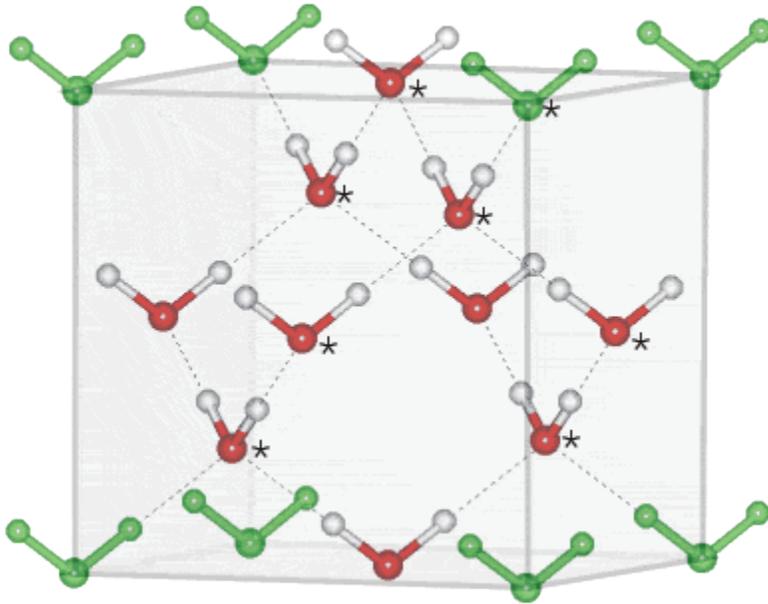


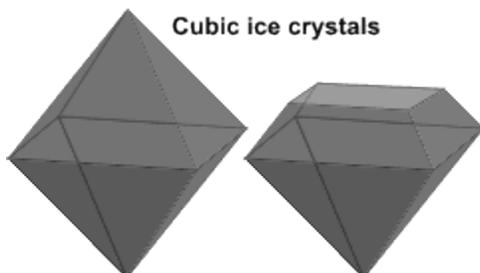
Cubic Ice (Ice Ic and Ice XIc)

Ice Ic is a metastable^b form of ice that can be formed, by condensation of water vapor, at ambient pressure but low temperatures (less than -80 °C, see Phase Diagram), or below about -38 °C in small droplets (~6 μm diameter) [1013] or by reducing the pressure on high-pressure ices at 77 K. Often (perhaps usually [1236c]) found are transitional states between hexagonal and cubic ice depending on the formation and history of the cubic ice [1236].

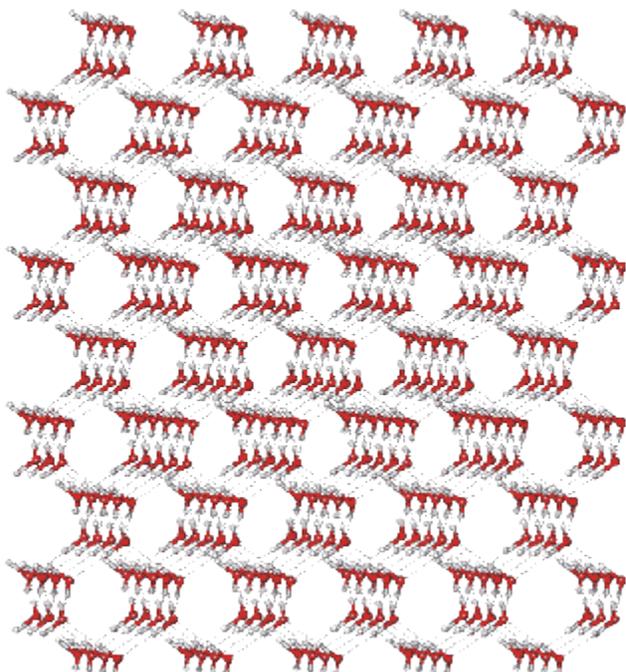


Cubic ice has a slightly higher vapor pressure than ice_h and may naturally form in the upper atmosphere [751] and is often found in freezing confined (porous) aqueous systems. There is evidence that it may be the preferred phase for ice formed from water droplets smaller than 15 nm radius at 160-220 K [856, 996], due to its lower interfacial free energy than hexagonal ice. Larger cubic ice crystals convert, irreversibly but extremely slowly in the temperature range 170-220 K, to hexagonal ice with up to 50 J mol⁻¹ heat evolution [493].

It consists of a face centered cubic lattice (Space group $Fd\bar{3}m$, **227**; Laue class symmetry $m\bar{3}m$; analogous to β -cristobalite silica) with half the tetrahedral holes filled. The starred molecules show the unit cell positions. The (H₂O)₁₀ cluster, shown in red, has been found in a super-molecular structure [32].



As with ice Ih, it possesses a fairly open low-density structure where the packing efficiency is low ($\sim 1/3$) compared with simple cubic ($\sim 1/2$) or true face centered cubic ($\sim 3/4$) structures.^a



In contrast to ice Ih, however, water molecules have a staggered arrangement of hydrogen bonding with respect to all of their neighbors, rather than to 3/4 of them. The result is that the density is almost the same as ice Ih.

All atoms have four tetrahedrally arranged nearest neighbors and twelve second neighbors, as ice Ih. The crystals may be thought of as sheets of chair-form hexamers in any one of the tetrahedrally-arranged planes. Please note that in both these structural diagrams 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 $O\cdots O$ 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). However, the ordered structure shown may exist in a proton ordered form (iceXIc; comparable to the relationship of ice XI to Ice-Ih) [1753].

The cubic crystal has unit cell dimension 6.358 \AA (a, b, c; 90° , 90° , 90° , 8 molecules) [383]. All molecules experience identical molecular environments. Interpenetrating ice Ic networks occur in the high pressure ices ice-seven and ice-eight.

There are differences in the numbers of water molecules in the hydration shells around water molecules in hexagonal and cubic ices. Notably, there is an extra water molecule in the second shell of hexagonal ice, which helps explain its greater stability. The cavities in cubic ice are formed from ten water molecules and are smaller than those in hexagonal ice; formed from twelve. These cavities form an identical network to the water molecules. Indeed if all the cavities contain a water molecule each, then the structure of ice-seven is formed.

Comparison of hexagonal and cubic ice						
Hydration shell	1	2	3	4	5	6
Radius, nm (approx.)	0.28	0.45 (0.46)	0.53	0.65	0.70 (0.74)	0.78
Hexagonal ice, No.	4	12 (+1)	9	12	9 (+2)	18
Cubic ice, No.	4	12	12	6	12	24

Cubic ice shows anomalous reduction in thermal conductivity with increasing pressure (as do hexagonal ice and low-density amorphous ice) but different from most crystals. This is due to changes in the hydrogen bonding decreasing the transverse sound velocity [617]. Cubic and hexagonal ices have been compared [996].

Interactive structures are available (Jmol).

Footnotes

^a The exact packing efficiency for ice Ic is low (
$$48 \times \left\{ \sin \left[\frac{\cos^{-1}(1/3)}{2} \right] \right\}^3 = 0.3401, \sim 1/3$$
) compared with simple cubic ($\frac{\pi}{6} = 0.5236, \sim 1/2$) or true face centered cubic ($\frac{\pi}{3\sqrt{2}} = 0.7408, \sim 3/4$) structure [811]. [Back]

^b The metastability of cubic ice relative to hexagonal ice is due to the greater symmetry of the cubic ice crystal. Although both crystal structures involve tetrahedrally placed oxygen atoms, cubic ice constricts the water H-O-H bond angle more strongly towards the tetrahedral angle (109.47°), relative to hexagonal ice, and further away from its gas phase value (104.47°). [Back]

Source: <http://www1.lsbu.ac.uk/water/ice1c.html>