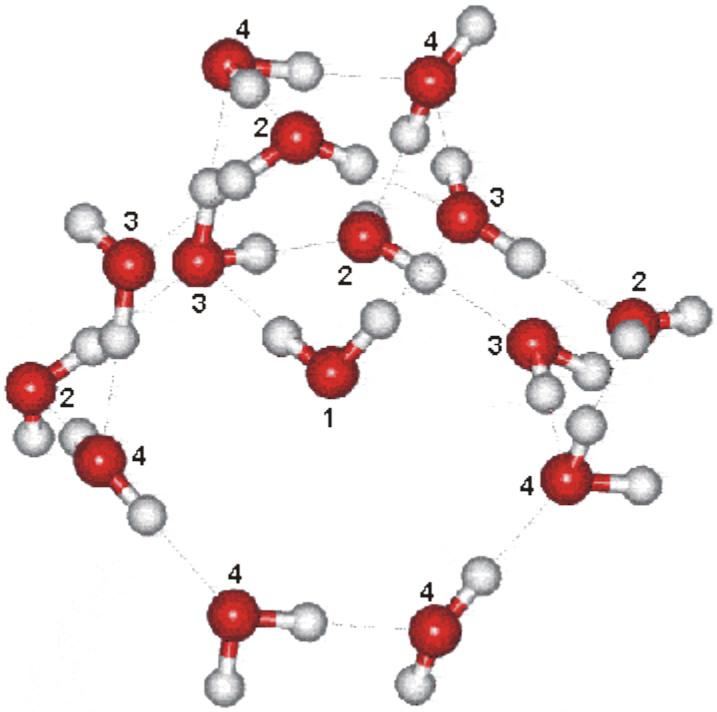
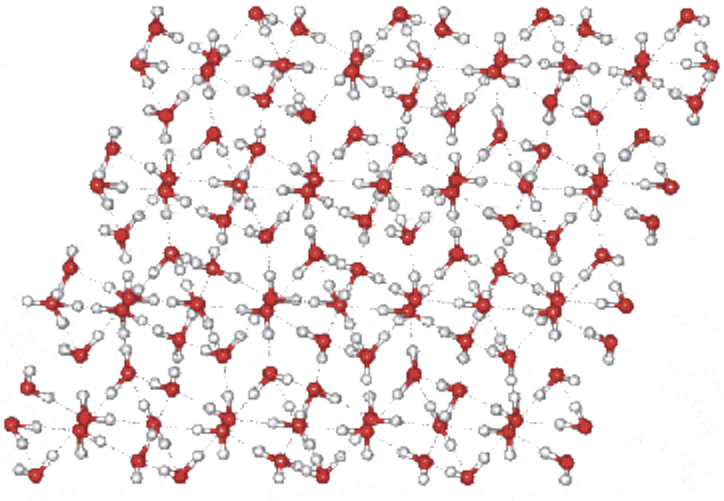
Ice-five (Ice V)



Ice-five (ice V) is formed from liquid water at 500 MPa by lowering its temperature to 253 K (see Phase Diagram). Its unit cell, which forms monoclinic crystals (Space group *C*2/*c*,**15**; Laue class symmetry 2/m), is shown opposite. Ice V contains four-, five-, six- and eight-membered rings (that is, the opposite sub-structure has two of each) and groups of seven molecules at four different lattice sites (three consisting of two molecules and one of a single molecule) with each experiencing a differing molecular environment. A chain of water molecules (O4), with each forming a corner of two condensed four-membered rings, runs parallel to the a-axis.

Also parallel run chains of two other alternating sites (O2 and O3) that are joined together through gaps in the first chain by the smaller number of the fourth type (O1). O4 water molecules are also hydrogen bonded to the O2 and O3 water molecules but not to the O1 molecules. These latter molecules form hydrogen bonds that penetrate (go through) the 8-membered rings structures.



All molecules form one connected lattice with a density of 1.24 g cm^{-3} (at 350 MPa where water density = 1.13 g cm^{-3}) [8].. The hydrogen bonding is disordered and constantly changing as in hexagonal ice. The crystal has cell dimensions a 9.22 Å, b 7.54 Å, and c 10.35 Å, (90°, 109.2°, 90°, 28 molecules; at atmospheric pressure and 98 K) and a unit cell contains 28 water molecules [359].

Ice-five has triple points with liquid water and ice-three (-16.986 °C, 350.1 MPa), liquid water and ice-six (0.16 °C, 632.4 MPa), ice-two and ice-three (-24.3 °C, 344.3 MPa) and ice-two and ice-six (estimated at -55 °C, 620 MPa). The dielectric constant of ice-five is about 144.

The melting curve for ice-five is given by $$P_m = 355.0 + 373.6 \times \left(\left(\frac{T_m}{256.43} \right)^{8.66} - 1 \right)$$ MPa [1320].

Note that in this structural diagram the hydrogen bonding is ordered whereas in reality it is random (obeying the 'ice rules': two hydrogen atoms near each oxygen, one hydrogen atom on each O···O bond). As the H-O-H angle does not vary much from that of the isolated molecule, the hydrogen bonds are not straight (although shown so in the figures).

The ordered hydrogen-bonding form of ice V is ice XIII (ice-thirteen).

Interactive Jmol structures are given.

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