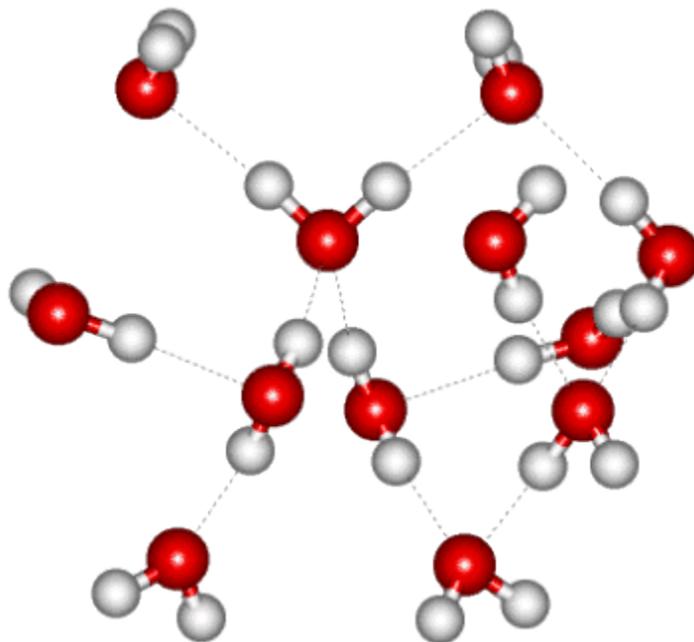
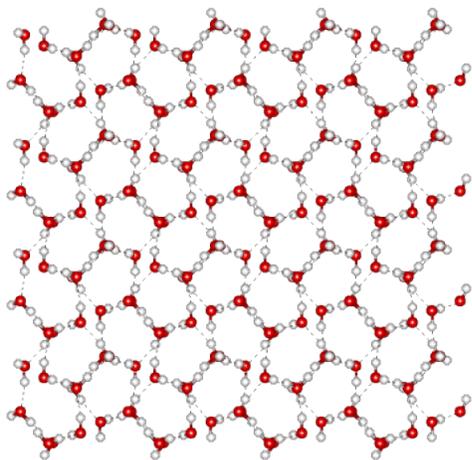


Ice-three (Ice III)



Ice-three (ice III) is formed from water at 300 MPa by lowering its temperature to 250 K (see Phase Diagram). It is stable over a relatively small range of conditions in the P - T phase space. Its unit cell, which forms tetragonal crystals (Space group $P4_12_12$, **92**; Laue class symmetry 4/mmm; analogous to keatite silica), is shown opposite. In the crystal, all water molecules are hydrogen bonded to four others, two as donor and two as acceptor. Ice III contains five membered rings joined as bicycloheptamers and has a density of 1.16 g cm⁻³ (at 350 MPa where water density = 1.13 g cm⁻³). The hydrogen bonding is disordered and constantly changing as in hexagonal ice. The tetragonal crystal (shown below) is pseudo-cubic with cell dimensions 6.666 Å (a) and 6.936 Å (c ; 90°, 90°, 90°; at 250 K and 280 MPa) [385] and contains 12 water molecules. Its structure consists of tight right-handed^afour-fold helices, containing two thirds of the water molecules, connected by the remaining water molecules which, thus, experience a differing molecular environment.



Metastable ice-three may be formed within the ice-two phase space by raising the compression rate in the density driven phase transition from hexagonal ice down to 170 K [1545].

Ice-three has triple points with liquid water and ice Ih (-21.985 °C, 209.9 MPa), liquid water and ice-five (-16.986 °C, 350.1MPa), ice Ih and ice-two (-34.7 °C, 212.9 MPa) and ice-two and ice-five (-24.3 °C, 344.3 MPa). The dielectric constant of ice-three is about 117.

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).

$$P_m = 209.5 + 101.1 \times \left(\left(\frac{T_m}{251.15} \right)^{42.86} - 1 \right) \text{ MPa}$$

The melting curve for ice-three is given by [1320].

The ordered hydrogen-bonding form of ice III is ice IX (ice-nine).

Interactive Jmol structures are given.

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