

# The many forms of ice

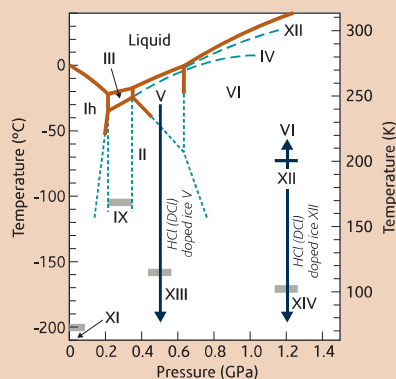
## ISIS Science

**You might think that the ice on Earth would be the same as that on Iapetus, Saturn's icy moon, but new research suggests they may be quite different. At high pressures and low temperatures ice starts to behave differently. Using neutron diffraction at ISIS, scientists have been discovering some new and unusual forms of ice.**

*The phase diagram of ice, including liquidus lines of metastable ices IV and XII (long dashed lines) and extrapolated equilibrium lines at low temperatures (short dashed lines). Hydrogen ordered ices XIII and XIV were prepared by isobaric cooling of HCl (DCl) doped H<sub>2</sub>O (D<sub>2</sub>O) ice V or XII to -196°C at 0.5 GPa or 1.2 GPa, respectively (indicated by arrows). Cooling of ice XII was started at -83°C, which is 10°C below the temperature where transition to stable ice VI would occur. The temperatures of the hydrogen ordering phase transitions are indicated by grey bars.*

As water freezes into ice, its molecules rearrange themselves. Freeze it at higher pressure and the molecular rearrangement can be different, enabling ice to form a number of different crystal structures. Ordinary ice has a honeycomb-like structure, but take this ice to a lower temperature or higher pressure and significant changes start to occur.

"At low temperatures the system tries to increase its degree of order," explains John Finney, a physicist at University College London, who has, together with Christoph Salzmann from Oxford University and Paolo Radaelli from ISIS, been using ISIS neutrons to study ice structures.

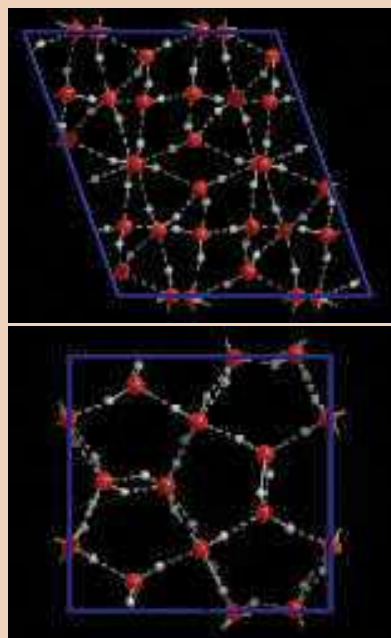


In order to increase order, the water molecules need to take on different orientations with respect to each other. By doping their ices with a small amount of hydrochloric acid, the scientists can free-up the molecules so they can re-order. This kick-starts the rearrangement process, which is usually prevented by the temperature being too low: these new ice phases form at around -160°C.

Using this technique, the team has discovered three new phases of ice, bringing the total number of known ice forms up to sixteen so far. "None of these phases are likely to occur naturally on Earth, but they might be found on some of the icy moons of the outer planets," says Salzmann.

A major advantage of using ISIS to study the ice was that the scientists could monitor how the structure changed over time. "The pulsed neutron source enabled us to take 'snapshots' of the structure and observe the phase transitions as they occurred," says Finney. The penetrating power of neutrons makes them ideal for experiments requiring thick-walled containers to study samples under pressure. The ability of neutrons to see light elements enables hydrogen bonding in substances such as ice to be studied.

Understanding the moons of outer planets is not the only application of ice research. "If we can understand the different forms and how they transform from one to another then it will help us to understand the water molecule better, which is essential if we are to understand the role of water in biological and chemical systems," explains Finney.



*The crystal structures of two new ice phases, ice XIII and ice XIV. Oxygen atoms are red, hydrogens are white. Each water molecule is bonded in a tetrahedral arrangement to four others. Ice XIII was formed at pressures of around 5000 atmospheres, ice XIV at around 12000 atmospheres.*

#### Further information:

*The preparation and structures of hydrogen ordered phases of ice,* CG Salzmann et al., *Science* 311 (2006) 1758.

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