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


# Supporting information for

## Energetics of Proton Configurations in Water Polyhedra and Clathrate Frameworks: Topology vs. Geometry

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**Table S1.** Potential energy U (kcal/mol) of the lowest-energy proton configurations for various polyhedra, total dipole moments (magnitude and direction) (Debyes), and potential energy per molecule U/N (kJ/mol). The data correspond to geometric optimization with the TIP4P potential. Calculations were performed with the Tinker molecular modeling package, version 6.2.

| Polyhedron | U | Dx | Dy | Dz | D | N | U/N |
|---|---|---|---|---|---|---|---|
| D ($5^{12}$) | -197.4744 | 0.598 | -0.934 | 0.764 | 1.347 | 20 | -41.3116 |
| T ($5^{12}6^{2}$) | -238.0425 | -0.01 | 0.006 | 0.809 | 0.809 | 24 | -41.4987 |
| K ($4^{6}6^{8}$) | -238.4780 | 0 | 0 | 0 | 0 | 24 | -41.5747 |
| 2 ($4^{1}5^{10}6^{3}$) | -237.3113 | -1.057 | -1.596 | -1.927 | 2.716 | 24 | -41.3713 |
| 3 ($4^{2}5^{8}6^{4}$) | -237.1987 | 0 | 0 | 0 | 0 | 24 | -41.3516 |
| 4 ($4^{2}5^{8}6^{4}$) | -236.9954 | 0.175 | -0.081 | 0.968 | 0.987 | 24 | -41.3162 |
| 5 ($4^{2}5^{8}6^{4}$) | -237.7371 | 1.234 | 1.4 | -0.029 | 1.866 | 24 | -41.4455 |
| 6 ($4^{2}5^{8}6^{4}$) | -237.1950 | -1.462 | 1.528 | 0.471 | 2.167 | 24 | -41.3510 |
| 12 ($4^{2}5^{8}6^{4}$) | -237.1119 | 2.393 | -1.486 | 0.026 | 2.817 | 24 | -41.3365 |
| 22 ($4^{3}5^{6}6^{5}$) | -237.2418 | 0 | -0.001 | 0.133 | 0.133 | 24 | -41.3592 |
| 31 ($4^{4}5^{4}6^{6}$) | -237.8472 | 1.469 | 1.996 | 0.041 | 2.479 | 24 | -41.4647 |

**Table S2.** Coordinates for lowest energy configuration of the pentagonal dodecahedron $(H_2O)_{20}$, (D-cage) calculated with the TIP4P potential

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | 2.30067113 | -0.13104076 | 2.82584946 |
| H | 1.76214871 | 0.64889392 | 2.95974246 |
| H | 1.6874594 | -0.86206297 | 2.90207113 |
| O | 0.69441656 | 2.0573317 | 3.02269116 |
| H | -0.24739382 | 1.89012746 | 3.05829725 |
| H | 0.8089749 | 2.62336633 | 2.25933474 |
| O | -2.00124588 | 1.51721923 | 3.18955217 |
| H | -1.9707806 | 0.56220662 | 3.13250281 |
| H | -2.2378076 | 1.69584056 | 4.09969766 |
| O | -1.90703361 | -1.15721308 | 3.02307599 |
| H | -1.04052038 | -1.56360388 | 3.00780579 |
| H | -2.35866953 | -1.52642442 | 2.264169 |
| O | 0.60352815 | -2.29742711 | 2.99110544 |
| H | 0.80710706 | -2.81319618 | 2.21086847 |
| H | 0.83545457 | -2.86843214 | 3.72349553 |
| O | 3.81526541 | 0.01554396 | 0.6190502 |
| H | 4.71330796 | 0.05629954 | 0.94782124 |
| H | 3.27296493 | -0.02557131 | 1.40673767 |
| O | 1.04587131 | 3.61638532 | 0.7888606 |
| H | 1.43495232 | 4.48287644 | 0.90735514 |
| H | 1.69459314 | 3.12948337 | 0.28061035 |
| O | -3.07237117 | 2.23014239 | 0.77783765 |
| H | -2.69599653 | 1.99270653 | 1.62530339 |
| H | -3.80423098 | 2.8080737 | 0.9937276 |
| O | -3.15484834 | -2.15000921 | 0.78950913 |
| H | -2.46331252 | -2.62107138 | 0.32463228 |
| H | -3.87683795 | -2.77609768 | 0.84406266 |
| O | 1.2221915 | -3.75084751 | 0.75586974 |
| H | 1.81632141 | -3.19807317 | 0.24824584 |
| H | 1.5301918 | -4.64314739 | 0.59722369 |
| O | 2.87421943 | 2.26122846 | -0.64860863 |
| H | 3.22106005 | 1.47756688 | -0.22221919 |
| H | 2.60438454 | 1.96243104 | -1.51702159 |
| O | -1.16955886 | 3.42500631 | -0.82394011 |
| H | -0.40856268 | 3.51735467 | -0.25071377 |
| H | -1.83433717 | 3.00895843 | -0.27511792 |
| O | -3.59253824 | 0.03924277 | -0.81346671 |
| H | -3.42125077 | 0.79637894 | -0.25343344 |
| H | -3.45677587 | -0.71706665 | -0.24268086 |
| O | -1.21590255 | -3.48084868 | -0.49840472 |
| H | -0.36156836 | -3.57556057 | -0.0772461 |
| H | -1.02100977 | -3.09491859 | -1.35239922 |
| O | 2.89875247 | -2.22026454 | -0.6817806 |
| H | 3.25392062 | -1.44525262 | -0.24652901 |
| H | 2.58530287 | -1.89835445 | -1.52697589 |
| O | 2.0752944 | 1.46211092 | -3.15898902 |
| H | 1.14627332 | 1.69175384 | -3.13859804 |
| H | 2.45925339 | 2.07111342 | -3.78980064 |
| O | -0.51782401 | 2.1025042 | -3.11305011 |
| H | -0.77944777 | 2.61767413 | -2.34990872 |
| H | -1.14563405 | 1.38052531 | -3.14190973 |
| O | -2.25483855 | -0.02715804 | -3.14775891 |
| H | -2.72561201 | 0.00372051 | -2.31490196 |
| H | -2.94360301 | -0.04637138 | -3.81218814 |
| O | -0.6214715 | -2.21703763 | -2.83135742 |
| H | -1.1881828 | -1.4587706 | -2.97313631 |
| H | 0.26714275 | -1.87237158 | -2.9196856 |
| O | 1.95940925 | -1.26674271 | -3.08907081 |
| H | 2.00583274 | -0.31094446 | -3.11201425 |
| H | 2.36071066 | -1.54632448 | -3.91188491 |

**Table S3.** Coordinates for lowest energy configuration of the T-cage $(H_2O)_{24}$ cluster calculated with the TIP4P potential

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | -2.81747714 | 0.17698371 | 2.87837948 |
| H | -2.31387461 | -0.6360862 | 2.8392175 |
| H | -3.35028183 | 0.09142275 | 3.66896807 |
| O | -4.30234235 | -0.00189396 | 0.57453218 |
| H | -3.78864972 | 0.07535666 | 1.37851232 |
| H | -4.12258965 | 0.80749337 | 0.0961882 |
| O | -3.71092135 | -2.30377398 | -0.75058959 |
| H | -3.9848243 | -1.50201673 | -0.30517482 |
| H | -3.25704998 | -1.99877989 | -1.5362175 |
| O | -2.3323937 | -3.93605243 | 0.85173336 |
| H | -2.99344799 | -4.51579814 | 1.23006387 |
| H | -2.82656931 | -3.35118694 | 0.27731655 |
| O | -1.51006973 | -2.17843612 | 2.80784787 |
| H | -1.7680322 | -2.79233903 | 2.12023576 |
| H | -0.55704684 | -2.25543186 | 2.85313436 |
| O | -3.75154159 | 2.33090634 | -0.78598047 |
| H | -4.50653948 | 2.85857054 | -1.0463274 |
| H | -3.23687243 | 2.9095501 | -0.22338035 |
| O | -2.2637698 | 3.98781939 | 0.79405977 |
| H | -1.49585635 | 4.12335801 | 0.2389291 |
| H | -2.44494505 | 4.85021322 | 1.16780334 |
| O | -1.20264248 | 2.39721135 | 2.77793834 |
| H | -1.74673887 | 1.61032317 | 2.80952881 |
| H | -1.58778697 | 2.92744115 | 2.08026225 |
| O | -2.3611554 | -1.46393717 | -2.99220294 |
| H | -2.83780777 | -1.60686949 | -3.80988546 |
| H | -2.29385685 | -0.51208118 | -2.91688427 |
| O | -2.27702401 | 1.22439748 | -2.83809971 |
| H | -2.77472357 | 1.61926666 | -2.12213511 |
| H | -1.47672584 | 1.74687192 | -2.89077935 |
| O | -0.13397983 | -4.43065097 | -0.69024447 |
| H | -0.89941793 | -4.26193387 | -0.14081669 |
| H | -0.21037438 | -5.35385069 | -0.93127973 |
| O | 0.11323965 | -2.64607601 | -2.77924831 |
| H | -0.73855396 | -2.21553574 | -2.85214939 |
| H | 0.0109776 | -3.25860926 | -2.05084092 |
| O | -0.01153466 | 2.77640896 | -2.99381334 |
| H | 0.77702533 | 2.24227627 | -2.8983815 |
| H | 0.12368764 | 3.26057814 | -3.80838499 |
| O | -0.12097687 | 4.36552973 | -0.75445249 |
| H | -0.06381122 | 3.81987586 | -1.53881578 |
| H | 0.69877002 | 4.20200115 | -0.28807788 |
| O | 2.14454849 | -3.71134099 | 0.68352449 |
| H | 1.35974383 | -3.97087816 | 0.20087147 |
| H | 1.81080816 | -3.28747897 | 1.4742142 |
| O | 1.21857623 | -2.46437891 | 2.94895845 |
| H | 1.67155664 | -1.62275353 | 2.89692658 |
| H | 1.54901298 | -2.86547374 | 3.75280317 |
| O | 2.48552022 | -1.37837762 | -2.93149912 |
| H | 1.62656223 | -1.79429925 | -2.85779565 |
| H | 2.85780478 | -1.73762245 | -3.73684327 |
| O | 2.27003442 | 1.35959814 | -2.78155294 |
| H | 2.32377083 | 0.40528067 | -2.83276239 |
| H | 2.84248282 | 1.59333488 | -2.05086709 |
| O | 3.85924057 | -2.07773776 | -0.6564576 |
| H | 3.2961464 | -2.7058809 | -0.20413803 |
| H | 3.37814846 | -1.85456728 | -1.45331214 |
| O | 3.91290459 | 2.08374309 | -0.68719224 |
| H | 4.14240364 | 1.3488011 | -0.11848994 |
| H | 4.75367626 | 2.47379787 | -0.92634095 |
| O | 2.13393977 | 3.72717845 | 0.62838364 |
| H | 2.75700179 | 3.16680348 | 0.16577641 |
| H | 1.92369521 | 3.24377391 | 1.42735117 |
| O | 1.48826696 | 2.3520587 | 2.9167638 |
| H | 1.66040453 | 2.85637926 | 3.71191239 |
| H | 0.53363039 | 2.32234987 | 2.85337418 |
| O | 4.5638237 | -0.03289194 | 0.91015458 |
| H | 4.31148152 | -0.76579331 | 0.34854008 |
| H | 5.39153854 | -0.30705927 | 1.30506249 |
| O | 2.60602005 | -0.1564591 | 2.8449793 |
| H | 2.19586508 | 0.70815669 | 2.86605739 |
| H | 3.27527931 | -0.08806264 | 2.16406388 |

**Table S4.** Coordinates for lowest energy configuration of the Kelvin polyhedron $(H_2O)_{24}$, $4^6 6^8$ calculated with the TIP4P potential

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | 1.84873224 | 3.74511918 | 0.0047781 |
| H | 1.26496892 | 3.79854776 | 0.7614799 |
| H | 1.26571816 | 3.79968332 | -0.75242014 |
| O | 3.93562769 | 2.0396277 | 0.00288185 |
| H | 3.17013829 | 2.61430788 | 0.00360052 |
| H | 4.68387504 | 2.63658423 | 0.00368266 |
| O | 3.75083609 | -0.01429738 | 1.83714229 |
| H | 3.80537814 | 0.74314764 | 1.25444679 |
| H | 3.80056095 | -0.77074437 | 1.25272186 |
| O | 2.05192285 | -0.01031183 | 3.92938327 |
| H | 2.62420553 | -0.01164608 | 3.16210067 |
| H | 2.65121237 | -0.01267494 | 4.67576006 |
| O | 0.00530022 | 1.83296491 | 3.75284813 |
| H | 0.76043289 | 1.24700274 | 3.80437305 |
| H | -0.75346047 | 1.25170098 | 3.80429038 |
| O | 0.01180696 | 3.9273422 | 2.05656753 |
| H | 0.00940921 | 3.15935104 | 2.62789552 |
| H | 0.01396724 | 4.67296905 | 2.65679063 |
| O | 0.01334599 | 3.93114634 | -2.0480806 |
| H | 0.01596805 | 4.67807791 | -2.64667746 |
| H | 0.0108198 | 3.16440242 | -2.62108078 |
| O | 0.00643842 | 1.84051697 | -3.74893257 |
| H | 0.76146695 | 1.25451986 | -3.80157442 |
| H | -0.7524255 | 1.25950269 | -3.8016563 |
| O | 2.0527522 | -0.00266696 | -3.92894964 |
| H | 2.65221844 | -0.00337872 | -4.67518791 |
| H | 2.62485446 | -0.00527771 | -3.16153577 |
| O | 3.75117518 | -0.00998466 | -1.83631371 |
| H | 3.80556087 | 0.74612094 | -1.25186666 |
| H | 3.80083574 | -0.76777132 | -1.25362593 |
| O | 3.92264456 | -2.06503424 | -0.00201447 |
| H | 4.66700813 | -2.66682679 | -0.00267336 |
| H | 3.15344752 | -2.6347421 | -0.00285748 |
| O | 1.82470363 | -3.75689643 | -0.00432569 |
| H | 1.24116783 | -3.80779573 | 0.75272587 |
| H | 1.24077729 | -3.80631802 | -0.76117401 |
| O | -0.01224901 | -3.93109453 | 2.04816778 |
| H | -0.01460309 | -4.67803058 | 2.64676015 |
| H | -0.00994737 | -3.16435334 | 2.62117258 |
| O | -0.00606888 | -1.84048278 | 3.7490846 |
| H | 0.75268157 | -1.25933076 | 3.80192327 |
| H | -0.76121175 | -1.25462506 | 3.80163767 |
| O | -2.0527325 | 0.00240056 | 3.92890005 |
| H | -2.65216803 | 0.0031904 | 4.67516291 |
| H | -2.62486573 | 0.00513909 | 3.16150973 |
| O | -3.75123666 | 0.01020733 | 1.83633644 |
| H | -3.80077106 | 0.76786815 | 1.25347431 |
| H | -3.80571922 | -0.74602376 | 1.2520608 |
| O | -3.92248957 | 2.06481354 | 0.00147922 |
| H | -4.66690229 | 2.66654543 | 0.001999 |
| H | -3.15333906 | 2.63458447 | 0.00212119 |
| O | -0.00566185 | -1.83289033 | -3.75323293 |
| H | 0.75321252 | -1.25176497 | -3.80456376 |
| H | -0.76067992 | -1.2467852 | -3.80481128 |
| O | -0.01289158 | -3.92696256 | -2.05656331 |
| H | -0.01027125 | -3.15906043 | -2.62800997 |
| H | -0.01530814 | -4.67268137 | -2.65667118 |
| O | -1.84870186 | -3.74508457 | -0.00374844 |
| H | -1.26520227 | -3.79976327 | 0.75306747 |
| H | -1.26540899 | -3.79823662 | -0.7608324 |
| O | -3.93578742 | -2.03984677 | -0.00230444 |
| H | -3.17024642 | -2.61445847 | -0.0027546 |
| H | -4.68398115 | -2.63687063 | -0.00300941 |
| O | -3.75081122 | 0.01360073 | -1.83712621 |
| H | -3.8004983 | 0.77016071 | -1.25284886 |
| H | -3.8053999 | -0.74373132 | -1.25428826 |
| O | -2.05193388 | 0.01084085 | -3.92940186 |
| H | -2.62421268 | 0.01154434 | -3.16211553 |
| H | -2.65122488 | 0.01448524 | -4.67577232 |
| O | -1.82472389 | 3.75691769 | 0.00341985 |
| H | -1.24125305 | 3.80645093 | 0.76061208 |
| H | -1.24074769 | 3.80787986 | -0.75328781 |

**Table S5.** Coordinates for lowest energy configuration of the $(H_2O)_{24}$ cluster No. 2 calculated with the TIP4P potential

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | -2.99192713 | 2.51213783 | -0.09927955 |
| H | -2.92883318 | 2.09876351 | 0.76175045 |
| H | -2.44540708 | 3.29494638 | -0.03029812 |
| O | -2.89372908 | 1.39672605 | 2.42309883 |
| H | -3.67123766 | 1.66727729 | 2.91147806 |
| H | -2.92392095 | 0.44007187 | 2.4346345 |
| O | -2.97808253 | 1.45153838 | -2.56192737 |
| H | -2.97042783 | 1.78537952 | -1.66486364 |
| H | -3.61384983 | 2.00306866 | -3.01782881 |
| O | -1.30990204 | 4.64494266 | 0.03701031 |
| H | -0.72368685 | 4.60197301 | -0.7184612 |
| H | -0.72827472 | 4.59216512 | 0.79540074 |
| O | -0.53578178 | 2.31423138 | 3.50241726 |
| H | -1.35078919 | 1.98392968 | 3.12440199 |
| H | -0.02236401 | 1.52840713 | 3.68980532 |
| O | -3.00783328 | -1.33247909 | 2.519103 |
| H | -3.66569709 | -1.89198051 | 2.93190465 |
| H | -2.93664509 | -1.66560092 | 1.62456741 |
| O | -0.52815486 | 2.32727075 | -3.46291121 |
| H | -1.36452331 | 1.98750998 | -3.14466243 |
| H | -0.00023448 | 1.54664779 | -3.63071975 |
| O | -2.85844195 | -1.27608249 | -2.4680943 |
| H | -3.67041586 | -1.54510537 | -2.89769514 |
| H | -2.88840704 | -0.31938298 | -2.47583971 |
| O | 0.50149276 | 4.35524464 | -2.0209257 |
| H | 0.15627066 | 3.62057776 | -2.52819103 |
| H | 0.67996474 | 5.03370174 | -2.67213653 |
| O | 0.51552987 | 4.34111216 | 2.08167747 |
| H | 0.693951 | 5.01591431 | 2.73668877 |
| H | 0.16667963 | 3.6050024 | 2.5843481 |
| O | 0.91768541 | 0.05359643 | 4.0485218 |
| H | 1.61146691 | -0.0236215 | 3.39358939 |
| H | 1.37902899 | 0.06036637 | 4.88718031 |
| O | -0.60030942 | -2.17640186 | 3.55553256 |
| H | -1.42360104 | -1.84700276 | 3.19508982 |
| H | -0.0874178 | -1.38962774 | 3.7403582 |
| O | -2.83599416 | -2.38788112 | 0.05806638 |
| H | -2.81480697 | -1.97011196 | -0.80289348 |
| H | -2.19511791 | -3.09623963 | -0.00307029 |
| O | 0.99116315 | 0.10281706 | -3.98638296 |
| H | 1.47667884 | 0.17452433 | -4.80818855 |
| H | 1.66644263 | -0.01384905 | -3.31808776 |
| O | -0.50545212 | -2.16086871 | -3.58485773 |
| H | -1.32538869 | -1.85260288 | -3.19897168 |
| H | -0.0033566 | -1.36297663 | -3.75068942 |
| O | 2.18260461 | 3.55095902 | 0.02201901 |
| H | 1.65514807 | 3.81731418 | -0.73102572 |
| H | 1.66221347 | 3.80899587 | 0.7828356 |
| O | 2.91974717 | -0.24626802 | 2.28511905 |
| H | 3.08522526 | 0.26926041 | 1.49576533 |
| H | 3.01720307 | -1.15563566 | 2.00265721 |
| O | 0.69033686 | -4.06456809 | 2.13947881 |
| H | 0.23451573 | -3.38520916 | 2.63639971 |
| H | 0.76997021 | -4.79660583 | 2.75104329 |
| O | -0.91176479 | -4.30762839 | -0.07717781 |
| H | -0.34621792 | -4.25278515 | 0.69313433 |
| H | -0.31237272 | -4.2391365 | -0.82032641 |
| O | 2.94048654 | -0.34052408 | -2.18628077 |
| H | 3.11438984 | 0.2086529 | -1.42182402 |
| H | 2.99356408 | -1.23695048 | -1.85486814 |
| O | 0.75191234 | -4.12930686 | -2.2650307 |
| H | 0.56389362 | -4.91480003 | -2.77872446 |
| H | 0.31058577 | -3.42283672 | -2.73658413 |
| O | 3.50667722 | 1.20144062 | 0.01829715 |
| H | 2.99859824 | 2.01266415 | 0.01630372 |
| H | 4.4171346 | 1.48866921 | 0.08757145 |
| O | 3.03102152 | -2.82174376 | 1.41493549 |
| H | 2.22685677 | -3.27425733 | 1.6694593 |
| H | 3.03647021 | -2.86169794 | 0.45858523 |
| O | 3.04054498 | -2.96019615 | -1.33437705 |
| H | 2.2415361 | -3.38259802 | -1.64964409 |
| H | 3.75010017 | -3.50793331 | -1.67015567 |

**Table S6.** Coordinates for lowest energy configuration of the $(H_2O)_{24}$ cluster No. 3 calculated with the TIP4P potential

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | 1.22880172 | -4.27757338 | 1.35762305 |
| H | 1.41167029 | -4.36496799 | 0.42212687 |
| H | 0.28189715 | -4.39783927 | 1.4293147 |
| O | 1.49606217 | -4.50197685 | -1.37747946 |
| H | 1.79355823 | -3.69287768 | -1.79351607 |
| H | 1.91330937 | -5.19936563 | -1.88323188 |
| O | 2.27582749 | -2.26393694 | -2.63248071 |
| H | 2.60551561 | -1.46818982 | -2.21495932 |
| H | 1.55878094 | -1.96275615 | -3.19048269 |
| O | 3.29398844 | 0.0062578 | -1.45535449 |
| H | 3.1328225 | -0.01302359 | -0.51201701 |
| H | 4.24761657 | -0.01034617 | -1.53628368 |
| O | 2.99133131 | -0.05850491 | 1.23225428 |
| H | 2.67026012 | -0.81073632 | 1.72953995 |
| H | 2.69890569 | 0.70288875 | 1.73325207 |
| O | 2.22506194 | -2.2230367 | 2.77519928 |
| H | 1.87019309 | -2.93261457 | 2.23966293 |
| H | 3.05557913 | -2.56468325 | 3.10648567 |
| O | -1.52292751 | -4.47635938 | 1.39869835 |
| H | -2.0769341 | -5.14131136 | 1.80753501 |
| H | -1.78057095 | -3.65676092 | 1.82072923 |
| O | -1.24323205 | -4.18536965 | -1.32856583 |
| H | -0.29932449 | -4.32159915 | -1.41049197 |
| H | -1.41984391 | -4.28539178 | -0.39313243 |
| O | -2.18151959 | -2.09768182 | -2.74529379 |
| H | -2.81086855 | -2.51275747 | -3.3350937 |
| H | -1.84950501 | -2.81492284 | -2.20532761 |
| O | 0.12738739 | -1.3841929 | -4.05099112 |
| H | -0.67906467 | -1.63290667 | -3.59931827 |
| H | 0.09641741 | -0.42822862 | -4.0884742 |
| O | -2.99133722 | 0.05851558 | -1.23226065 |
| H | -2.69891185 | -0.70288122 | -1.73325382 |
| H | -2.67026451 | 0.81074383 | -1.72955011 |
| O | -2.2250617 | 2.22304049 | -2.77521321 |
| H | -3.05557696 | 2.56469154 | -3.10649981 |
| H | -1.8701919 | 2.93261428 | -2.23967208 |
| O | -0.00932139 | 1.36000605 | -4.12220049 |
| H | -0.09797805 | 1.74484354 | -4.99413624 |
| H | -0.791562 | 1.64839984 | -3.65192347 |
| O | 2.17374552 | 2.20182706 | -2.66941294 |
| H | 2.54704605 | 1.4324543 | -2.23936165 |
| H | 1.44398663 | 1.8582369 | -3.1848056 |
| O | -1.22879973 | 4.27756549 | -1.35762134 |
| H | -0.28189511 | 4.39783161 | -1.42931196 |
| H | -1.41166942 | 4.36496071 | -0.42212543 |
| O | 1.52292892 | 4.47635565 | -1.3986949 |
| H | 1.78057369 | 3.6567602 | -1.82073082 |
| H | 2.07692931 | 5.1413121 | -1.80753266 |
| O | -1.49606255 | 4.50197414 | 1.37748089 |
| H | -1.91331063 | 5.19936407 | 1.88323101 |
| H | -1.79355723 | 3.69287599 | 1.79352046 |
| O | 1.24323172 | 4.18536973 | 1.32856999 |
| H | 1.41984481 | 4.28538962 | 0.39313657 |
| H | 0.29932397 | 4.32159887 | 1.41049449 |
| O | -2.27582551 | 2.26393722 | 2.63248877 |
| H | -2.60551214 | 1.46819187 | 2.21496285 |
| H | -1.55878148 | 1.96275398 | 3.19049267 |
| O | -3.29398572 | -0.00625072 | 1.45534919 |
| H | -4.24761358 | 0.01035447 | 1.53628133 |
| H | -3.13282262 | 0.01303332 | 0.51201127 |
| O | 0.00932505 | -1.36001329 | 4.12219881 |
| H | 0.79156468 | -1.64839936 | 3.65191541 |
| H | 0.09797091 | -1.74488624 | 4.99412 |
| O | -0.1273907 | 1.38418726 | 4.05100422 |
| H | -0.09641787 | 0.42822313 | 4.08848887 |
| H | 0.67906003 | 1.63290263 | 3.59932987 |
| O | 2.18151226 | 2.09768156 | 2.74530193 |
| H | 2.81086134 | 2.51275609 | 3.33510249 |
| H | 1.84949949 | 2.81492317 | 2.20533542 |
| O | -2.17373995 | -2.20182164 | 2.66940191 |
| H | -2.54704118 | -1.43244851 | 2.2393519 |
| H | -1.44398142 | -1.85823167 | 3.18479521 |

**Table S7.** Coordinates for lowest energy configuration of the $(H_2O)_{24}$ cluster No. 4 calculated with the TIP4P potential

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | 1.20238644 | -3.44726581 | -2.2713668 |
| H | 1.48876638 | -4.21298752 | -2.7692509 |
| H | 1.10712294 | -3.76639411 | -1.373974 |
| O | 0.87509286 | -4.4574663 | 0.2042385 |
| H | 1.338712 | -4.09577828 | 0.9595337 |
| H | -0.03863208 | -4.50763625 | 0.4849903 |
| O | 1.9413271 | -3.42159615 | 2.5230992 |
| H | 1.05806725 | -3.3730413 | 2.8887853 |
| H | 2.39880572 | -4.04871438 | 3.0831598 |
| O | 2.67066578 | -0.81495135 | 2.0294862 |
| H | 2.44521099 | -1.73252025 | 2.1826831 |
| H | 2.09055766 | -0.32478717 | 2.6121057 |
| O | 3.52001049 | 0.00336344 | -0.4039907 |
| H | 3.16564875 | -0.28336752 | 0.437701 |
| H | 4.46911168 | -0.06617432 | -0.3010186 |
| O | 2.60138069 | -1.12580103 | -2.7392611 |
| H | 2.14257962 | -1.9340861 | -2.5103317 |
| H | 2.89021417 | -0.7677979 | -1.8998322 |
| O | -1.38919905 | -2.72687994 | -2.8504822 |
| H | -0.48181888 | -2.96431431 | -2.6593854 |
| H | -1.32618304 | -1.8920887 | -3.3145775 |
| O | -2.8763713 | -2.74880288 | -0.5702929 |
| H | -2.40429269 | -2.75447002 | -1.4029642 |
| H | -3.09505577 | -1.82836799 | -0.4246613 |
| O | -1.71771305 | -4.44722544 | 1.151816 |
| H | -2.13764756 | -3.81527689 | 0.5682683 |
| H | -2.28676939 | -5.21633042 | 1.1220795 |
| O | -0.592423 | -3.32412736 | 3.3991702 |
| H | -1.08020936 | -3.70518429 | 2.6690387 |
| H | -0.92468165 | -2.42913821 | 3.4686716 |
| O | -1.36342492 | -0.71502227 | 3.7253678 |
| H | -1.71547091 | -0.60909216 | 4.6091519 |
| H | -0.50525792 | -0.29216818 | 3.7566034 |
| O | 1.0815924 | 0.49499331 | 3.8729278 |
| H | 1.66447913 | 0.56670392 | 4.6287932 |
| H | 0.91805349 | 1.40050223 | 3.6092225 |
| O | 0.58629485 | 3.05402982 | 3.2298397 |
| H | 1.09323882 | 3.48543527 | 2.541996 |
| H | -0.32614353 | 3.23866539 | 3.0071342 |
| O | 1.8255984 | 4.31809106 | 1.1170662 |
| H | 2.42065204 | 5.06746651 | 1.1411376 |
| H | 2.23210789 | 3.70853912 | 0.5010886 |
| O | 2.95142907 | 2.68335662 | -0.6898883 |
| H | 3.11381142 | 1.74528086 | -0.5905018 |
| H | 2.48690646 | 2.75952446 | -1.5233444 |
| O | 1.48149157 | 2.85598403 | -2.9764316 |
| H | 1.40929004 | 2.04721789 | -3.4833005 |
| H | 0.57729796 | 3.08811145 | -2.7648125 |
| O | 1.35335401 | 0.52720476 | -4.4355227 |
| H | 1.97478863 | 0.64943483 | -5.1532348 |
| H | 1.80164132 | -0.0605538 | -3.8274025 |
| O | -1.23099237 | -0.3240753 | -4.1978904 |
| H | -0.32804989 | -0.0206358 | -4.2919711 |
| H | -1.56712915 | -0.35854678 | -5.093466 |
| O | -3.60483194 | -0.12054498 | -0.2176234 |
| H | -3.19619191 | 0.35801927 | -0.9388872 |
| H | -4.54249869 | -0.08479948 | -0.4066609 |
| O | -2.90309098 | 0.98191417 | 2.1952174 |
| H | -2.38054335 | 0.31999418 | 2.6480283 |
| H | -3.12470842 | 0.57953186 | 1.3554519 |
| O | -1.99962037 | 3.50760876 | 2.3890557 |
| H | -2.32966532 | 2.61581529 | 2.2794812 |
| H | -2.71029446 | 3.97416253 | 2.8289441 |
| O | -0.74779473 | 4.51715691 | 0.1472741 |
| H | 0.16156136 | 4.50223863 | 0.4457381 |
| H | -1.24936731 | 4.17849736 | 0.8888714 |
| O | -1.10313618 | 3.53111342 | -2.3305289 |
| H | -0.98838065 | 3.8530084 | -1.4364111 |
| H | -1.44789215 | 4.28213764 | -2.8135794 |
| O | -2.56728421 | 1.20136497 | -2.330448 |
| H | -2.10855524 | 0.66700474 | -2.9787217 |
| H | -2.06978637 | 2.01846186 | -2.2975787 |

**Table S8.** Coordinates for lowest energy configuration of the $(H_2O)_{24}$ cluster No. 5 calculated with the TIP4P potential

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | 3.4712931 | 0.04462068 | -1.78762322 |
| H | 4.32063162 | -0.14244542 | -2.18745092 |
| H | 2.92228149 | -0.70091203 | -2.03052048 |
| O | 1.98576928 | -2.05108663 | -2.6050266 |
| H | 1.66347501 | -2.74597752 | -2.03101885 |
| H | 1.25222083 | -1.86421947 | -3.19087571 |
| O | 1.02979195 | -4.06946919 | -1.00496443 |
| H | 1.34138807 | -4.95990641 | -1.16701763 |
| H | 1.25785859 | -3.89796197 | -0.09128903 |
| O | 1.64038 | -3.69186697 | 1.5883521 |
| H | 2.17324023 | -2.95768797 | 1.89375841 |
| H | 0.87164348 | -3.68403853 | 2.15862811 |
| O | 3.02361483 | -1.54331271 | 2.63092843 |
| H | 3.8844254 | -1.67351668 | 3.02877757 |
| H | 3.15098782 | -0.82284516 | 2.01372955 |
| O | 3.48986696 | 0.49410698 | 0.92400274 |
| H | 3.46241114 | 0.33249754 | -0.01905633 |
| H | 3.14424062 | 1.38091922 | 1.02568034 |
| O | 2.1795447 | 2.08170816 | -3.09634456 |
| H | 2.63594557 | 1.37836608 | -2.63456539 |
| H | 1.99621572 | 2.73354541 | -2.41978671 |
| O | -0.10557805 | 1.17919883 | -4.26190004 |
| H | 0.71234643 | 1.53415763 | -3.91371097 |
| H | -0.79115532 | 1.61630693 | -3.75677416 |
| O | -0.07571948 | -1.49334751 | -4.34728868 |
| H | -0.09400702 | -0.53699235 | -4.31148083 |
| H | 0.23562698 | -1.69455042 | -5.22979229 |
| O | -2.3408857 | -2.17711412 | -2.98327362 |
| H | -1.54346373 | -1.95045514 | -3.46178774 |
| H | -2.92046338 | -2.55181551 | -3.6465386 |
| O | -1.71279416 | -3.9019432 | -0.93443402 |
| H | -0.75806687 | -3.96253194 | -0.96694001 |
| H | -1.93942132 | -3.3008953 | -1.64409125 |
| O | -2.51605125 | -2.9514807 | 1.48536016 |
| H | -2.28615669 | -3.32581015 | 0.63491452 |
| H | -2.86535197 | -2.08441508 | 1.2794037 |
| O | -0.55351684 | -3.47368694 | 3.24000032 |
| H | -1.2571521 | -3.25278079 | 2.62981204 |
| H | -0.90675872 | -4.19309444 | 3.76335953 |
| O | 0.74538468 | -1.22048103 | 4.15451457 |
| H | 1.56035523 | -1.28071685 | 3.65609056 |
| H | 0.24509541 | -1.99271607 | 3.89070493 |
| O | -0.56591276 | 1.12249366 | 4.33173395 |
| H | -0.09527094 | 0.29481424 | 4.2333729 |
| H | -0.74278788 | 1.18793598 | 5.27017113 |
| O | 0.50106793 | 3.22129491 | 2.89797469 |
| H | 0.21544453 | 2.48007045 | 3.43205092 |
| H | -0.29913956 | 3.53718098 | 2.47831314 |
| O | 2.64623864 | 3.09979188 | 1.28087375 |
| H | 1.87620976 | 3.10800152 | 1.84939813 |
| H | 3.34159309 | 3.48645286 | 1.813046 |
| O | 1.66987662 | 3.93887635 | -1.13158487 |
| H | 2.01786002 | 3.6346563 | -0.29337872 |
| H | 2.10154521 | 4.78032078 | -1.27945422 |
| O | -2.11755951 | 2.33795467 | -2.79028697 |
| H | -2.82564731 | 2.70576961 | -3.31901722 |
| H | -2.50311953 | 1.565557 | -2.37679312 |
| O | -3.24363733 | 0.11993054 | -1.75698693 |
| H | -2.93744709 | -0.69838093 | -2.1479418 |
| H | -3.34897763 | -0.0828531 | -0.82746337 |
| O | -3.61439251 | -0.49684418 | 0.8979868 |
| H | -4.53377761 | -0.53245921 | 1.16198386 |
| H | -3.22851712 | 0.17332355 | 1.4620854 |
| O | -2.64651273 | 1.42131963 | 2.53358647 |
| H | -1.95411682 | 1.24254337 | 3.16987162 |
| H | -2.43403985 | 2.28692098 | 2.18455721 |
| O | -1.85381442 | 3.91839411 | 1.65120466 |
| H | -2.37167724 | 4.71322826 | 1.77883156 |
| H | -1.60304157 | 3.94105566 | 0.72771602 |
| O | -1.07362087 | 4.04878421 | -0.9159299 |
| H | -0.12503719 | 3.99921533 | -1.03409828 |
| H | -1.42867531 | 3.44604505 | -1.56928562 |

**Table S9.** Coordinates for lowest energy configuration of the $(H_2O)_{24}$ cluster No. 6 calculated with the TIP4P potential

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | -2.62952357 | 3.49454471 | -0.8483742 |
| H | -2.93289081 | 2.61534268 | -0.6220913 |
| H | -3.42862178 | 3.97701664 | -1.06025796 |
| O | -0.65490008 | 4.5624207 | 0.75805878 |
| H | -1.38924426 | 4.18384221 | 0.27468646 |
| H | -0.02693409 | 4.81519808 | 0.08130613 |
| O | 0.42389795 | 3.31405381 | 2.87971707 |
| H | 0.02909634 | 3.72770269 | 2.11208556 |
| H | 0.15227462 | 3.86365592 | 3.6148294 |
| O | -0.94483925 | 0.96693595 | 3.37642378 |
| H | -0.45669946 | 1.75771567 | 3.14703585 |
| H | -0.27363786 | 0.2926815 | 3.48178729 |
| O | -3.20738361 | 0.01651774 | 2.26320343 |
| H | -2.39365292 | 0.36630189 | 2.62614315 |
| H | -3.86216769 | 0.17831396 | 2.94240269 |
| O | -3.56506146 | 1.04186614 | -0.25823584 |
| H | -3.4425262 | 0.68593781 | 0.62183914 |
| H | -3.37414353 | 0.30815351 | -0.84257133 |
| O | -0.55098367 | 3.33670369 | -2.65750368 |
| H | -1.3176216 | 3.34556691 | -2.08442465 |
| H | 0.05761417 | 3.95544049 | -2.25376455 |
| O | 1.12199531 | 5.05447167 | -1.29355814 |
| H | 1.50869616 | 5.85679276 | -1.64423629 |
| H | 1.87263032 | 4.51459152 | -1.04595294 |
| O | 3.1874252 | 3.5172335 | -0.56344833 |
| H | 3.13087687 | 3.18761412 | 0.33342691 |
| H | 3.1921091 | 2.73036634 | -1.10847124 |
| O | 2.93782859 | 2.64554197 | 2.03570646 |
| H | 3.52130081 | 3.10846408 | 2.6369511 |
| H | 2.0569699 | 2.87560717 | 2.33132415 |
| O | 3.02683547 | -0.10355151 | 2.11757263 |
| H | 3.03077494 | 0.85040276 | 2.03891144 |
| H | 3.18314089 | -0.4184144 | 1.22725706 |
| O | 0.9877282 | -0.96758111 | 3.64463566 |
| H | 1.7038769 | -0.69916318 | 3.06903623 |
| H | 1.41149901 | -1.16072148 | 4.48090531 |
| O | -0.12581854 | -3.32350304 | 2.76315718 |
| H | 0.25368429 | -2.49089499 | 3.04417903 |
| H | -1.04358781 | -3.12015841 | 2.58265128 |
| O | -2.6766406 | -2.66908437 | 2.06873892 |
| H | -2.86589375 | -1.73263582 | 2.12772371 |
| H | -2.86598755 | -2.89529889 | 1.15813112 |
| O | -3.23882881 | -3.4019817 | -0.52594213 |
| H | -2.44969469 | -3.89330368 | -0.75420052 |
| H | -3.91603952 | -4.07042291 | -0.4220006 |
| O | -3.12830259 | -1.07607383 | -1.95881582 |
| H | -3.16098834 | -1.88263255 | -1.44439721 |
| H | -3.85220906 | -1.15792172 | -2.57969599 |
| O | 0.64780511 | 1.04491007 | -3.42665479 |
| H | 0.18581227 | 1.82630387 | -3.1229803 |
| H | 0.91181114 | 1.25513036 | -4.32238918 |
| O | 3.00627615 | 1.23301476 | -2.02126801 |
| H | 2.16848499 | 1.0999871 | -2.46471075 |
| H | 3.13021063 | 0.44013151 | -1.49953222 |
| O | 3.54106218 | -0.95970435 | -0.44445951 |
| H | 4.46123555 | -1.18639763 | -0.57908107 |
| H | 3.06381535 | -1.76510747 | -0.64394165 |
| O | 2.31838346 | -3.29370973 | -1.02649401 |
| H | 1.89273999 | -3.8181459 | -0.34824172 |
| H | 1.74212487 | -3.3713404 | -1.78684351 |
| O | 0.91036664 | -4.82376335 | 0.79467848 |
| H | 1.23001869 | -5.6070212 | 1.24251946 |
| H | 0.55885444 | -4.27367021 | 1.49472744 |
| O | -1.03235587 | -4.79443332 | -1.15585051 |
| H | -0.39558846 | -4.87612742 | -0.44586095 |
| H | -0.53074867 | -4.43589363 | -1.88801944 |
| O | 0.50611163 | -3.58650609 | -3.09192348 |
| H | 0.05264728 | -2.75330177 | -3.21987852 |
| H | 0.70022307 | -3.89261442 | -3.97784124 |
| O | -0.81704208 | -1.27434873 | -3.44355139 |
| H | -1.58945762 | -1.13629039 | -2.89533066 |
| H | -0.33293372 | -0.45046698 | -3.38796553 |

**Table S10.** Coordinates for lowest energy configuration of the $(H_2O)_{24}$ cluster No. 12 calculated with the TIP4P potential

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | 3.73575223 | -0.00402335 | 2.30040352 |
| H | 3.84050564 | 0.05689074 | 1.35090469 |
| H | 4.62809824 | 0.04165994 | 2.643716 |
| O | 2.11551566 | 2.04182267 | 3.1870911 |
| H | 2.67769014 | 1.33029524 | 2.88062671 |
| H | 1.92674829 | 2.55415512 | 2.40088873 |
| O | 4.04332906 | 0.14165556 | -0.40956532 |
| H | 4.84466924 | 0.13650741 | -0.933072 |
| H | 3.57109726 | -0.64375658 | -0.68589253 |
| O | 2.10972593 | -2.08191526 | 3.09996055 |
| H | 2.68354683 | -1.372397 | 2.81091859 |
| H | 1.91498355 | -2.57328373 | 2.30192278 |
| O | 1.54217101 | 3.50317935 | 0.93602826 |
| H | 0.58903528 | 3.43274166 | 0.88308807 |
| H | 1.70713373 | 4.43761633 | 1.06191181 |
| O | -0.17082668 | 1.31998741 | 4.47250414 |
| H | 0.6537589 | 1.6048203 | 4.07859973 |
| H | -0.08687459 | 0.36915062 | 4.54387133 |
| O | 2.58756702 | 2.30634606 | -1.3013949 |
| H | 3.06067306 | 1.54382726 | -0.96827692 |
| H | 2.21750143 | 2.71893525 | -0.52097613 |
| O | 2.78646488 | -2.10548079 | -1.16155418 |
| H | 2.29826217 | -2.58691553 | -0.49363911 |
| H | 2.261095 | -2.19816772 | -1.95630412 |
| O | 1.47216759 | -3.48176654 | 0.82321509 |
| H | 1.62003973 | -4.42686428 | 0.85721404 |
| H | 0.51961733 | -3.38760888 | 0.82698246 |
| O | 0.04016521 | -1.41938139 | 4.68097189 |
| H | 0.77277863 | -1.65340655 | 4.11111082 |
| H | 0.3513706 | -1.61544139 | 5.56468198 |
| O | -1.14248034 | 3.38619302 | 0.85848833 |
| H | -1.56077212 | 2.99176355 | 1.62379168 |
| H | -1.63708086 | 3.04626894 | 0.11279819 |
| O | -2.27440741 | 2.26702758 | 3.10089783 |
| H | -1.52129678 | 1.93070779 | 3.58663975 |
| H | -2.71239447 | 2.8562855 | 3.71504299 |
| O | 1.25566188 | 2.33746422 | -3.64673295 |
| H | 1.69611642 | 2.29626372 | -2.79789012 |
| H | 1.65630449 | 3.08592376 | -4.08891577 |
| O | 1.35569311 | -2.38486669 | -3.48776687 |
| H | 1.35486705 | -1.55621518 | -3.96689924 |
| H | 1.70901976 | -3.02119011 | -4.10944574 |
| O | -1.2096201 | -3.30300973 | 0.95429701 |
| H | -1.57272169 | -2.87029377 | 1.72704921 |
| H | -1.7553793 | -2.99769234 | 0.22961775 |
| O | -2.18097635 | -2.09194694 | 3.23159191 |
| H | -2.70419701 | -2.63134887 | 3.82448105 |
| H | -1.41300012 | -1.84479954 | 3.74672541 |
| O | -2.6462252 | 2.45283116 | -1.24338925 |
| H | -2.96381055 | 1.58999473 | -0.97714749 |
| H | -3.43869582 | 2.98091668 | -1.3400735 |
| O | -3.64828854 | 0.03734925 | 2.27177489 |
| H | -3.18704033 | 0.82070552 | 2.57149955 |
| H | -3.12559423 | -0.69155357 | 2.60602505 |
| O | 1.13497052 | -0.11424956 | -4.91334501 |
| H | 1.26654481 | 0.72742452 | -4.47687648 |
| H | 0.19850849 | -0.13881275 | -5.10998515 |
| O | -1.40035251 | -2.35695484 | -3.40287703 |
| H | -0.44702882 | -2.43325638 | -3.36307948 |
| H | -1.55769726 | -1.62019671 | -3.99335305 |
| O | -2.80770285 | -2.44369965 | -1.10721398 |
| H | -2.28608587 | -2.39910589 | -1.9085622 |
| H | -3.55266132 | -2.99935181 | -1.33638508 |
| O | -1.49963298 | 2.12340906 | -3.70962763 |
| H | -0.5610968 | 2.27631465 | -3.60007602 |
| H | -1.86509013 | 2.23551262 | -2.83207097 |
| O | -3.65061844 | 0.09205533 | -0.44502573 |
| H | -3.71622051 | 0.06012702 | 0.50938969 |
| H | -3.33654416 | -0.77742311 | -0.69321201 |
| O | -1.62013236 | -0.17727511 | -5.0895171 |
| H | -1.66195765 | 0.63134677 | -4.57901428 |
| H | -2.21296916 | -0.0271363 | -5.82588298 |

**Table S11.** Coordinates for lowest energy configuration of the $(H_2O)_{24}$ cluster No. 22 calculated with the TIP4P potential

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | 0.08612143 | -2.42043152 | -3.06344178 |
| H | -0.76758051 | -2.00353512 | -2.94672744 |
| H | 0.02135974 | -3.24089319 | -2.57468784 |
| O | 2.54717153 | -1.36700614 | -2.92082388 |
| H | 3.0310451 | -1.90403318 | -3.54827919 |
| H | 1.65040145 | -1.69918383 | -2.96197291 |
| O | -2.42757467 | -1.31276148 | -2.80840686 |
| H | -2.44832672 | -0.35608489 | -2.8323045 |
| H | -2.93553634 | -1.58300735 | -3.57337349 |
| O | -0.04014153 | -4.66588578 | -1.53723581 |
| H | -0.79739619 | -4.66182976 | -0.95176098 |
| H | 0.71649706 | -4.66649533 | -0.95095131 |
| O | 3.30086535 | -2.24612029 | -0.42098546 |
| H | 3.03701184 | -1.8968565 | -1.27223628 |
| H | 3.37279665 | -1.47580119 | 0.14263339 |
| O | 2.42036113 | 1.35660849 | -2.79375133 |
| H | 2.92635806 | 1.63880582 | -3.55569857 |
| H | 2.44103249 | 0.40042361 | -2.83267452 |
| O | -3.32467794 | -2.22029105 | -0.37211529 |
| H | -3.01340263 | -1.88813099 | -1.21414214 |
| H | -3.38825459 | -1.44352876 | 0.18360965 |
| O | -2.55465619 | 1.41250644 | -2.89250467 |
| H | -1.65798829 | 1.74530567 | -2.93075632 |
| H | -3.04013171 | 1.95927914 | -3.51023031 |
| O | -2.09157025 | -4.51573033 | 0.30336073 |
| H | -2.52468734 | -3.68800198 | 0.09477692 |
| H | -2.80479281 | -5.15127353 | 0.36361234 |
| O | 2.02568005 | -4.51262775 | 0.28597884 |
| H | 2.73213068 | -5.1534418 | 0.36670492 |
| H | 2.4688324 | -3.69342591 | 0.06517081 |
| O | 3.57722806 | -0.03789571 | 1.19373673 |
| H | 2.91261721 | -0.04099309 | 1.88258698 |
| H | 4.41069975 | -0.04588833 | 1.66436706 |
| O | 3.32375348 | 2.22590872 | -0.34587059 |
| H | 3.01030379 | 1.90696274 | -1.19218885 |
| H | 3.38874171 | 1.44054503 | 0.19746379 |
| O | -0.09396018 | 2.468085 | -3.02494713 |
| H | 0.76003061 | 2.04942935 | -2.9169702 |
| H | -0.02792349 | 3.28079738 | -2.52357943 |
| O | -3.57414882 | 0.01913378 | 1.2033813 |
| H | -4.40640452 | 0.019742 | 1.6762258 |
| H | -2.90776459 | 0.01146172 | 1.89048031 |
| O | -3.30189312 | 2.25237 | -0.37728022 |
| H | -3.04023986 | 1.91647918 | -1.23457059 |
| H | -3.37239187 | 1.47332097 | 0.17439394 |
| O | -0.02570524 | -4.14950749 | 2.09483604 |
| H | -0.78548656 | -4.28396183 | 1.52836785 |
| H | 0.7283799 | -4.27877238 | 1.51961605 |
| O | 1.8084472 | -0.04479522 | 3.23176917 |
| H | 1.23949672 | -0.79684706 | 3.39591918 |
| H | 1.25595752 | 0.71692212 | 3.40719344 |
| O | 2.09243968 | 4.51047315 | 0.3686185 |
| H | 2.52500039 | 3.68611864 | 0.14599165 |
| H | 2.80582903 | 5.14500824 | 0.4369755 |
| O | 0.03627918 | 4.68937804 | -1.4641118 |
| H | 0.79503967 | 4.6761743 | -0.88072513 |
| H | -0.71884638 | 4.68079366 | -0.87594214 |
| O | -1.80011987 | -0.00583283 | 3.23670476 |
| H | -1.24719604 | -0.77019161 | 3.3987626 |
| H | -1.23073382 | 0.74356892 | 3.4111421 |
| O | -2.0248418 | 4.50755517 | 0.36179567 |
| H | -2.73106825 | 5.14701424 | 0.45435998 |
| H | -2.4685788 | 3.69190224 | 0.12933144 |
| O | -0.01694808 | -2.04690765 | 3.77316188 |
| H | -0.02111815 | -2.76949611 | 3.14540368 |
| H | -0.02131869 | -2.47342705 | 4.63007141 |
| O | 0.02669735 | 1.98759672 | 3.8046833 |
| H | 0.0332511 | 2.40065128 | 4.66815004 |
| H | 0.02927534 | 2.71992276 | 3.18830373 |
| O | 0.03118938 | 4.11620932 | 2.15945729 |
| H | 0.7895119 | 4.25953039 | 1.59320835 |
| H | -0.72437217 | 4.25444598 | 1.588275 |

**Table S12.** Coordinates for lowest energy configuration of the $(H_2O)_{24}$ cluster No. 31 calculated with the TIP4P potential

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | 1.4982977 | -4.05719759 | -1.62471492 |
| H | 1.88080849 | -3.24746932 | -1.96273485 |
| H | 1.95925152 | -4.75378502 | -2.09217547 |
| O | 2.63819464 | -1.82930757 | -2.62003065 |
| H | 2.15470527 | -1.24329623 | -3.20231974 |
| H | 3.12374151 | -1.24355706 | -2.03919297 |
| O | 1.29017632 | -4.03050338 | 1.12598433 |
| H | 1.44282646 | -4.02978192 | 0.18103499 |
| H | 0.35175336 | -4.19556245 | 1.21736095 |
| O | -1.25923476 | -3.97814626 | -1.50393521 |
| H | -0.30871331 | -3.99686205 | -1.61524797 |
| H | -1.39472578 | -4.13915208 | -0.57015197 |
| O | 1.33735105 | 0.01009327 | -4.21279142 |
| H | 1.43843625 | 0.00102958 | -5.16459574 |
| H | 0.39065758 | -0.00194357 | -4.07187153 |
| O | 3.98625619 | 0.00298294 | -1.05815238 |
| H | 3.70340386 | 0.02052619 | -0.14386652 |
| H | 4.94189251 | -0.02811317 | -1.01316237 |
| O | -1.4370699 | -4.41356381 | 1.21398902 |
| H | -1.85513666 | -5.15612224 | 1.64994659 |
| H | -1.75841085 | -3.64576176 | 1.68669595 |
| O | 2.20646116 | -2.1298813 | 2.79892276 |
| H | 1.88579364 | -2.77348463 | 2.16711668 |
| H | 2.76269994 | -2.63350579 | 3.39322289 |
| O | -2.73663355 | -2.05623184 | -2.67810878 |
| H | -3.3758281 | -2.56998285 | -3.17179093 |
| H | -2.18658367 | -2.7092573 | -2.2454025 |
| O | -1.34102919 | -0.0221688 | -3.91511995 |
| H | -1.77616471 | -0.77908836 | -3.52274043 |
| H | -1.77964138 | 0.73480304 | -3.52673248 |
| O | 2.63640104 | 1.8426068 | -2.60819921 |
| H | 2.15370259 | 1.26075242 | -3.19529336 |
| H | 3.13073076 | 1.25288946 | -2.03889839 |
| O | 3.30680805 | 0.06194296 | 1.55386003 |
| H | 2.91389276 | -0.70580462 | 1.96908656 |
| H | 2.88443089 | 0.80777019 | 1.97997166 |
| O | -2.28831896 | -2.29928224 | 2.63116487 |
| H | -1.56690897 | -1.99473693 | 3.18166612 |
| H | -2.67586204 | -1.49820703 | 2.27857347 |
| O | -0.13645843 | -1.40121538 | 4.0346797 |
| H | 0.67986018 | -1.65229482 | 3.60245884 |
| H | -0.10901812 | -0.44481047 | 4.06240207 |
| O | -3.59171005 | -0.01074171 | -1.02744392 |
| H | -3.31399612 | -0.77080394 | -1.53872878 |
| H | -3.31502474 | 0.74306512 | -1.54845481 |
| O | -2.73352241 | 2.02175146 | -2.6938832 |
| H | -2.18097758 | 2.67248455 | -2.26090226 |
| H | -3.36178043 | 2.53812291 | -3.19874381 |
| O | 1.50590781 | 4.06133263 | -1.58506252 |
| H | 1.88717133 | 3.25349402 | -1.92896184 |
| H | 1.94121978 | 4.75942812 | -2.07434569 |
| O | 2.23864035 | 2.24536701 | 2.86669966 |
| H | 3.00721358 | 2.67994153 | 3.23639142 |
| H | 1.89107885 | 2.87163971 | 2.23170727 |
| O | -3.47899614 | -0.00933097 | 1.67120625 |
| H | -3.47056677 | -0.01054973 | 0.71404414 |
| H | -4.40673893 | -0.05124651 | 1.90308604 |
| O | -1.25139141 | 3.93322001 | -1.50567607 |
| H | -0.29992363 | 3.96386388 | -1.60568529 |
| H | -1.39961304 | 4.08519733 | -0.57231383 |
| O | 1.25803626 | 4.07968537 | 1.16249457 |
| H | 1.42899682 | 4.06486715 | 0.22080208 |
| H | 0.31523765 | 4.22936265 | 1.23291716 |
| O | -0.02088065 | 1.34393297 | 4.11450241 |
| H | 0.04682653 | 1.69112344 | 5.00394401 |
| H | 0.77514793 | 1.64658356 | 3.67749788 |
| O | -2.18797847 | 2.20950491 | 2.65008488 |
| H | -2.62557402 | 1.43417408 | 2.29851115 |
| H | -1.46085131 | 1.86138385 | 3.16615625 |
| O | -1.48356139 | 4.3650179 | 1.20828385 |
| H | -2.00708559 | 5.07342266 | 1.58287288 |
| H | -1.76013134 | 3.58340914 | 1.68664421 |

**Table S13.** Atomic coordinates in the unit cell for the lowest-energy configuration of clathrate structure. sL_I. The unit cell size- and coordinate-optimization was performed using the AMOEBA potential.

| Atom | X(Å) | Y(Å) | Z(Å) |
|---|---|---|---|
| O | -0.887873 | -2.729329 | 1.169712 |
| H | -1.481742 | -1.961664 | 1.169712 |
| H | -1.481742 | -3.496994 | 1.169712 |
| O | -2.729329 | -0.671743 | 1.169712 |
| H | -2.729329 | -0.077875 | 0.402047 |
| H | -2.729329 | -0.077875 | 1.937378 |
| O | 3.227298 | -2.729329 | 1.169712 |
| H | 3.821167 | -1.961664 | 1.169712 |
| H | 3.821167 | -3.496994 | 1.169712 |
| O | -2.729329 | 3.011168 | 1.169712 |
| H | -2.729329 | 2.4173 | 0.402047 |
| H | -2.729329 | 2.4173 | 1.937378 |
| O | 1.169713 | -0.887873 | -2.729329 |
| H | 1.169712 | -1.481742 | -1.961664 |
| H | 1.169713 | -1.481742 | -3.496994 |
| O | 3.011168 | 1.169712 | -2.729329 |
| H | 2.4173 | 0.402047 | -2.729329 |
| H | 2.4173 | 1.937378 | -2.729329 |
| O | 1.169713 | 3.227298 | -2.729329 |
| H | 1.169713 | 3.821167 | -1.961664 |
| H | 1.169713 | 3.821167 | -3.496994 |
| O | -0.671743 | 1.169712 | -2.729329 |
| H | -0.077875 | 0.402047 | -2.729329 |
| H | -0.077875 | 1.937378 | -2.729329 |
| O | -2.729329 | 1.169712 | -0.887873 |
| H | -1.961664 | 1.169712 | -1.481742 |
| H | -3.496994 | 1.169712 | -1.481742 |
| O | -2.729329 | 1.169712 | 3.227298 |
| H | -3.496994 | 1.169712 | 3.821167 |
| H | -1.961664 | 1.169713 | 3.821167 |
| O | 1.169713 | -2.729329 | 3.011168 |
| H | 0.402047 | -2.729329 | 2.4173 |
| H | 1.937378 | -2.729329 | 2.4173 |
| O | 1.169712 | -2.729329 | -0.671743 |
| H | 0.402047 | -2.729329 | -0.077875 |
| H | 1.937378 | -2.729329 | -0.077875 |