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Geometry of the magic number $H^+(H_2O)_{21}$ water cluster by proxy

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Supplementary Information

Experiments

Abundance spectra

Figure S1 shows the abundance for $H^+(TB)_m(H_2O)_n$ clusters with m = 0–10, taken from a mass spectrum produced with a 250 mM TB solution and with a reduction in the rate with which the TB solution is fed to the ESI unit. The reduction in flow rate (20 μL min^{-1} here compared to the 30 μL min^{-1} used for the measurement presented in Fig. 3) resulted in a slight reduction in the average number of TB in the clusters.

The eleven cluster series in Fig. S1 are split between three panels in order to improve clarity. Figure S1a shows the same clusters as Fig. 2; however, the trends in overall abundance of the different cluster series m = 0–3 is now reversed owing to the higher TB concentration in the solution. Again, magic numbers are observed for $m + n$ = 21, 28 and, to a smaller degree, for m = 30. The new magic number at $m + n$ = 25 is also observed to emerge as m increases from zero to three. The markedly increased intensity for $H^+(H_2O)_{10}$ and $H^+(H_2O)_{15}$ observed in Fig. S1a is not magic numbers as such, they are artefacts. They have been observed for other measurements using the 250 mM TB solution, and are due to isobaric overlap (not separable) with unidentified contaminants.

Figure S1b covers the series m = 4–6, all of which have an identical detailed structure in the region of the magic numbers (allowing for the shift in n due to the replacement of water molecules). The same is true for m = 7–10 in Fig. S1c, with the exception for $H^+(TB)_{10}(H_2O)_{11}$ and $H^+(TB)_{10}(H_2O)_{12}$ (as discussed in the Experimental results).

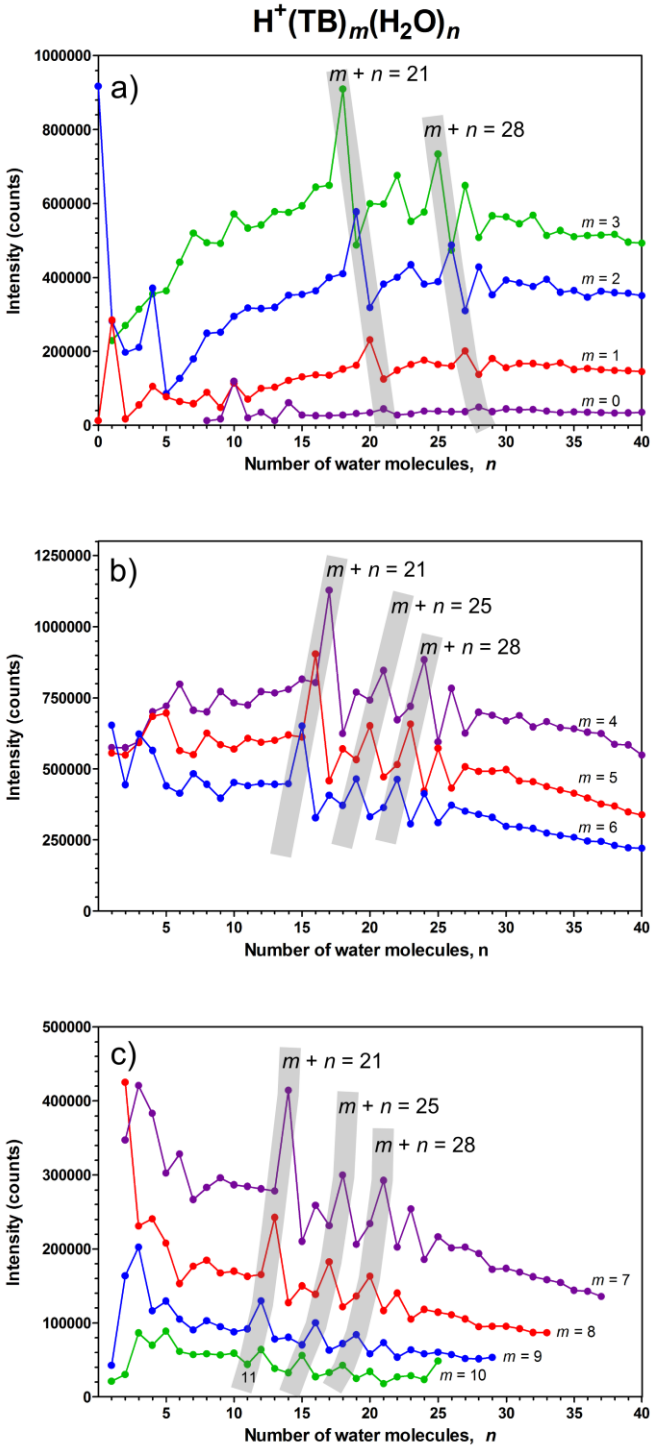

Figure S1. Abundance of $H^+(TB)_m(H_2O)_n$ clusters with m = 0–10 in a QTOF spectrum produced from a solution of 250 mM tert-butyl alcohol in water. In order to improve clarity, the cluster series are presented in different panels: a) m = 0–3, b) m = 4–6 and c) m = 7–10. Grey bands indicate where the total number of water- and tert-butyl alcohol molecules equals 21, 25 and 28. The cluster $H^+(TB)_{10}(H_2O)_{11}$ is indicated by "11" in panel c).

Collision induced dissociation

Collision induced dissociation measurement was performed, wherein the $H^+(TB)_{10}(H_2O)_{11}$ cluster and the $H^+(TB)_{10}(H_2O)_{11}$ cluster was collided with Ar at a collision energy of 10 eV (in the lab-frame). Results are showed in Fig. S2 and Fig. S3, respectively. The clusters were produced using the same solution and experimental conditions as used in the experiment presented in Fig. 3, and singled out from the resulting cluster distribution by the quadrupole mass filter on the QTOF instrument. Isobaric overlaps occurred in the form of clusters containing one TB. For example, the cluster $H^+(TB)_1(H_2O)_{48}$, having a mass of 939.61 overlaps with $H^+(TB)_{10}(H_2O)_{11}$. Fortunately, the overlapping clusters have a very small abundance compared to our main peaks, and their presence in Fig. S2 and Fig. S3 can be neglected.

The cluster $H^+(TB)_{10}(H_2O)_{11}$ is observed to be anti-magic in Fig. 3 and Fig. S1, which we have interpreted as a consequence of the clusters inability to form hydrogen bonds to all ten TB without disrupting the core cluster structure corresponding to the original magic $H^+(H_2O)_{21}$ cluster. Given this, one might suspect that $H^+(TB)_{10}(H_2O)_{11}$ would be prone to lose a TB upon collision induced dissociation. Interestingly enough, this is not the case, as it is evident that loss of one or two H_2O is still the preferred collision product.

The cluster $H^+(TB)_{10}(H_2O)_{12}$ on the other hand, is observed to be a magic cluster. However, also this cluster is observed to lose almost exclusively water molecules upon collision induced dissociation.

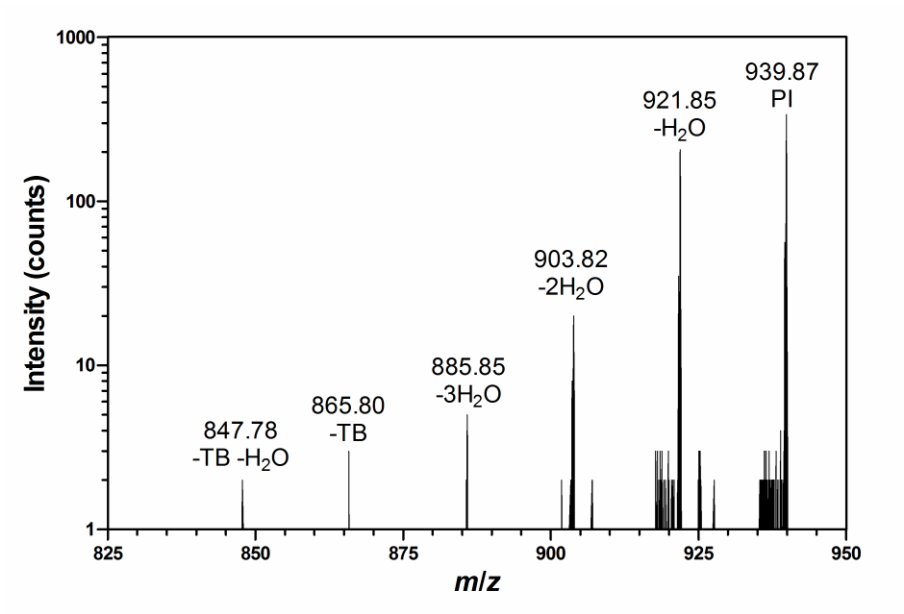

Figure S2. Mass spectrum of a collision induced dissociation experiment wherein the $H^+(TB)_{10}(H_2O)_{11}$ cluster (marked PI) collides with Ar after being accelerated to 10 eV nominal collision energy (lab frame).

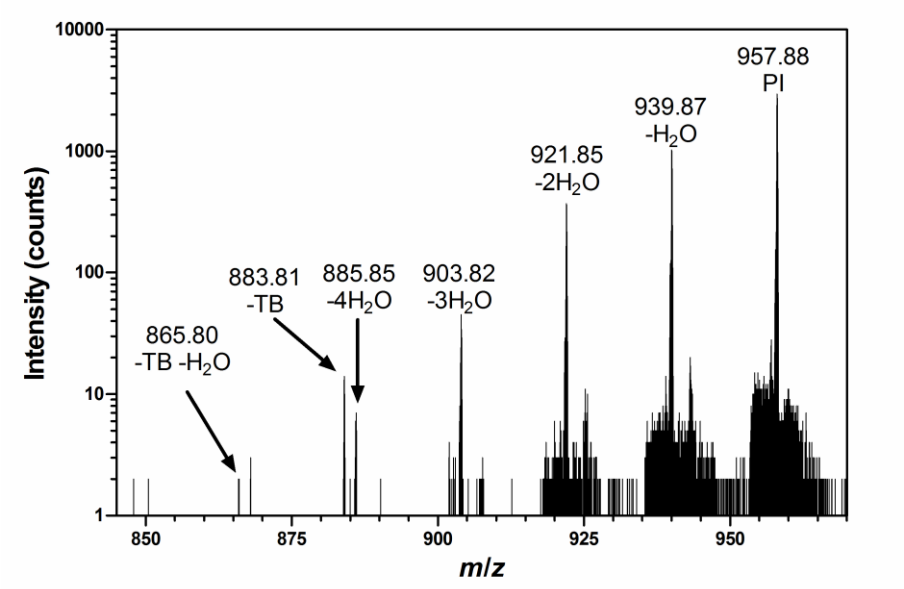

Figure S3. Mass spectrum of a collision induced dissociation experiment wherein the $H^+(TB)_{10}(H_2O)_{12}$ cluster (marked PI) collides with Ar after being accelerated to 10 eV nominal collision energy (lab frame).

Computations

Electrostatic potential mappings of clusters

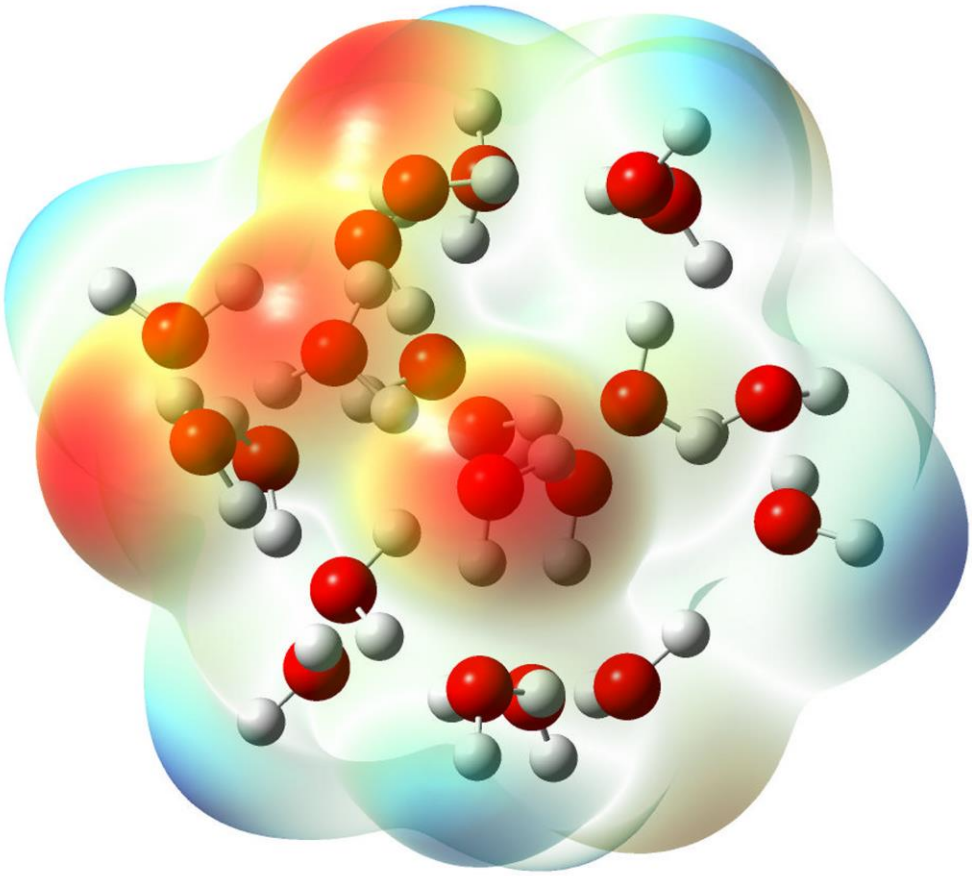

Figure S4. Isodensity plot of the geometry optimized $H^+(H_2O)_{21}$ cluster mapping the electrostatic potential by indicating electronegative regions as red and electropositive regions as blue. Colours indicating intermediate charge values have been faded to enhance visibility.

Notes on the geometry optimized structure of $H^+(H_2O)_{21}$ and other clusters

Within the geometry optimized $H^+(H_2O)_{21}$ cluster structure we identify a central axis that is surrounded by three similar cluster units. The axis is defined by the central oxygen atom of the $(H_3O^+)(H_2O)_3$ structure on the surface and the centre of dodecahedron, which we define to be the oxygen atom of the lone water molecule inside the cage. The axis continues (approximately) through a hydrogen bond to the oxygen of a water molecule diametrically opposite the hydronium ion. This situation is depicted in Fig. S5.

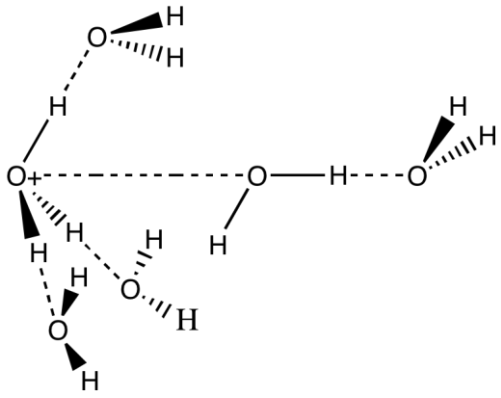

Figure S5. The central binding motif and axis of the geometry optimized $H^+(H_2O)_{21}$ cluster.

In addition to this central motif the slightly degenerated dodecahedron consists of three additional motifs that surround the central axis by quasi threefold rotation, as shown in Fig. S6. The symbol X refers to a hydrogen atom pointing outwards, into the void, thereby giving rise to a so-called dangling O–H group. These units each contain 5 water molecules, and are slight variations of each other. The structures wcunit1 and wcunit2 are almost mirror images to each other, while wcunit3 is somewhat different in that it's lacking a hydrogen bond contact to the leftmost water molecule. All structures contain at least one hydrogen atom which is connected to another wcunit structure on the cluster surface; this is just indicated with a regular straight line pointing out of the ring.

There is also one hydrogen atom in each structure that points towards the central axis, either to the middle water, or towards the water molecule at the end of the axis (i.e., not towards the hydroxonium part); this H is connected with a hashed wedge in the wcunit figures. The rest of the interactions are mediated by the oxygen atoms of the cluster units, and the hydrogen atoms of the axis.

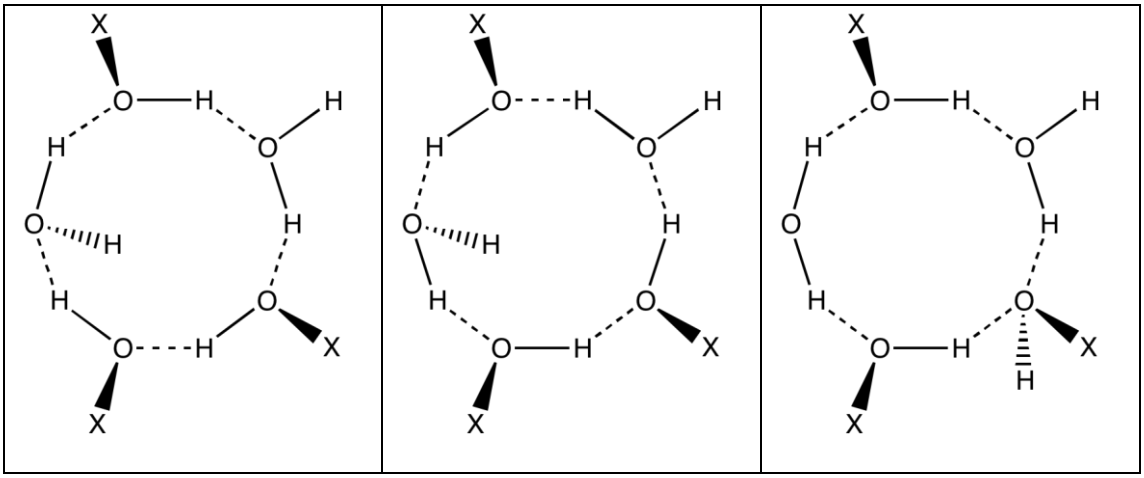

Figure S6. The three surrounding binding motifs of the geometry optimized $H^+(H_2O)_{21}$. From left to right: , wcunit1, wcunit2 and wcunit3. The symbol X refers to a hydrogen atom pointing outwards, into the void, thereby giving rise to a so-called dangling O–H group.

For the geometry optimizations with TB or TMA, the X in Fig. S6 was replaced by either tert-butyl or a hydrogen atom forming a hydrogen bond to TMA. In addition, we performed calculations for these clusters removing or adding one TB or TMA unit. This corresponds to removing (or adding) an X unit on the above figures. If an X unit has to be removed for a calculation, it is removed from the remotest site from the H_3O^+, while an extra X is positioned immediately above the H_3O^+ before geometry optimization.

Larger versions of Figs. 4–6

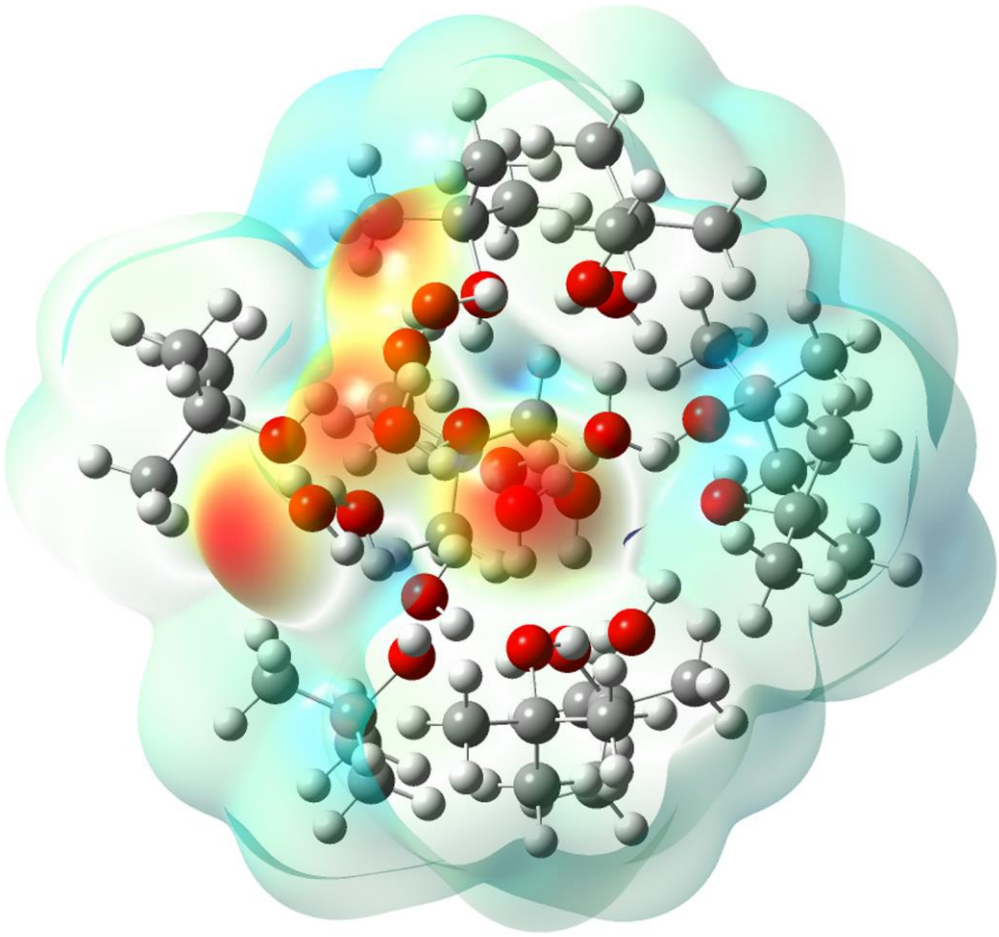

Figure S7. Larger version of Fig. 4.

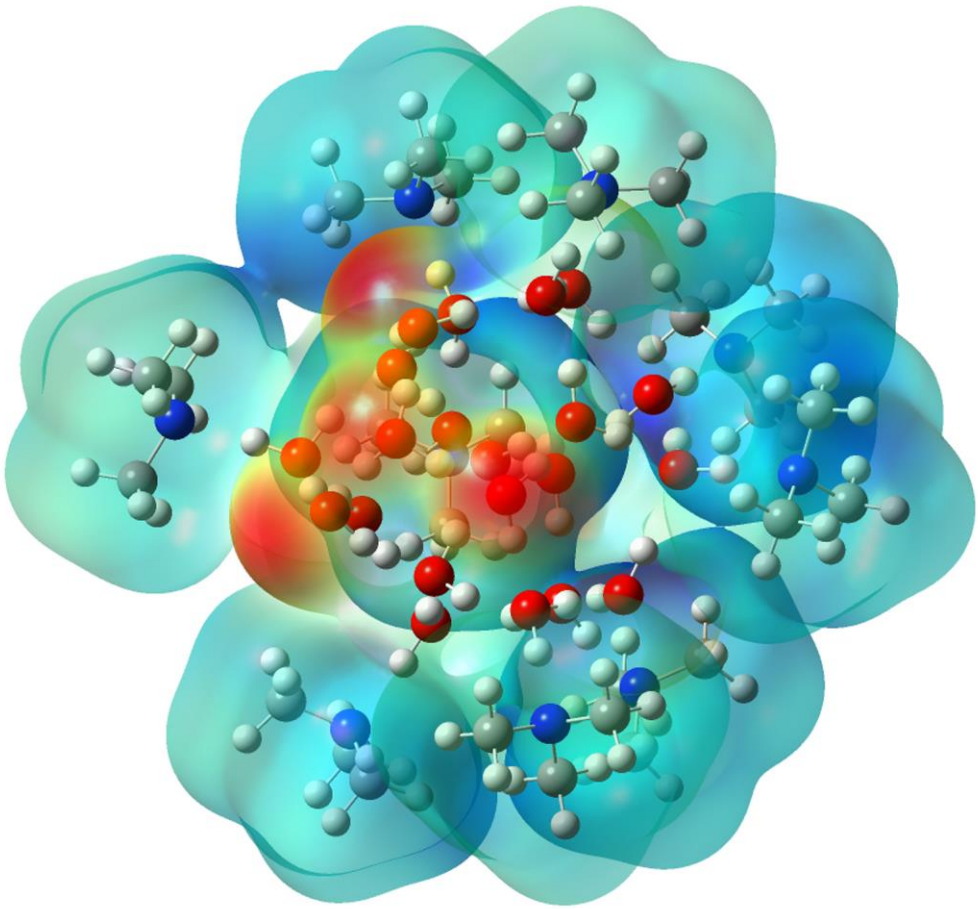

Figure S8. Larger version of Fig. 5.

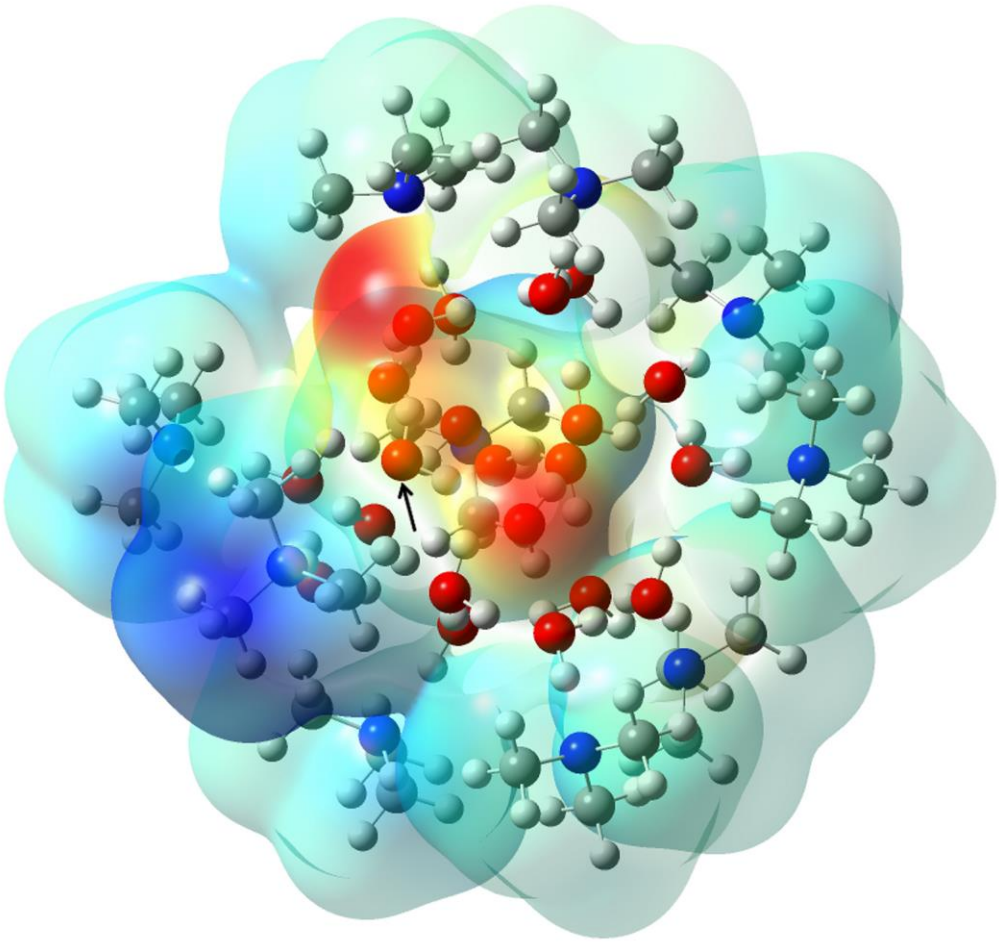

Figure S9. Larger version of Fig. 6.

A note on the convergence criteria for the calculations (as specified in ref. [36] in the main paper)

Convergence is obtained when the following four quantities:

- the root-mean-square of the gradient,
- the maximum absolute value of the gradient,
- the root-mean square of the step vector,
- and the maximum absolute element (in internal or Cartesian coordinates) of the step vector,

are smaller than the four respective convergence criteria, namely epsilon, 5 epsilon, 3 epsilon and 15 epsilon.

Cartesian coordinates of structures

The water cluster (Fig. S4)

H -2.56307 -2.14399 -0.624282
H -2.33813 -2.16272 -2.17406
H 0.0211769 0.114043 -1.70258
H 0.883576 0.448283 -2.97546
H 0.27658 -4.70329 1.24196
H -0.363294 -3.25346 1.03379
H -0.45046 2.55887 1.85084
H -0.893045 3.04164 0.386771
H -0.975371 -1.28037 0.571946
H -2.00487 -1.8218 1.63988
H -0.635099 4.78352 -1.30858
H 0.40939 3.58209 -1.24404
H 2.28562 2.28601 -1.7658
H 2.35297 2.82302 -0.281373
H 0.588631 -0.877665 3.45798
H 0.283113 0.676025 3.56159
H -1.34281 1.35628 -2.80735
H -1.68215 2.71608 -2.11262
H 4.20105 -1.88539 -1.66147
H 2.62416 -2.11337 -1.57341
H 1.39389 -2.8614 2.26973
H 2.37816 -2.57271 3.48014
H -3.3157 0.403998 1.87754
H -2.64512 1.67665 1.25663
H 3.04126 0.0175705 -2.47557
H 3.18528 1.04049 -3.68014
H -0.344128 0.88416 0.399513
H 0.925911 -0.07924 0.351929
H 1.11454 -3.46309 -0.650549
H 0.635626 -3.01511 -2.10096
H 0.887633 3.03255 3.87206
H 1.6828 2.46699 2.6207
H 3.8621 2.55503 1.62296
H 3.00053 1.26555 1.27065
H -0.838826 -2.71243 -4.01462
H -0.465424 -1.42139 -3.1555
H -3.12474 -1.17013 3.7549
H -1.69575 -0.572714 3.37921
H 3.02797 -0.771349 0.100265
H 2.51055 -1.02419 1.59813
H -3.13981 1.12234 -1.78668
H -3.49203 -0.484341 -1.41318
H -3.70031 0.718144 -0.252592
O -3.00176 -1.93855 -1.48352
O -0.0137014 0.15712 -2.69593
O 0.496927 -3.77156 1.08277
O -0.996525 2.32878 1.06517

O -1.50946 -2.08181 0.824493
O -0.555652 3.83127 -1.14231
O 1.97638 2.99927 -1.16862
O -0.090142 -0.218104 3.71003
O -2.09501 1.94498 -2.56219
O 3.36403 -1.42125 -1.50024
O 1.83851 -2.14418 2.79704
O -3.45114 1.11131 1.20819
O 2.66452 0.837889 -2.88702
O 0.000122854 0.0289643 0.0225463
O 1.42639 -3.1724 -1.53511
O 0.831393 2.4155 3.12541
O 2.96438 2.25053 1.41596
O -0.750954 -2.37542 -3.10913
O -2.58156 -0.861169 3.01323
O 2.60189 -0.344519 0.886147
O -3.77852 0.499698 -1.26225

The TB-water cluster (Fig. 4)

H -2.55671 -2.08736 -0.557693
H -2.2847 -2.09224 -2.09624
H 0.0543254 0.0944451 -1.67846
H 0.990323 0.429564 -2.88625
H -0.312056 -3.25517 1.04967
H -0.281923 2.49062 1.83393
H -0.759406 3.02051 0.383339
H -0.931786 -1.2868 0.57325
H -1.95546 -1.76255 1.67076
H 0.53741 3.51816 -1.17042
H 2.36786 2.1997 -1.63162
H 2.44723 2.76126 -0.155728
H 0.657862 -0.916713 3.30171
H 0.411396 0.642933 3.44771
H -1.22333 1.37509 -2.78486
H -1.49065 2.72103 -2.0409
H 2.63986 -2.04943 -1.59113
H 1.47158 -2.90431 2.25583
H -3.18201 0.443799 1.9054
H -2.54586 1.73644 1.30092
H 3.12966 0.048107 -2.51128
H -0.301002 0.875371 0.410336
H 0.97344 -0.0870859 0.339251
H 1.10149 -3.39238 -0.592567
H 0.552372 -2.93375 -2.01305
H 1.78658 2.45178 2.64425
H 3.06912 1.24927 1.27848
H -0.459064 -1.42824 -3.10528
H -1.59219 -0.527267 3.31339
H 3.03902 -0.785577 0.0306042
H 2.50828 -1.06431 1.52775
H -2.98264 1.18595 -1.7305
H -3.3872 -0.419716 -1.353

H -3.56807 0.79727 -0.189697
H 5.69227 -3.41152 -3.12266
H 3.93387 -3.33626 -3.34525
H 4.94314 -1.91707 -3.71139
H 5.41639 -4.06576 -0.619489
H 4.31945 -3.11156 0.394695
H 3.66752 -4.10814 -0.923701
H 6.75582 -1.91244 -1.23873
H 5.86182 -0.487794 -1.79959
H 5.67974 -1.05047 -0.123672
H 4.49963 -3.80889 4.14581
H 3.53337 -4.28683 2.73851
H 4.52208 -2.81193 2.67926
H 2.36935 -0.754735 4.94728
H 3.86527 -1.60141 5.39035
H 3.77483 -0.715555 3.8576
H 2.38613 -3.74428 5.68375
H 0.957265 -2.85338 5.11836
H 1.46771 -4.34417 4.29456
H -1.78956 -4.80807 2.19131
H -1.19186 -6.45854 2.42603
H -0.402136 -5.10594 3.26144
H 1.11232 -7.12792 1.31384
H 2.04284 -5.85536 0.497442
H 1.83293 -5.81637 2.26339
H 0.0426227 -5.49482 -1.02465
H -1.00691 -6.62434 -0.146816
H -1.50137 -4.93363 -0.345103
H -1.61919 -4.92455 -5.0096
H -0.765677 -4.95158 -3.45276
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H -2.20068 6.63081 -1.25326
H -2.63749 5.01535 -1.84066

H -2.34465 5.28364 -0.10669
H -4.17705 -0.448353 5.90866
H -2.59759 0.236442 5.47894
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H -1.5889 -2.08638 5.18998
H -5.27818 -2.17758 4.25093
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H 4.57575 1.92169 3.67122
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H 0.671296 5.43614 4.49519
H -0.610913 1.91834 5.20967
H -0.808825 3.62093 5.67067
H -1.40054 3.05838 4.09653
C 4.50063 -3.46451 -0.625476
C 5.80408 -1.37631 -1.1625
C 3.88537 -3.42939 3.32181
C 3.20707 -1.33997 4.55538
C 1.82498 -3.43735 4.79444
C -0.88477 -5.41152 2.32775
C 1.34162 -6.05728 1.31455
C -0.641621 -5.59181 -0.175876
C -1.47192 -4.3843 -4.0686
C 0.439054 -3.02621 -5.00935
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C 4.73891 1.59941 -3.92409
C 2.48914 2.62443 -4.43273
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C 0.331685 5.96769 -0.287177
C -2.0207 5.55931 -1.11677
C -3.54605 -0.131418 5.07069
C -2.54727 -2.43945 4.79248
C -4.60686 -1.78568 3.47973
C 4.49111 4.10883 1.954
C 5.1422 1.79621 2.74219
C 5.25492 2.37777 0.287312
C 1.89744 3.03509 5.20602
C 0.778191 4.71642 3.67627
C -0.597971 2.94669 4.83423

C 4.52211 2.62183 1.61122
C 0.758458 3.28351 4.21484
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C 3.24367 1.33411 -4.11149
C 4.64909 -2.28065 -1.58689
C 2.71177 -2.60898 3.86202
C 0.0647566 -5.23955 1.1384
C -0.938607 -2.97941 -4.34114
C -3.30325 -1.29662 4.10757
C 4.81325 -2.76413 -3.02982
O -2.98243 -1.88418 -1.42697
O 0.0639173 0.158281 -2.67175
O 0.495387 -3.83919 1.08008
O -0.90599 2.33065 1.08307
O -1.49003 -2.0642 0.846939
O -0.417319 3.79978 -1.09257
O 2.12422 2.96354 -1.06248
O 0.0400187 -0.242211 3.66105
O -1.94882 1.99564 -2.53087
O 3.44204 -1.45251 -1.5099
O 1.89876 -2.14638 2.73247
O -3.36211 1.18139 1.27367
O 2.6853 0.86868 -2.83841
O 0.0374351 0.0184092 0.0314697
O 1.374 -3.11866 -1.49818
O 0.907294 2.35738 3.08797
O 3.12115 2.22355 1.45546
O -0.794451 -2.35923 -3.02355
O -2.49418 -0.806807 2.99178
O 2.63406 -0.364984 0.835639
O -3.63772 0.579772 -1.20348

The TMA-water cluster (Fig. 5)

H -2.51186 -2.08757 -0.559136
H -2.21668 -2.09555 -2.09314
H 0.0718957 0.115751 -1.66457
H 1.00888 0.450996 -2.87166
H -0.23635 -3.25664 0.995984
H -0.266393 2.46595 1.89499
H -0.675385 3.01436 0.421766
H -0.90227 -1.29543 0.569857
H -1.89001 -1.77252 1.69087
H 0.659182 3.53667 -1.18519
H 2.48802 2.29116 -1.73518
H 2.56475 2.85591 -0.267752
H 0.709371 -0.938094 3.48956
H 0.444928 0.611504 3.64546
H -1.18744 1.39174 -2.74567
H -1.41217 2.73039 -1.97907
H 2.6209 -2.18037 -1.6082
H 1.45662 -2.83515 2.1909
H -3.08342 0.414244 1.94782

H -2.49847 1.72626 1.33321
H 3.04807 -0.00579643 -2.40784
H -0.291312 0.88397 0.44696
H 0.98694 -0.0728369 0.358727
H 1.17853 -3.57202 -0.670973
H 0.657606 -3.12157 -2.09572
H 1.76187 2.35644 2.59947
H 2.99574 1.27472 1.20462
H -0.384475 -1.45535 -3.03826
H -1.50242 -0.561349 3.40671
H 2.99453 -0.817311 0.0154971
H 2.4976 -1.0424 1.53973
H -2.91398 1.2027 -1.67656
H -3.31451 -0.415964 -1.33453
H -3.49515 0.775505 -0.138451
H 6.59028 -4.16087 -3.14731
H 4.81651 -3.98267 -3.27818
H 5.87766 -2.62537 -3.71508
H 6.21017 -4.77029 -0.672943
H 5.27391 -3.60558 0.30827
H 4.4597 -4.5372 -0.964829
H 7.75666 -2.79135 -1.29619
H 6.96722 -1.34668 -1.98601
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H 5.19376 -4.11501 5.21524
H 4.21284 -4.71286 3.84842
H 5.16287 -3.22172 3.66912
H 2.92458 -1.17297 5.67192
H 4.39475 -1.93487 6.34998
H 4.42784 -1.18965 4.72634
H 3.01848 -4.09607 6.60685
H 1.63756 -3.19141 5.92144
H 2.18239 -4.69596 5.14785
H -1.98229 -5.85095 2.18214
H -1.57468 -7.58148 2.35192
H -0.644886 -6.34515 3.24404
H 0.656046 -8.35438 1.32588
H 1.64696 -7.1062 0.51972
H 1.44462 -7.07313 2.28622
H -0.166758 -6.41808 -0.913575
H -1.27579 -7.63316 -0.210444
H -1.70909 -5.89932 -0.205592
H -1.71222 -5.37981 -6.16669
H -0.817777 -5.37806 -4.61975
H -2.48663 -4.76935 -4.67711
H 0.212953 -3.97089 -7.13541
H 0.634759 -2.47316 -6.25895
H 0.978448 -4.05366 -5.52235
H -2.20802 -3.0854 -7.22403
H -2.95233 -2.62382 -5.66699
H -1.62899 -1.64689 -6.33668
H 2.47498 0.453596 -6.27939
H 3.85093 1.09201 -7.22217
H 4.10058 -0.224873 -6.04246

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H 5.35391 2.62585 -4.15957
H 5.7602 1.02747 -4.82492
H 3.14552 3.54151 -4.48336
H 3.28 3.41862 -6.26306
H 1.93242 2.62525 -5.39883
H -0.329015 7.79003 -3.1115
H 0.855005 6.46125 -2.94841
H -0.784757 6.11691 -3.54189
H 0.0668817 8.27672 -0.611664
H -0.150775 6.90981 0.517249
H 1.22037 6.91161 -0.613942
H -2.31391 7.78307 -1.47138
H -2.64414 6.11178 -2.00874
H -2.3749 6.44815 -0.285672
H -4.86041 -0.865246 6.81685
H -3.24742 -0.246485 6.35995
H -4.67746 0.234091 5.42035
H -3.88162 -3.23471 6.5629
H -3.09664 -3.61772 5.00483
H -2.33452 -2.45895 6.11604
H -5.95915 -2.54378 5.20343
H -5.71062 -1.33493 3.91189
H -5.03834 -2.96942 3.73298
H 6.6654 4.83505 2.07519
H 5.11005 4.95866 1.20437
H 5.12358 4.63277 2.95168
H 6.18337 1.16786 2.61393
H 7.32622 2.50097 2.94358
H 5.74079 2.44866 3.76343
H 5.69367 3.21165 -0.350458
H 7.30074 2.9804 0.402263
H 6.16372 1.6093 0.25125
H 2.71524 4.11428 5.72398
H 1.60145 4.49653 7.06527
H 1.76614 2.81596 6.48242
H 1.64318 5.67178 4.22883
H -0.0965478 5.52588 3.89585
H 0.45708 6.16908 5.46765
H -0.594292 2.62502 6.02848
H -0.913593 4.2948 6.58329
H -1.384 3.78171 4.93739
H -2.96754 -1.14625 3.77658
H 2.45057 -2.50851 3.43509
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H 3.96053 2.50913 1.56318
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H -0.409489 4.75458 -1.20254
H 3.15803 1.04215 -3.65445
H 4.21212 -1.97014 -1.58146
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C 6.83904 -2.17695 -1.2839
C 4.55747 -3.81132 4.36537

C 3.81291 -1.7635 5.42735
C 2.516 -3.7941 5.6714
C -1.15713 -6.56059 2.3006
C 0.942316 -7.28808 1.33728
C -0.880588 -6.60764 -0.106135
C -1.54198 -4.82566 -5.22696
C 0.265567 -3.49717 -6.13917
C -2.01009 -2.66673 -6.22177
C 3.54174 0.695973 -6.23893
C 5.2089 1.95491 -5.01205
C 2.9953 2.88029 -5.34236
C -0.20203 6.72624 -2.84404
C 0.166582 7.18313 -0.494362
C -2.07106 6.71948 -1.3017
C -4.21006 -0.590107 5.96794
C -3.2926 -2.81819 5.72671
C -5.24613 -2.1677 4.44889
C 5.6389 4.4344 2.00629
C 6.25996 2.24008 2.82243
C 6.23721 2.68544 0.440281
C 1.74729 3.86516 6.1713
C 0.670307 5.43427 4.67156
C -0.624059 3.67391 5.71759
C 5.7445 -3.46239 -3.02207
N -3.99051 -1.71789 5.05764
N 3.4023 -3.02172 4.79635
N -0.217516 -6.40646 1.18727
N 0.685763 4.06066 5.18098
N 5.6284 2.99391 1.73777
N -1.03897 -3.47077 -5.47367
N -0.640028 6.44986 -1.47267
N 3.78265 1.65538 -5.15868
N 5.65228 -2.95063 -1.6519
O -2.92875 -1.88484 -1.43487
O 0.0809015 0.170878 -2.65836
O 0.601943 -3.79234 1.02511
O -0.885045 2.34491 1.12761
O -1.46057 -2.07259 0.845578
O -0.304827 3.7632 -1.05757
O 2.31967 3.0973 -1.19261
O 0.117084 -0.27749 3.91941
O -1.89941 2.02552 -2.478
O 3.33602 -1.48237 -1.51665
O 1.87664 -2.10423 2.71613
O -3.30279 1.14957 1.32057
O 2.69258 0.837841 -2.78746
O 0.0488946 0.0348388 0.0520316
O 1.46582 -3.40775 -1.60195
O 0.919899 2.27718 3.11776
O 3.00707 2.2499 1.38394
O -0.717578 -2.38752 -2.97505
O -2.38883 -0.812926 3.02325
O 2.64102 -0.362602 0.827879
O -3.5678 0.580466 -1.16063

The TMA-water cluster with an additional TMA (Fig. 6)

H -2.5587 -2.48268 -0.42406
H -2.27799 -2.65749 -1.94426
H -0.163098 0.18644 -1.69385
H 0.865175 0.391284 -2.84679
H -0.286244 -3.0544 0.986494
H -0.17245 2.52296 1.91407
H -0.53196 3.14494 0.471052
H -1.0895 -1.14537 0.515113
H -1.91463 -1.66172 1.75148
H 0.978976 3.68753 -1.08603
H 2.60437 2.24941 -1.68424
H 2.76763 2.80964 -0.220766
H 0.809894 -0.949595 3.55738
H 0.529653 0.589932 3.74423
H -1.10098 1.69639 -2.86734
H -1.09713 3.02833 -2.0648
H 2.53527 -2.23846 -1.65017
H 1.45713 -2.79056 2.18785
H -2.96054 0.560965 2.23013
H -2.49215 1.90196 1.59702
H 2.94394 -0.0602283 -2.41462
H -0.402729 1.0075 0.424104
H 0.838253 0.0071576 0.307257
H 1.0888 -3.52245 -0.688114
H 0.562651 -3.1319 -2.12167
H 1.84027 2.30529 2.66699
H 3.00868 1.22039 1.21108
H -0.595832 -1.45143 -2.94214
H -1.36831 -0.610791 3.56244
H 2.86675 -0.816529 -0.0559691
H 2.41768 -1.01366 1.47813
H -2.76067 1.45901 -1.57417
H -3.23098 0.996274 -0.130158
H 6.54037 -4.29712 -3.00774
H 4.77133 -4.12778 -3.20078
H 5.84227 -2.77925 -3.63939
H 6.05878 -4.84026 -0.519902
H 5.08273 -3.64472 0.382691
H 4.32413 -4.61218 -0.896501
H 7.63891 -2.87568 -1.14234
H 6.87393 -1.45429 -1.90582
H 6.548 -1.8223 -0.198078
H 5.19108 -4.00122 5.41022
H 4.31111 -4.67077 4.00856
H 5.24992 -3.17201 3.83022
H 2.85684 -1.08311 5.59984
H 4.28983 -1.79729 6.40171
H 4.41954 -1.11134 4.75726
H 2.93613 -3.96348 6.65609
H 1.58833 -3.10692 5.85162
H 2.19738 -4.63427 5.17518
H -2.15694 -5.73523 2.00439

H -1.75059 -7.47398 2.05583
H -0.849297 -6.30728 3.06355
H 0.517385 -8.16309 1.02593
H 1.52118 -6.84585 0.355031
H 1.26806 -6.96016 2.11162
H -0.245497 -6.05825 -1.06943
H -1.38562 -7.31589 -0.500542
H -1.80445 -5.57905 -0.37782
H -1.49386 -5.34293 -6.28576
H -0.738505 -5.31039 -4.66648
H -2.43604 -4.82553 -4.85868
H 0.397423 -3.78186 -7.0554
H 0.624659 -2.27063 -6.12918
H 1.02414 -3.83181 -5.38117
H -2.06829 -3.05788 -7.34167
H -2.97446 -2.69659 -5.84652
H -1.67629 -1.60648 -6.37567
H 2.34759 0.580228 -6.34042
H 3.76433 1.2407 -7.20384
H 3.95256 -0.142169 -6.08976
H 5.5213 2.48095 -5.76316
H 5.18986 2.57264 -4.00914
H 5.59261 1.00892 -4.75495
H 3.01688 3.5529 -4.35857
H 3.2037 3.52191 -6.13793
H 1.81507 2.71217 -5.35679
H -0.428445 7.82384 -3.21682
H 0.977437 6.75203 -2.95716
H -0.570107 6.06378 -3.49713
H -0.132825 8.58563 -0.770275
H -0.105961 7.30276 0.471178
H 1.24714 7.45628 -0.671598
H -2.3827 7.5987 -1.56557
H -2.40131 5.85151 -1.94599
H -2.20638 6.38642 -0.264898
H -4.83623 -0.764479 6.91653
H -3.17395 -0.240862 6.52202
H -4.53139 0.30415 5.51569
H -3.96386 -3.19351 6.72791
H -3.13985 -3.62813 5.20363
H -2.36643 -2.49781 6.33387
H -5.95672 -2.40199 5.27395
H -5.58177 -1.22358 3.98476
H -4.99414 -2.89713 3.85321
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H 5.08709 4.81713 1.06437
H 5.25313 4.57199 2.81727
H 6.44825 1.14379 2.53286
H 7.5501 2.53788 2.71054
H 6.04224 2.45372 3.66313
H 5.61332 3.03558 -0.45774
H 7.28915 2.9098 0.161837
H 6.21248 1.48362 0.160374
H 2.64659 4.2373 5.80457

H 1.46374 4.57378 7.09885
H 1.74372 2.89758 6.54723
H 1.55145 5.70683 4.24431
H -0.162004 5.45864 3.84409
H 0.289705 6.15907 5.42453
H -0.587056 2.5737 6.01463
H -1.01411 4.2328 6.52842
H -1.3962 3.66847 4.87571
H -2.84652 -1.156 3.93907
H 2.50138 -2.49204 3.41197
H 0.212697 -4.57609 1.08733
H 0.965388 2.93452 3.88923
H 4.05482 2.38985 1.59018
H -0.930216 -2.72224 -3.88275
H -0.0741093 4.92362 -1.10054
H 3.00444 1.01763 -3.63244
H 4.12411 -2.04362 -1.57903
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H -6.77985 -0.709595 -0.25334
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H -5.74719 -3.24174 -2.75457
H -5.88196 -3.52704 -1.00436
H -7.15709 -2.59586 -1.85815
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C 3.76722 -1.66785 5.43768
C 2.48739 -3.70676 5.68018
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C 0.327479 -3.32157 -6.05377
C -1.98662 -2.65447 -6.31675
C 3.41665 0.798819 -6.25305
C 5.06406 1.95657 -4.90514
C 2.88003 2.94203 -5.25587
C -0.11088 6.82709 -2.86126
C 0.160873 7.54078 -0.563496
C -1.9529 6.61579 -1.30441
C -4.13617 -0.537023 6.09318
C -3.32518 -2.81335 5.91088
C -5.18912 -2.07499 4.54987
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O -1.56236 -1.9509 0.866931
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O 2.60184 3.08189 -1.1545
O 0.244866 -0.305818 4.04688
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O 1.92065 -2.08027 2.70553
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O -3.29716 0.786473 -1.08972