

# Hydrogen-Stuffed, Quartz-like Water Ice

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## Scientific Achievement

The structure of a new phase in the  $\text{H}_2+\text{H}_2\text{O}$  system (“ $\text{C}_0$ ”) was experimentally resolved using single-crystal X-ray diffraction.

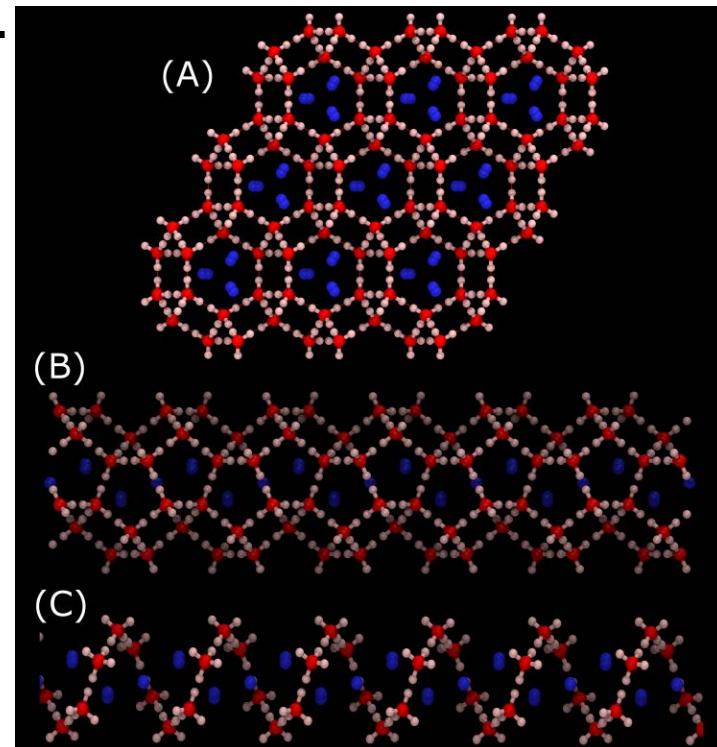
## Significance and Impact

The oxygen topology of this phase shows strong similarities with the mineral quartz, strengthening analogies between ice and silicate minerals.  $\text{C}_0$  holds  $>5\text{wt}\%$   $\text{H}_2$  in large channels that provide mobility.

## Research Details

- Single crystals grown at 400 MPa and 280 K within diamond anvil cells and probed using Raman spectroscopy and single-crystal X-ray diffraction.
- Composition is  $(\text{H}_2\text{O})_2\text{H}_2$  with three formula units per unit cell. Chiral hexagonal structure, space group  $P6_522$ .

(A) Supercell of the  $\text{C}_0$  structure viewed down the crystallographic  $c$ -axis.  $\text{H}_2$  molecules are shown in blue. (B) Single channel along the  $c$ -axis is a tube constructed of hydrogen-bonded water molecules with pentagonal tiling. (C) Tubes consist of interpenetrating spiral chains of  $\text{H}_2\text{O}$  and  $\text{H}_2$ .



T.A. Strobel, M. Somayazulu, P. Dera, S. Sinogeikin, R.J. Hemley, Hydrogen-Stuffed, Quartz-like Water Ice, *J. Am. Chem. Soc.* 138, 13768 (2016).



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