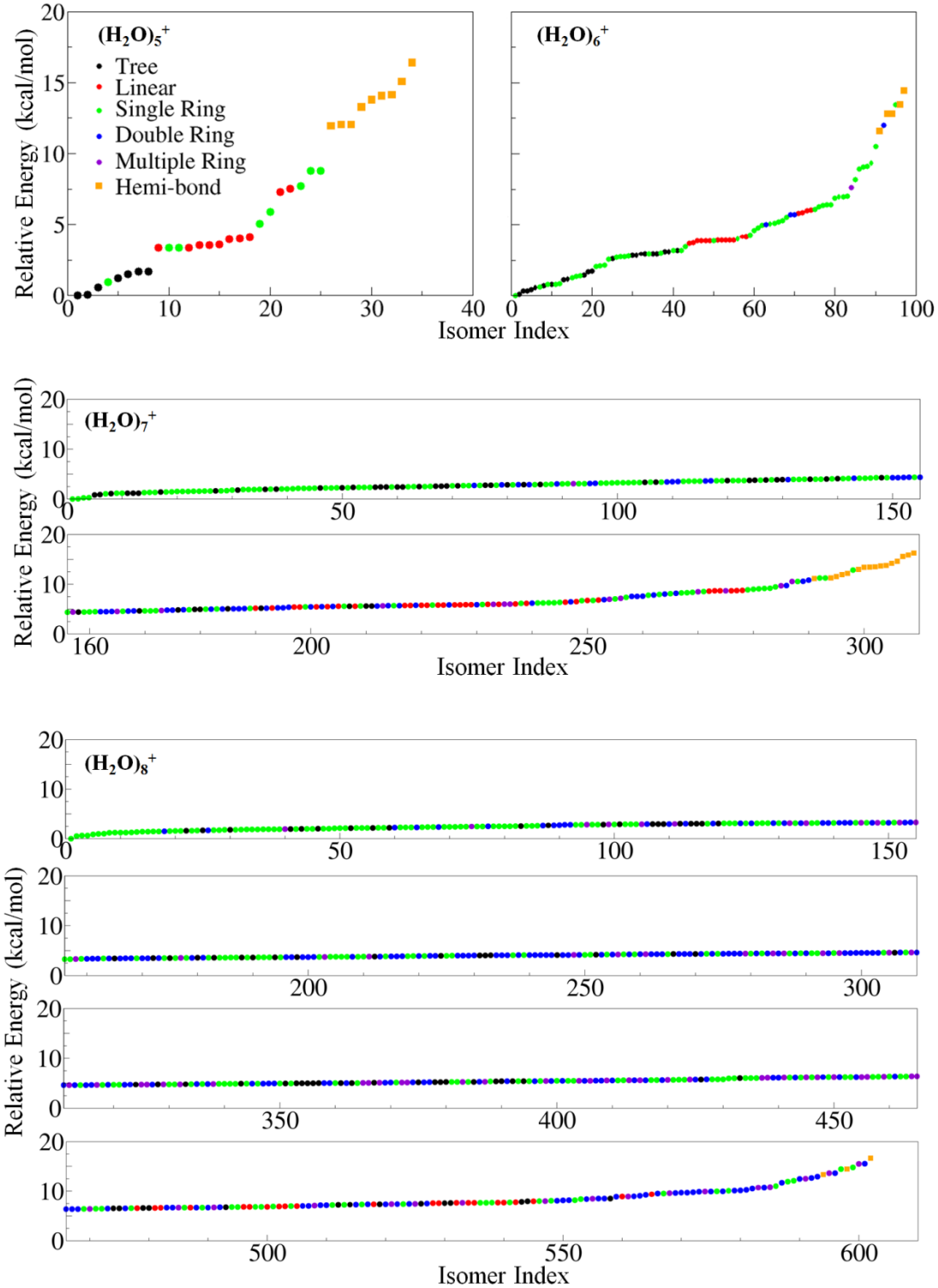
## Supporting Information

En-Ping Lu,[a] Piin-Ruey Pan,[a] Ying-Cheng Li,[a]
Ming-Kang Tsai, *[b] and Jer-Lai Kuo*[a]

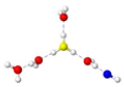
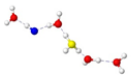
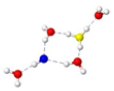
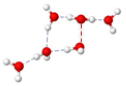
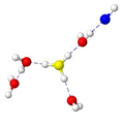
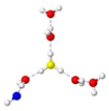
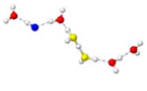
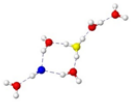
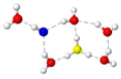
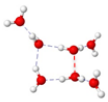
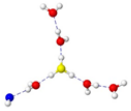
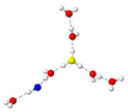
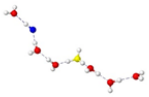
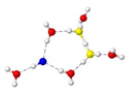
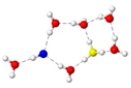
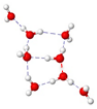
a. *Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan. E-mail: jlkuo@pub.iams.sinica.edu.tw*
b. *Department of Chemistry, National Taiwan Normal University, Taipei 10677, Taiwan. E-mail: mktsai@ntnu.edu.tw*

Contents Page #

Relative energy of the stable isomers of $(H_2O)_n^+$ found by our searching method at BH&HLYP/aug-cc-pVDZ.



Comparison on the ZPE corrected relative energy of isomers in Figure 3 using BH&HLYP/aug-cc-pvDZ, B3LYP/6-311++G** B3LYP-D3/6-311++G** and MP2/6-311++G**) to address the role of dispersion on the relative stability. One can find from the following figure that BH&HLYP/aug-cc-pvDZ (1) yield the same ground state structures and (2) the order of the relative stability between multiple ring and single ring is the same for BH&HLYP/aug-cc-pvDZ, B3LYP-D3/6-311++G** and MP2/6-311++G**.

| | Tree | Linear | Single ring | Double ring | Multiple ring | Hemi-bonded | Besley's minimum |
|---|---|---|---|---|---|---|---|
| $(H_2O)_6^+$ |  |  |  |  |  |  |  |
| BH&HLYP | 0.12 | 3.70 | 0.0 | 5.02 | 7.62 | 11.61 | 0.33 |
| B3LYP | 1.22 | 3.93 | 0.0 | 4.68 | 7.26 | 2.41 | 1.43 |
| B3LYP-D3 | (1.27) | (4.27) | (0.0) | (3.91) | (5.53) | (2.09) | (1.48) |
| MP2 | 0.13 | 4.28 | 0.0 | 3.83 | 3.58 | 7.07 | 0.31 |
| $(H_2O)_7^+$ |  |  |  |  |  |  |  |
| BH&HLYP | 0.81 | 5.16 | 0.0 | 2.70 | 3.04 | 11.15 | 1.08 |
| B3LYP | 1.82 | 4.77 | 0.0 | 2.04 | 2.79 | 0.89 | 1.73 |
| B3LYP-D3 | (2.02) | (5.01) | (0.0) | (1.48) | (0.98) | (0.45) | (2.23) |
| MP2 | 0.69 | 5.31 | 0.0 | 1.96 | 1.59 | 18.46 | 0.90 |
| $(H_2O)_8^+$ |  |  |  |  |  |  |  |
| BH&HLYP | 1.59 | 6.59 | 0.0 | 1.48 | 1.93 | 13.34 | 1.86 |
| B3LYP | 2.92 | 7.20 | 0.0 | 1.32 | 1.70 | 3.56 | 1.42 |
| B3LYP-D3 | (3.76) | (7.80) | (0.0) | (1.02) | (0.05) | (2.54) | (1.04) |
| MP2 | 2.67 | 7.47 | 0.0 | 1.49 | 1.59 | 22.93 | 1.55 |

The coordinate of the most stable structures of $(H_2O)_n^+$ at BH&HLYP/aug-cc-pVDZ in different topological groups. The relative energies are corrected with zero-point energy.

# $(H_2O)_5^+$

#1 (Tree): +0 kcal/mol

| | | | |
|---|---|---|---|
| O | -0.057328 | 1.193976 | 2.894928 |
| O | 2.461812 | -1.559880 | 0.677465 |
| O | -0.466720 | 0.838900 | -1.391776 |
| O | 0.310472 | -0.170393 | 0.757134 |
| O | -2.708089 | -0.377490 | -2.508975 |
| H | 0.020541 | 0.270108 | -0.107929 |
| H | -0.152747 | 1.619141 | -1.840064 |
| H | -3.258512 | -0.243096 | -3.293417 |
| H | 3.356982 | -1.293847 | 0.480242 |
| H | 0.414895 | 1.953155 | 3.229046 |
| H | 1.165938 | -0.674466 | 0.711687 |
| H | 0.200835 | 0.383475 | 1.575009 |
| H | 2.458238 | -2.511160 | 0.760262 |
| H | -1.240566 | 0.501360 | -1.861273 |
| H | -0.718486 | 0.960597 | 3.543137 |

#4 (Single ring): +0.95 kcal/mol

| | | | |
|---|---|---|---|
| O | -0.178028 | -0.206007 | -2.013116 |
| O | -2.445543 | -1.255147 | -0.465090 |
| O | 1.124926 | 0.207223 | 0.131668 |
| O | -0.640452 | -0.615542 | 1.767706 |
| O | 2.085835 | 2.546643 | 0.503180 |
| H | -0.541714 | -1.020674 | 2.626128 |
| H | 1.460732 | 1.135317 | 0.273513 |
| H | 0.495704 | -0.100989 | 0.847726 |
| H | -1.424865 | -0.978232 | 1.352789 |
| H | -3.346506 | -1.579533 | -0.611308 |
| H | 0.133121 | -0.424891 | -2.888376 |
| H | -1.028410 | -0.628837 | -1.882100 |
| H | 3.018120 | 2.708957 | 0.631152 |
| H | 1.638739 | 3.389006 | 0.544576 |

| | | | |
|---|---|---|---|
| H | 0.692448 | 0.073676 | -0.762204 |

#9 (Linear): +3.34 kcal/mol

| | | | |
|---|---|---|---|
| O | 2.015109 | -0.757209 | -0.391385 |
| O | -3.850406 | 1.398359 | 0.178189 |
| O | -0.097592 | -0.894047 | 0.787394 |
| O | -2.258616 | -0.789889 | -0.422842 |
| O | 3.747510 | 1.201513 | -0.032903 |
| H | 0.809737 | -0.854043 | 0.246999 |
| H | 2.320524 | -1.337556 | -1.083181 |
| H | 4.513124 | 1.169245 | 0.535817 |
| H | -0.097512 | -1.543185 | 1.490433 |
| H | 2.655985 | -0.027801 | -0.268599 |
| H | -4.745857 | 1.688557 | -0.046664 |
| H | -2.639947 | -1.430183 | -1.017352 |
| H | -2.891726 | -0.072191 | -0.283666 |
| H | 3.794418 | 2.024421 | -0.513596 |
| H | -0.977711 | -0.878854 | 0.267345 |

#26 (Hemi-bonded): +11.95 kcal/mol

| | | | |
|---|---|---|---|
| O | -2.939732 | -1.394718 | 0.500327 |
| H | -3.489074 | -0.636696 | 0.692525 |
| H | -3.506946 | -2.162798 | 0.467705 |
| O | 3.539561 | -0.778650 | -0.383026 |
| H | 3.970582 | -1.561948 | -0.716969 |
| H | 4.199271 | -0.089276 | -0.362951 |
| O | 1.095726 | -0.599322 | 0.607256 |
| H | 1.118815 | -0.870529 | 1.522414 |
| H | 2.003085 | -0.676412 | 0.245008 |
| O | -1.485347 | 1.085666 | -0.516968 |
| H | -1.616818 | 1.409734 | -1.408412 |
| H | -0.764315 | 1.599438 | -0.151905 |
| O | -0.831990 | -1.000718 | -0.852510 |
| H | -1.687581 | -1.174039 | -0.325523 |
| H | -0.012054 | -0.855264 | -0.193268 |

# $(H_2O)_6^+$

#1 (Single ring): +0 kcal/mol

| | | | |
|---|---|---|---|
| O | -1.323273 | -1.376950 | -0.169223 |
| O | 1.412724 | 1.221442 | 0.653241 |
| O | -3.203974 | -3.150396 | -0.789942 |
| O | 2.836133 | 2.835320 | -0.747823 |
| O | -1.104468 | 1.378355 | 0.438760 |
| O | 1.493102 | -1.239162 | 0.065674 |
| H | 0.601408 | -1.589510 | -0.033157 |
| H | -3.068170 | -4.067221 | -1.016869 |
| H | -4.140873 | -2.984568 | -0.862216 |
| H | -2.022826 | -2.036345 | -0.403219 |
| H | 3.485199 | 3.422409 | -0.366380 |
| H | 2.836128 | 2.981715 | -1.690903 |
| H | 1.945046 | 1.832742 | 0.077608 |
| H | -1.738138 | 1.889765 | 0.935333 |
| H | -1.480976 | 0.509117 | 0.264674 |
| H | 0.423928 | 1.397472 | 0.606729 |
| H | 1.563587 | 0.249974 | 0.442566 |
| H | 2.059409 | -1.936108 | 0.386911 |

#2 (Tree); +0.12 kcal/mol

| | | | |
|---|---|---|---|
| O | -0.068876 | -3.121768 | -2.878808 |
| O | -2.642961 | 1.920860 | -0.264933 |
| O | -0.514919 | 0.456402 | -0.107379 |
| O | 1.773634 | -0.247815 | 3.713182 |
| O | 0.260944 | -0.532013 | -2.256483 |
| O | 1.275097 | 1.330267 | 1.450221 |
| H | -0.691801 | -3.460101 | -3.517223 |
| H | 0.151953 | -1.473675 | -2.475965 |
| H | 0.461215 | -3.862365 | -2.595230 |
| H | -3.462547 | 1.676301 | 0.159111 |
| H | 1.506373 | 0.872991 | 2.267598 |
| H | -2.838266 | 2.638466 | -0.862944 |
| H | -0.170213 | 0.071696 | -0.983965 |
| H | -1.313313 | 1.031595 | -0.201562 |
| H | 1.685249 | 2.190347 | 1.462380 |

| | | | |
|---|---|---|---|
| H | 0.904692 | -0.160971 | -2.852978 |
| H | 2.309064 | -0.163228 | 4.514583 |
| H | 0.190108 | 0.836332 | 0.496687 |

#44 (Linear): +3.70 kcal/mol

| | | | |
|---|---|---|---|
| O | 1.071200 | -2.515128 | 1.248692 |
| O | 0.356314 | 1.428529 | -0.014583 |
| O | -1.797413 | 1.456002 | -1.593337 |
| O | 3.141355 | -3.732463 | 2.383700 |
| O | 0.401394 | -0.225428 | 1.787889 |
| O | -2.808116 | 2.987796 | -3.553195 |
| H | -3.640636 | 2.783039 | -3.971933 |
| H | 0.779999 | -3.021430 | 0.495410 |
| H | 0.680333 | -1.193914 | 1.524721 |
| H | -0.382723 | -0.211547 | 2.336406 |
| H | -2.131650 | 2.042833 | -2.310568 |
| H | 3.080467 | -4.384913 | 3.077259 |
| H | 1.841074 | -2.959622 | 1.652246 |
| H | -0.388155 | 1.543405 | -0.635447 |
| H | 0.365085 | 0.480389 | 1.022539 |
| H | 4.061441 | -3.676760 | 2.137742 |
| H | -2.474749 | 3.775464 | -3.975133 |
| H | 0.892891 | 2.216475 | -0.007972 |

#63 (Double ring): +5.02 kcal/mol

| | | | |
|---|---|---|---|
| O | 1.066033 | 2.098122 | -0.576439 |
| O | -2.387310 | -1.658168 | 0.217014 |
| O | 1.509034 | -0.113944 | -2.383697 |
| O | 0.313850 | 0.637723 | 1.359168 |
| O | 0.601863 | -1.545035 | -0.101333 |
| O | -2.140542 | 0.648663 | 1.764117 |
| H | 1.442264 | 2.972872 | -0.633055 |
| H | 2.390538 | -0.276712 | -2.718672 |
| H | 0.940812 | -0.133439 | -3.153632 |
| H | 1.342090 | 1.588901 | -1.342899 |
| H | 0.482606 | -0.244015 | 0.951323 |
| H | 0.596041 | 1.321284 | 0.682838 |
| H | -1.469567 | -1.861556 | -0.030298 |

| | | | |
|---|---|---|---|
| H | 1.102114 | -2.324194 | 0.136576 |
| H | 0.953794 | -1.232020 | -0.945999 |
| H | -2.527058 | -0.132806 | 1.349896 |
| H | -0.679065 | 0.708994 | 1.594344 |
| H | -2.654914 | 0.888750 | 2.530932 |

#84 (Multiple ring): +7.62 kcal/mol

| | | | |
|---|---|---|---|
| O | 0.445270 | 2.864108 | -0.550480 |
| O | -0.601949 | -2.698523 | 0.590441 |
| O | -0.881621 | -0.302242 | 1.286057 |
| O | -1.409714 | 0.875147 | -0.938944 |
| O | 1.567678 | 0.443866 | 0.846499 |
| O | 0.810312 | -1.081434 | -1.386565 |
| H | -0.906777 | 1.706187 | -0.921928 |
| H | -2.260903 | 1.061893 | -1.331182 |
| H | 0.087253 | -0.535267 | -1.704099 |
| H | 1.689098 | -0.113239 | 0.066187 |
| H | 1.087557 | 2.433885 | 0.037841 |
| H | -1.260468 | 0.160652 | 0.484719 |
| H | 2.346087 | 0.354831 | 1.394051 |
| H | -0.871307 | -1.294354 | 1.102555 |
| H | -0.113051 | -2.742320 | -0.232043 |
| H | 1.314833 | -1.328716 | -2.159601 |
| H | 0.065720 | -0.007677 | 1.338639 |
| H | -0.971262 | -3.554867 | 0.791183 |

#91 (Hemi-bonded): +11.61 kcal/mol

| | | | |
|---|---|---|---|
| O | -1.369546 | -0.415267 | -1.054107 |
| H | -1.720240 | -1.280048 | -0.675013 |
| H | -1.506090 | 0.331488 | -0.372050 |
| O | 1.092102 | 1.227276 | 1.346771 |
| H | 1.773613 | 1.861833 | 1.059819 |
| H | 1.298687 | 1.013973 | 2.254777 |
| O | -1.558049 | 1.408508 | 0.673349 |
| H | -2.121494 | 2.177716 | 0.680638 |
| H | -0.694426 | 1.638119 | 1.038936 |
| O | -2.275240 | -2.615419 | -0.102595 |
| H | -3.041016 | -3.091576 | -0.416230 |

| | | | |
|---|---|---|---|
| H | -1.720795 | -3.236872 | 0.363952 |
| O | 0.464993 | -0.950134 | -0.166469 |
| H | 0.954720 | -0.970220 | -0.989618 |
| H | 0.767156 | -0.163431 | 0.330939 |
| O | 2.967446 | 2.975982 | 0.517582 |
| H | 2.889337 | 3.926983 | 0.531481 |
| H | 3.889300 | 2.785003 | 0.361287 |

# $(H_2O)_7^+$

#1 (Single ring): +0 kcal/mol

| | | | |
|---|---|---|---|
| O | 3.559490 | 4.088010 | -0.640270 |
| O | 0.918515 | -1.833192 | 0.333041 |
| O | -1.896177 | -2.212994 | 0.323477 |
| O | 0.691350 | 0.707300 | 0.519327 |
| O | -1.863397 | 0.621098 | 0.473627 |
| O | -3.661982 | -4.197424 | 0.093851 |
| O | 1.833762 | 2.105651 | -1.201686 |
| H | -2.550854 | -2.948050 | 0.236198 |
| H | -2.167984 | -0.291917 | 0.468821 |
| H | 3.349644 | 5.012166 | -0.531954 |
| H | 0.904419 | -0.265424 | 0.459897 |
| H | 1.143569 | 1.261597 | -0.201959 |
| H | 0.051917 | -2.251116 | 0.357536 |
| H | -2.515719 | 1.152638 | 0.921833 |
| H | -0.302201 | 0.798580 | 0.520406 |
| H | 1.552770 | -2.435156 | 0.712941 |
| H | -4.611206 | -4.111798 | 0.049076 |
| H | -3.464595 | -5.126127 | -0.000445 |
| H | 4.507088 | 4.011773 | -0.563317 |
| H | 2.458040 | 2.823009 | -0.999765 |
| H | 1.747096 | 2.039113 | -2.147949 |

#5 (Tree): +0.81 kcal/mol

| | | | |
|---|---|---|---|
| O | -4.580233 | 1.289197 | 0.126075 |
| O | -0.483997 | -0.751729 | -0.277218 |
| O | 3.092488 | -1.046039 | 2.770026 |
| O | 0.614649 | -1.901384 | 1.716519 |
| O | 2.642533 | 1.489156 | -2.978727 |
| O | -1.886054 | 1.254313 | 0.298188 |
| O | 0.963124 | -0.528087 | -2.320908 |
| H | -5.087665 | 1.692895 | -0.573438 |
| H | 0.346860 | -2.767794 | 2.009941 |
| H | -0.022416 | -1.184756 | 0.492980 |
| H | -1.024381 | 0.060542 | -0.025117 |
| H | 1.461887 | -1.696252 | 2.126397 |

| | | | |
|---|---|---|---|
| H | 3.656709 | -1.361897 | 3.489701 |
| H | 0.810707 | -1.061760 | -3.095421 |
| H | 1.559035 | 0.196924 | -2.568260 |
| H | 3.594007 | 1.419712 | -2.976600 |
| H | 2.428994 | 2.260013 | -3.498515 |
| H | -2.855566 | 1.260874 | 0.242985 |
| H | 0.101362 | -0.627580 | -1.087891 |
| H | -1.616429 | 2.009283 | 0.812611 |
| H | -5.209063 | 0.943883 | 0.754565 |

#74 (Double ring): +2.70 kcal/mol

| | | | |
|---|---|---|---|
| O | -3.424290 | -3.218864 | 0.714352 |
| O | 1.525094 | -1.812852 | 0.652495 |
| O | 1.872899 | 0.283245 | -0.749654 |
| O | -1.271683 | -1.798183 | 0.069499 |
| O | -0.662855 | 0.505458 | -1.452313 |
| O | 2.207017 | 2.360234 | 0.550421 |
| O | -0.358506 | 3.009424 | 0.154198 |
| H | 1.856409 | -0.540777 | -0.182224 |
| H | 2.102652 | 1.132023 | -0.210089 |
| H | -4.320060 | -3.091883 | 0.411173 |
| H | -1.096450 | -0.250494 | -1.035104 |
| H | -2.079630 | -2.318437 | 0.305846 |
| H | 2.092062 | -2.545657 | 0.877193 |
| H | -0.972358 | 0.540011 | -2.355522 |
| H | 0.971903 | 0.389287 | -1.137582 |
| H | 0.614526 | -2.118600 | 0.632155 |
| H | 1.347951 | 2.813048 | 0.523774 |
| H | 2.900329 | 3.003643 | 0.426838 |
| H | -3.438948 | -3.963046 | 1.311582 |
| H | -0.806811 | 2.352532 | -0.378114 |
| H | -1.006431 | 3.652358 | 0.427852 |

#92 (Multiple ring): +3.04 kcal/mol

| | | | |
|---|---|---|---|
| O | 0.018209 | -0.881430 | -1.857051 |
| O | 0.462743 | -2.744616 | -0.180059 |
| O | 1.034251 | 1.834619 | 1.133772 |
| O | -1.753823 | 1.219216 | 1.443677 |

| | | | |
|---|---|---|---|
| O | 0.314118 | -0.769946 | 1.888598 |
| O | 1.754973 | 0.898454 | -1.392409 |
| O | -2.140160 | 0.259633 | -1.168121 |
| H | 0.604692 | -2.453136 | 0.722351 |
| H | 0.729121 | -0.178618 | -1.752844 |
| H | -1.500507 | 0.456206 | 1.968536 |
| H | 1.485674 | 2.544085 | 1.586861 |
| H | 2.261309 | 1.424323 | -2.005663 |
| H | -2.433407 | 1.674295 | 1.937960 |
| H | 0.921183 | -0.006988 | 1.896507 |
| H | 1.622099 | 1.401745 | -0.579467 |
| H | 0.800485 | -3.631291 | -0.275425 |
| H | 0.090492 | 2.009778 | 1.212558 |
| H | 0.212406 | -1.661482 | -1.262071 |
| H | -3.010439 | 0.216425 | -1.554584 |
| H | -0.874247 | -0.482703 | -1.635220 |
| H | -2.205416 | 0.635185 | -0.282021 |

#190 (Linear): +5.16 kcal/mol

| | | | |
|---|---|---|---|
| O | -0.939452 | -1.134303 | 1.537574 |
| O | -0.080008 | -2.733132 | 3.358952 |
| O | -0.884886 | 2.383173 | -2.863998 |
| O | -0.050232 | 1.081209 | 1.256731 |
| O | 2.138207 | -4.322478 | 3.334614 |
| O | -0.870049 | 3.450053 | -5.338296 |
| O | 0.885983 | 1.710736 | -0.952169 |
| H | -0.835832 | 2.773321 | -3.765970 |
| H | 0.705737 | -3.299124 | 3.354803 |
| H | 2.164840 | -5.238207 | 3.068958 |
| H | 1.785005 | 1.997723 | -1.084597 |
| H | -1.676085 | 3.608535 | -5.823451 |
| H | 0.345045 | 1.994894 | -1.709888 |
| H | 0.328696 | 1.353369 | 0.346496 |
| H | 2.937039 | -4.162683 | 3.830709 |
| H | -0.153090 | 3.745140 | -5.893584 |
| H | -1.355597 | -1.629115 | 0.837218 |
| H | -0.647427 | 1.745368 | 1.599199 |
| H | -0.582073 | -2.945218 | 4.140121 |

| | | | |
|---|---|---|---|
| H | -0.443360 | 0.078283 | 1.347409 |
| H | -0.592103 | -1.758866 | 2.223743 |

#291 (Hemi-bonded): +11.15 kcal/mol

| | | | |
|---|---|---|---|
| O | -1.247106 | 3.130030 | -1.041523 |
| H | -0.782800 | 3.571039 | -1.749248 |
| H | -1.859298 | 3.764787 | -0.676881 |
| O | -2.173965 | -2.885123 | 1.379567 |
| H | -2.026094 | -3.826368 | 1.428563 |
| H | -2.701088 | -2.654241 | 2.140383 |
| O | 2.982992 | 1.614962 | 1.006959 |
| H | 2.697424 | 1.596925 | 1.916854 |
| H | 3.887711 | 1.917374 | 0.999256 |
| O | -0.179894 | 1.056499 | 0.214706 |
| H | -0.575787 | 1.835605 | -0.236836 |
| H | -0.638047 | 0.254846 | -0.116236 |
| O | -1.359598 | -1.253074 | -0.611486 |
| H | -2.090985 | -1.211829 | -1.223797 |
| H | -1.652229 | -1.834163 | 0.112773 |
| O | 1.259265 | -1.387351 | -1.495667 |
| H | 0.348696 | -1.663738 | -1.349539 |
| H | 1.641442 | -1.932029 | -2.177985 |
| O | 1.433779 | 1.145988 | -1.051809 |
| H | 1.442069 | 0.167643 | -1.250596 |
| H | 2.014301 | 1.308108 | -0.266485 |

# $(H_2O)_8^+$

#1 (Single ring): +0 kcal/mol

| | | | |
|---|---|---|---|
| O | 0.157198 | 0.989409 | 1.883699 |
| O | -1.906599 | -0.330939 | 1.050173 |
| O | -1.665446 | -1.189471 | -1.647636 |
| O | 0.996821 | -0.132887 | -2.058394 |
| O | -0.407143 | 3.453840 | 2.593415 |
| O | 4.354108 | -0.238888 | 1.039515 |
| O | -3.340972 | -2.537488 | -3.242296 |
| O | 1.950003 | 0.766743 | 0.287966 |
| H | -2.287483 | -1.685406 | -2.231864 |
| H | 0.971774 | 0.886369 | 1.182617 |
| H | 5.167364 | 0.257436 | 0.995748 |
| H | -2.473510 | -0.860762 | 1.603547 |
| H | 4.589258 | -1.122965 | 1.308498 |
| H | 1.690224 | 0.445196 | -0.592138 |
| H | -0.055107 | 1.920407 | 2.112846 |
| H | 1.267013 | 0.094162 | -2.943169 |
| H | -4.248642 | -2.769779 | -3.062548 |
| H | -0.320741 | 3.767305 | 3.490490 |
| H | -3.140734 | -2.867995 | -4.114602 |
| H | -0.521683 | 4.221783 | 2.039205 |
| H | -0.649730 | 0.492353 | 1.596336 |
| H | 0.118009 | -0.514789 | -2.113854 |
| H | -1.941463 | -0.694345 | 0.158656 |
| H | 2.797723 | 0.371410 | 0.543315 |

#18 (Double ring): +1.48 kcal/mol

| | | | |
|---|---|---|---|
| O | 1.029317 | 1.553842 | 1.164090 |
| O | -1.480510 | 1.150761 | 1.350207 |
| O | -2.295530 | -1.325491 | 0.267349 |
| O | 0.343395 | -2.363289 | -0.241746 |
| O | 1.792653 | 2.997571 | -0.712863 |
| O | 3.333915 | 0.997534 | -1.578590 |
| O | -4.735605 | -2.312110 | -0.160396 |
| O | 2.228115 | -0.665382 | 0.558312 |
| H | 1.488916 | 0.685691 | 1.002634 |

| | | | |
|---|---|---|---|
| H | 3.180942 | 0.228272 | -1.027453 |
| H | -1.900315 | 0.345756 | 1.026079 |
| H | 3.866216 | 0.725683 | -2.320234 |
| H | 2.787182 | -1.084796 | 1.209078 |
| H | 1.298370 | 2.219466 | 0.433060 |
| H | 0.418817 | -3.143885 | -0.782829 |
| H | -4.948842 | -3.203919 | -0.424243 |
| H | 2.426204 | 2.439602 | -1.195285 |
| H | -5.561565 | -1.837974 | -0.102185 |
| H | -3.200226 | -1.690442 | 0.106982 |
| H | 2.167229 | 3.870084 | -0.622823 |
| H | 0.040708 | 1.421775 | 1.238208 |
| H | 1.587684 | -1.341279 | 0.259125 |
| H | -2.048204 | 1.542303 | 2.008285 |
| H | -0.592334 | -2.168721 | -0.142860 |

#22 (Tree): +1.59 kcal/mol

| | | | |
|---|---|---|---|
| O | -1.308925 | -4.534739 | -1.496473 |
| O | 1.407655 | 1.158699 | -0.609522 |
| O | -0.113504 | 2.526210 | -2.408396 |
| O | 0.553949 | -0.719116 | 3.100797 |
| O | 0.250379 | -0.740648 | 0.591238 |
| O | -1.372649 | 0.032450 | 4.847195 |
| O | 0.667965 | -2.988748 | -0.482644 |
| O | 0.088281 | 4.813222 | -3.854876 |
| H | 0.378359 | -0.760345 | 1.587143 |
| H | 2.166486 | 1.644998 | -0.301406 |
| H | 0.927813 | 1.716619 | -1.242899 |
| H | -1.570485 | -5.388443 | -1.161148 |
| H | 0.805384 | 5.432286 | -3.963193 |
| H | 0.433332 | -1.624140 | 0.147967 |
| H | -2.155145 | -0.448762 | 5.103364 |
| H | 1.478318 | -3.243322 | -0.914417 |
| H | -0.606514 | 5.093608 | -4.445283 |
| H | 1.189464 | -1.237299 | 3.585893 |
| H | 0.720056 | 0.027648 | 0.145385 |
| H | -0.146816 | -0.459290 | 3.719842 |
| H | -1.367486 | 0.836912 | 5.359532 |

| | | | |
|---|---|---|---|
| H | -0.044599 | -3.533682 | -0.853181 |
| H | 0.000947 | 3.358762 | -2.916328 |
| H | -1.832354 | -4.376540 | -2.277833 |

#40 (Multiple ring): +1.93 kcal/mol

| | | | |
|---|---|---|---|
| O | -0.110006 | -1.820632 | 1.293493 |
| O | -2.312812 | -0.062844 | 0.934628 |
| O | -2.323240 | -1.034834 | -1.753520 |
| O | 0.262367 | -1.357112 | -1.460996 |
| O | 1.570555 | 1.770564 | 0.322312 |
| O | 2.242229 | 0.592429 | -1.829018 |
| O | -0.917634 | 2.246324 | 0.272522 |
| O | 1.730356 | 0.068519 | 2.192858 |
| H | 0.099796 | -1.910794 | 0.354014 |
| H | 2.435745 | -0.129862 | 2.802486 |
| H | 1.194361 | -0.722995 | 2.058985 |
| H | 1.726653 | 1.125067 | 1.074277 |
| H | 1.711389 | -0.169144 | -2.076906 |
| H | -1.661663 | -0.710199 | 1.236428 |
| H | 1.859567 | 1.370512 | -0.548601 |
| H | -2.654566 | -0.640060 | -0.942945 |
| H | -1.512330 | 1.540363 | 0.563568 |
| H | -0.214123 | -2.706576 | 1.634959 |
| H | -1.333418 | 3.086607 | 0.446060 |
| H | -3.027281 | -0.081078 | 1.567655 |
| H | 0.597295 | 2.022406 | 0.301118 |
| H | -2.964869 | -0.892006 | -2.443338 |
| H | -0.680212 | -1.309504 | -1.764426 |
| H | 2.744989 | 0.881666 | -2.585521 |

#478 (Linear): +6.59 kcal/mol

| | | | |
|---|---|---|---|
| O | -0.469618 | 2.605832 | 4.059467 |
| O | -1.128444 | 4.278627 | 6.100177 |
| O | -1.379548 | -5.098440 | -5.290567 |
| O | 0.333736 | -3.329624 | -4.097596 |
| O | 0.498547 | 2.819699 | 1.492827 |
| O | 1.567682 | 0.673810 | 0.491864 |
| O | -0.348468 | -1.286588 | -2.649654 |

| | | | |
|---|---|---|---|
| O | 0.161305 | -1.161249 | -0.272920 |
| H | -0.470155 | -0.529548 | -3.215296 |
| H | -0.699472 | 3.239222 | 4.772943 |
| H | -0.081920 | -2.057709 | -3.202994 |
| H | -1.098327 | 5.229523 | 6.164114 |
| H | -1.625766 | -5.959636 | -4.963297 |
| H | 0.161747 | 2.863407 | 2.399114 |
| H | 1.214368 | -3.553857 | -4.382063 |
| H | 2.412175 | 0.494960 | 0.896651 |
| H | 1.199456 | 1.501599 | 0.879946 |
| H | -0.628366 | -1.284617 | 0.252140 |
| H | 0.754200 | -0.365336 | 0.075672 |
| H | 0.651473 | 3.711728 | 1.196408 |
| H | -1.437267 | 3.957723 | 6.943643 |
| H | -1.752524 | -5.024730 | -6.165156 |
| H | -0.272645 | -3.955954 | -4.517446 |
| H | -0.044711 | -1.183761 | -1.303166 |

#594 (Hemi-bonded): +13.34 kcal/mol

| | | | |
|---|---|---|---|
| O | -1.591104 | 1.740558 | -0.405788 |
| O | -4.219121 | -2.760543 | -0.099107 |
| O | 3.599816 | 2.642123 | -0.146518 |
| O | 0.831229 | 1.196647 | 0.781496 |
| O | 0.382393 | -1.390096 | 1.297398 |
| O | -1.978793 | -1.189425 | 0.199456 |
| O | 2.368044 | -1.413934 | -0.569502 |
| O | 1.757078 | 1.026732 | -1.048821 |
| H | 3.649874 | 2.932178 | 0.760843 |
| H | -1.543488 | 1.944835 | -1.338500 |
| H | -0.005178 | 1.458906 | 0.352989 |
| H | 0.722481 | 0.250518 | 1.035952 |
| H | -4.393065 | -3.351414 | -0.827270 |
| H | -0.536190 | -1.458686 | 0.955889 |
| H | 0.386297 | -1.745299 | 2.182715 |
| H | -4.863782 | -2.966512 | 0.572900 |
| H | -2.205036 | -0.298938 | -0.061499 |
| H | -2.764215 | -1.742136 | 0.097031 |
| H | -2.157660 | 2.408045 | -0.022151 |

| | | | |
|---|---|---|---|
| H | 1.725701 | -1.762306 | 0.060571 |
| H | 2.625734 | -2.112001 | -1.164955 |
| H | 4.347596 | 3.014765 | -0.606786 |
| H | 2.045670 | 0.073931 | -0.916909 |
| H | 2.469006 | 1.623861 | -0.702458 |

The parameters $\alpha$ and $\beta$ in the width equation:

$\Gamma = \alpha(\Delta\omega)^{\beta} = \alpha(\omega_{free\ OH} - \omega_{H-bonded\ OH})^{\beta}$

| Size | $\alpha$ | $\beta$ |
|---|---|---|
| $(H_2O)_5^+$ | 0.00269 | 1.66324 |
| $(H_2O)_6^+$ | 0.00112 | 1.81286 |
| $(H_2O)_7^+$ | 0.00476 | 1.65940 |
| $(H_2O)_8^+$ | 0.04640 | 1.29963 |