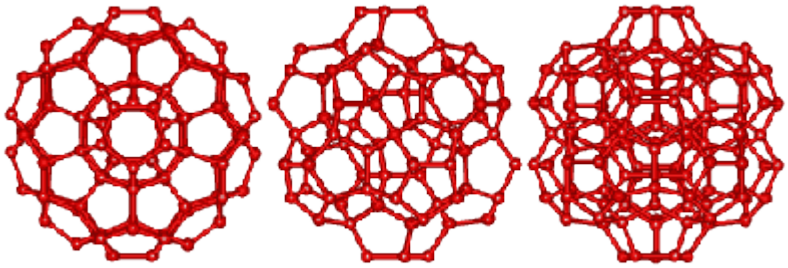
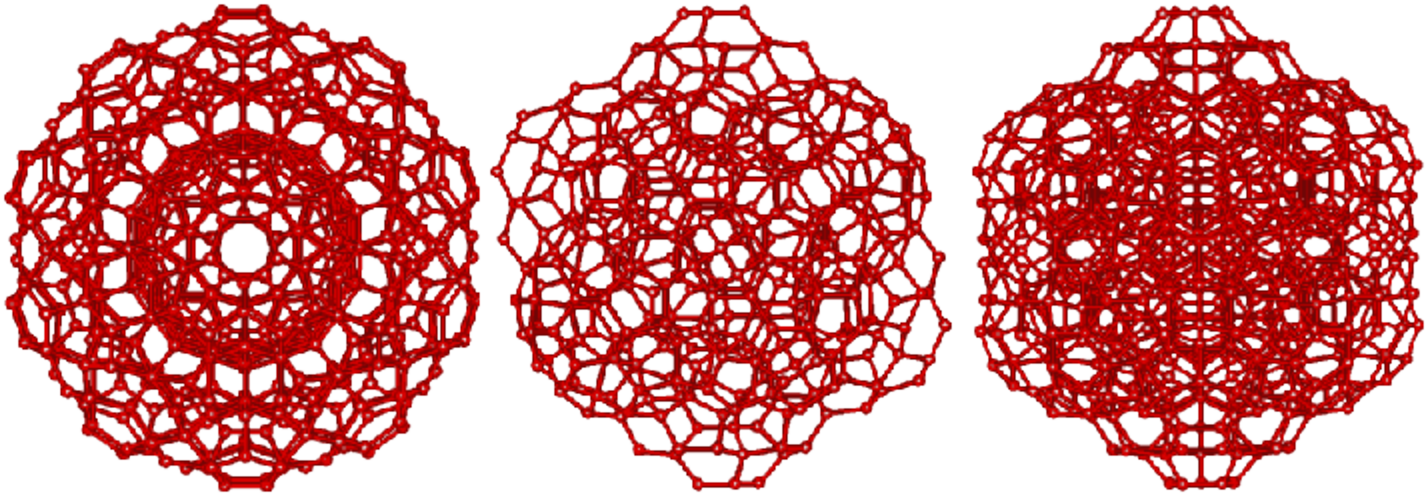
Alternative Icosahedral Water Cluster Architecture

Dodecahedral clusters of water, $(H_2O)_{20}$, can tessellate with only slight distortion of the preferred hydrogen bonding parameters, so long as the tessellation is not too extensive. This low density structure may occur when a solute is available to stabilize the structuring by occupying the cavities and when the water concentration is low. It provides one interstitial site for every five water molecules and a mole fraction of water (x_w) of 0.83. It is likely that solutes, soluble at this level, may well distort the dodecahedra but such a structuring shows the possiblility of retaining complete hydrogen bonding even at high concentrations of small solutes.



Shown above is an icosahedron of twelve dodecahedral structures surrounding a central dodecahedron; $(H_2O)_{130}$. Only the oxygen atoms of the constituent water molecules are shown. For interactive Figures, see Jmol.

The icosahedral model of water, $(H_2O)_{280}$, consists of water dodecahedra separated by two pentagonal boxes. It is also possible that a tessellated structure may arise from water dodecahedra separated by only one pentagonal box (shown below). Such a structure possesses higher energy than the icosahedral model and a lower density, due to the relatively greater number of large cavities. It may hower arise when a solute is available to stabilize the structuring by occupying the large cavities and when the water concentration is low. It provides one large interstitial site for every 25 water molecules and a mole fraction of water (x_w) of 0.96. It is likely that solutes soluble at this level may well distort the dodecahedra but such a structuring shows the possiblility of retaining complete hydrogen bonding even at moderately high concentrations of small solutes. Concentrated salts may provide water-separated ions that occupy the larger interstitial dodecahedral sites and show partial occupancy of the associated pentagonal boxes to produce water-separated ion pairs.



Shown above is an icosahedron of twelve dodecahedral structures surrounding a central dodecahedron, all separated from each other by a pentagonal box; $(H_2O)_{650}$. Only the oxygen atoms of the constituent water molecules are shown. For interactive Figures, see Jmol.

Source : http://www1.lsbu.ac.uk/water/alticos.html