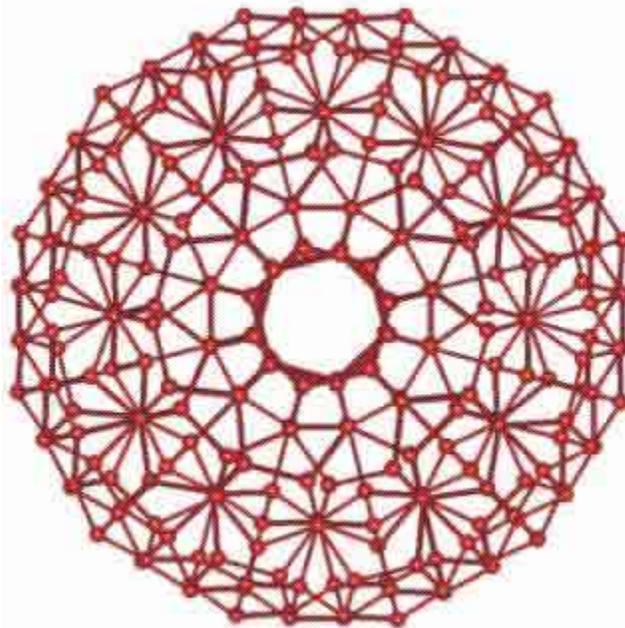
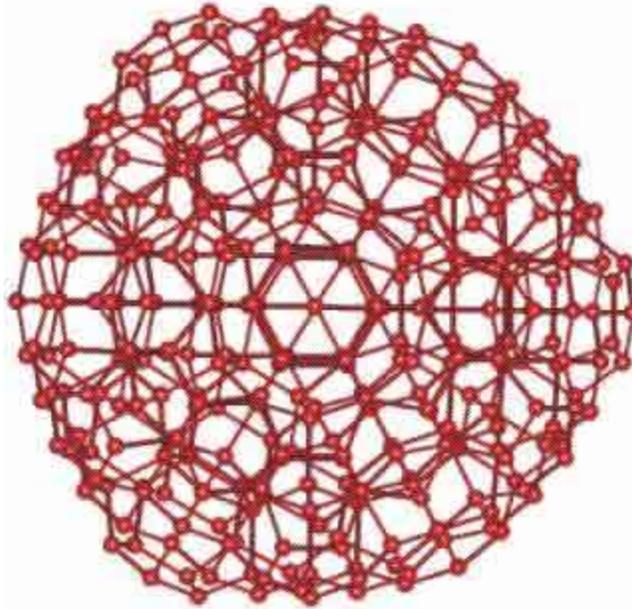


Water Cluster Architecture, Based on Gas Clathrates

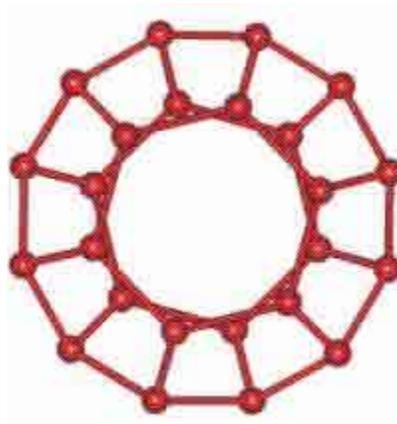
As well as forming [icosahedral water clusters](#), [14-water-molecule water tetrahedra](#) can form large regular, and relatively undistorted^a, clusters around other clathrate cavities ('Bucky-ice' structures such as the tetrakaidecahedral ($5^{12}6^2$) and hexakaidecahedral ($5^{12}6^4$) cavities found in crystalline gas [clathrate structures sI and sII](#) respectively). Such structuring would allow icosahedral-like network structuring around larger guest molecules as the cavities have radii 4.33 Å and 4.68 Å (compare pentagonal dodecahedral cavity (5^{12}) at 3.91 Å). They are also capable of forming an infinite network without further hydrogen-bond distortion (see [below](#)) in the same way gas hydrates form regular crystalline solids. Although both non-crystalline [ES](#) clusters and crystalline [gas-containing clathrates](#) both have similar inner-shell water clustering, the topology of the outer clustering is very different. The lack of evidence for the partial formation of crystalline clathrates in liquid water containing clathrate-forming solutes cannot, therefore, be used to indicate the lack of formation of other clathrate structuring as suggested by some authors.



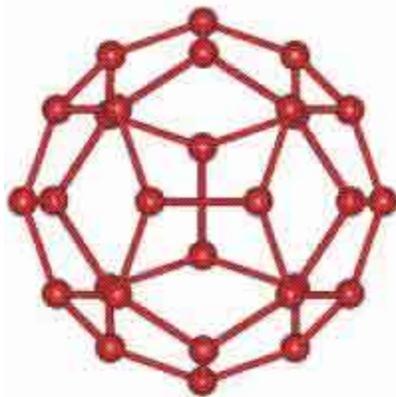


Twenty-four 14-molecule water [tetrahedra](#) arranged around the clathrate-I cavity, given below. Only the 336 oxygen atoms are shown.

Twenty-eight 14-molecule water [tetrahedra](#) arranged around the clathrate-II cavity, given below. Only the 392 oxygen atoms are shown.

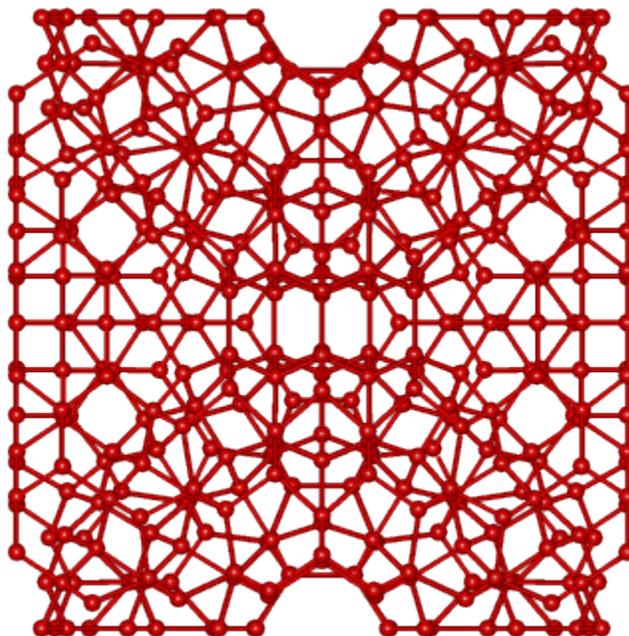


5¹²6² cavity



5¹²6⁴ cavity

For interactive Figures, see [Jmol](#).



The use of such clathrate cages in the formation of solid gas hydrate ices is [shown on another page](#).

[280-molecule icosahedra](#) plus [336-molecule tetrakaidecahedra](#)(5¹²6²) can be arranged in a similar cubic network to give a fully tessellated structure (only the oxygen atoms of water are shown.). A unit cell of such a structure is shown above. It is not known whether such a structure actually exists, as it does involve some distortion with standard deviations of 2.4% in the O···O nearest neighbor distances and 4.4% in the tetrahedral hydrogen bonded angles.

For interactive Figures, see [Jmol](#).

Source : <http://www1.lsbu.ac.uk/water/clathrate.html>