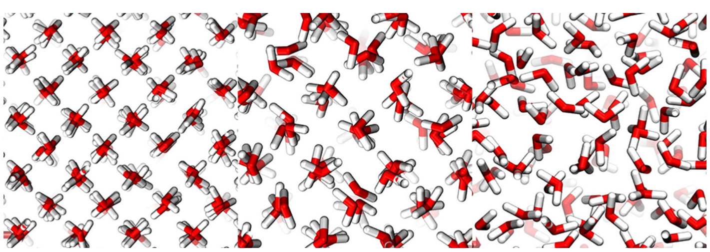
Plastic Ice Observed

A neutron-scattering experiment has confirmed the existence of an unusual phase of ice that forms at high temperature and high pressure.

By **Charles Day**

Above a pressure of 2 gigapascals (GPa), water ice adopts a body-centered cubic (BCC) structure known as ice VII. When the temperature and the pressure of this structure increase, the hydrogen atoms start to move and eventually become mobile protons. But before the temperature gets high enough to liberate protons, the water molecules can rotate within the BCC lattice, creating a phase of ice known as plastic ice VII. This unusual phase was first predicted in 2008. Now Livia Bove of Sorbonne University in France and her collaborators have confirmed its existence through neutron-scattering experiments [**1**].

The telltale rotation of the water molecules in plastic ice VII primarily manifests in the rapid movement of hydrogen atoms. Neutrons scatter readily off hydrogen atoms, making them an ideal structural probe in neutron-scattering experiments. What's more, the neutrons produced at neutron-scattering facilities tend to have low energies, meaning that a small but potentially measurable change in energy results from the additional kick. But plastic ice VII is still challenging to observe, and not just because of the need to reach temperatures higher than 450 K and pressures higher than 3 GPa. Attaining those pressures requires a diamond-anvil cell, which, being small, reduces the sample volume to the point that a typical neutron beam would struggle to deliver enough neutrons to form a crisp diffraction pattern.



Snapshots from molecular-dynamics simulations of heated, pressurized water. In ice VII (left) the water molecules jiggle somewhat but occupy a body-centered cubic lattice (BCC). In plastic ice VII (middle) the molecules remain in the BCC lattice but rotate. In liquid water (right) the molecules both move and rotate.
Credit: M. Rescigno *et al*. [1]; adapted by APS

To overcome that challenge, Bove and her collaborators used the powerful neutron beams available at the Institut Laue—Langevin in France. In their experiments, the researchers recorded neutron diffraction patterns at five temperatures between 471 and 523 K and at three pressures between 4.6 and 5.9 GPa. The energy that neutrons lost or gained when they scattered off a moving hydrogen atom was detected through the neutrons' flight times from the sample to the detector. When the conditions favored the liquid state, the researchers recorded a signal indicating the molecules were both changing positions and rotating. In crystalline ice VII those two motions appeared frozen. In plastic ice VII the researchers observed signals indicating a crystalline structure and active molecular rotations.

To characterize the rotations in plastic ice VII, the researchers performed molecular-dynamics simulations of water under the same temperature and pressure conditions as in the experiments. The simulations reproduced the neutron-scattering data in all three phases. What's more, the combination of data and simulations revealed that the water molecules in plastic ice VII do not rotate freely. Rather, they jump randomly between a few favored directions. Such jumps are also seen in pressurized crystals of neopentyl glycol and certain other organic molecules [**2**].

The range of conditions under which plastic ice VII exists is considerably narrower than for ice VII, which is expected to exist on Jupiter's moons Callisto and Ganymede and on Saturn's moon Titan, sandwiched between the moons' rocky cores and liquid oceans. Whether or not the properties of plastic ice VII influenced the formation or structure of those moons of Jupiter and Saturn is unclear.

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REFERENCES

1. M. Rescigno *et al.*, "Observation of plastic ice VII by quasi-elastic neutron scattering," **Nature (2025).**
2. B. Li *et al.*, "Colossal barocaloric effects in plastic crystals," **Nature 567, 506 (2019).**