

The hidden complexities of ice

Water molecules (H_2O) in an ice crystal cannot fit together in any old way, because of their tetrahedral shape and the particular way they are held together. Using a branch of mathematics called combinatorics we can work out how many possible arrangements there are.

There are six ways of choosing two out of the four corners of the tetrahedron for the two hydrogen atoms. So there are a total of six possible orientations of a water molecule sitting within a larger ice crystal.



But not every potential arrangement of tetrahedra is possible, as each hydrogen atom of the water molecules must bond with a lone electron pair of an adjacent molecule. In fact, when the constraints of hydrogen-bonding are taken into account, the number of possible orientations for a given molecule is no longer six, but 3/2. Therefore, for a crystal of ice with N molecules there are $(3/2)^N$ possible ways to arrange the water molecules.

Produced by the LMS-IMA Mathematics Promotion Unit in conjunction with Plus magazine, the *A* molecule's eye view of water project and the Royal Society. Find out more about the maths inside science at http://plus.maths.org/inside.

Front Image by Kenneth Libbrecht, Caltech and Ben Slater, UCL



The ice cube in your drink has a volume of about 2cm^3 , containing about $6x10^{22}$ molecules. Our maths tells us that there are about $(3/2)^{6x10^{22}}$ ways that the water molecules could be arranged in that ice cube. That is more possibilities than the number of ways you could have drawn the lotto numbers every week since the Big Bang! Therefore, every single ice cube ever created will probably have a different arrangement of water molecules within it.

To find out more about "A molecule's eye view of water" visit http://www.chem.ucl.ac.uk/ice

