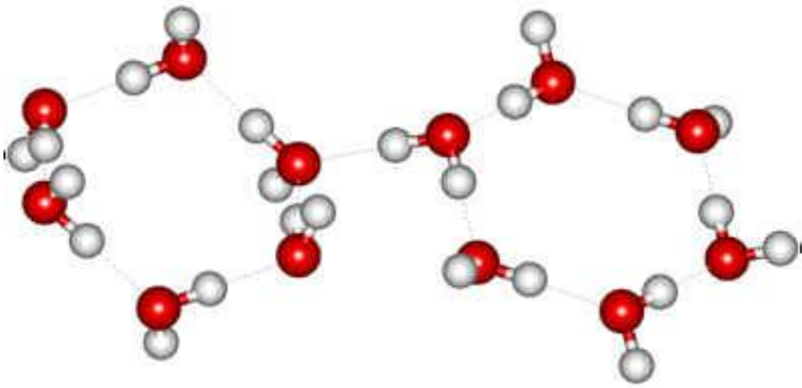
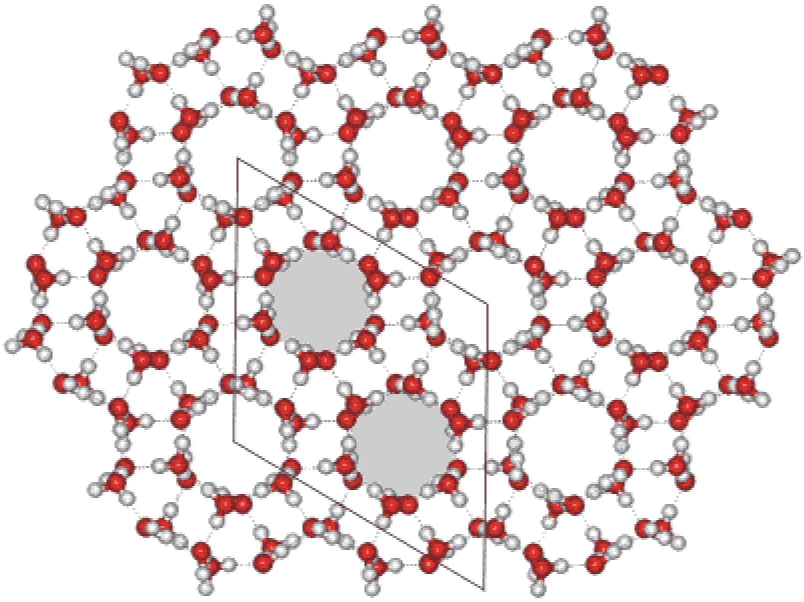
Ice-two (Ice II)

Ice-two (ice II) may be synthesized from hexagonal ice at 198 K and 300 MPa or by decompressing ice-five (ice V) at 238 K but is not easily formed by cooling ice-three (ice III) (see Phase Diagram). It may form a major proportion of icy moons such as Jupiter's Gannymede [839].



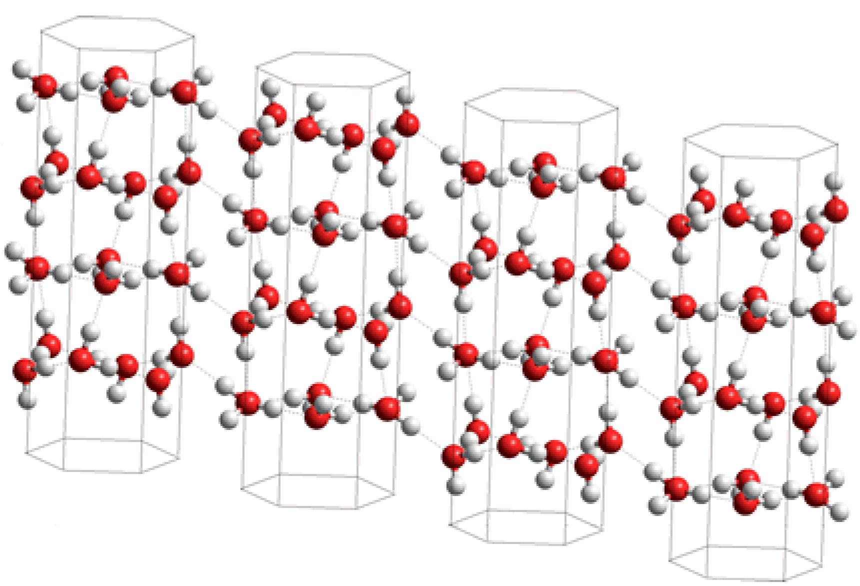
Its unit cell, which forms rhombohedral crystals, (Space group $R\bar{3}$) is shown opposite. In the crystal, all water molecules are hydrogen bonded to four others, two as donor and two as acceptor. Ice-two may exist metastably below ~100 K between ambient pressure and ~5 GPa. At ambient pressure it irreversibly transforms into ice Ic above 160 K. 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).

Half the open hexagonal channels of ice Ih have collapsed in ice II. The relationship of the ice II structure to ice Ih can be visualized by detaching the columns of hexameric ice Ih rings, moving them relatively up or down at right angles to their plane, rotating them about 30° around this axis and re-linking the hydrogen bonds in a more compact way to give a density of 1.16 g cm^{-3}. The hydrogen bonding is ordered and fixed in ice-two, as can be seen in the linkages round the hexamers. There is no corresponding disordered phase, in contrast to the other ordered ices VIII, IX, XI and XV. The lack of a disordered phase has been correlated with the high energy difference between the most and the second most stable ice configurations [1655]. Some of ice-two's hydrogen bonds are bent and, consequentially, much weaker than the hydrogen bonds in hexagonal ice.



View down the hexagonal *c* axis.

The unit cell consists of two hydrogen bonded hexamers, one chair-form (above left) and one almost flat (above right). Two molecules (center bottom in the above diagram) are shown closely approaching (3.23 Å) but they are not hydrogen bonded. The rhombohedral crystal has unit cell dimensions 7.78 Å (a, b, c; 113.1°, 113.1°, 113.1°, 12 mols) [384] each containing 12 water molecules. It may be easier to visualize the crystal as hexagonal, each unit cell containing 36 water molecules (as shown opposite, with dimensions a, b, c; 12.935 Å, 12.935 Å, 6.233 Å; 225 K. 0.25 GPa, [839]).



The hexagonal channels (as indicated gray above) form columns of alternating puckered and flat rings going away from the viewer, and remain from the conversion from hexagonal ice.

Opposite shows the view almost perpendicular to the *c* axis, showing the hydrogen bonding between these hexagonal channels.

Ice-two has triple points with ice Ih and ice-three (-34.7 °C, 212.9 MPa), ice-three and ice-five (-24.3 °C, 344.3 MPa) and ice-five and ice-six (estimated at -55 °C, 620 MPa). The dielectric constant of ice-two is about 3.7 [94].

Interactive Jmol structures are given.

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