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Near-infrared spectroscopic sensing of hydrogen order  
in ice XIII

Christina M. Tonauer *et al.*  
Phys. Rev. Lett. **135**, 018002 (2025)

Published 2 July 2025

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Yours sincerely,

A blue ink signature of Hugues Chaté.

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Robert Garisto  
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PHYSICAL REVIEW LETTERS



## Near-Infrared Spectroscopic Sensing of Hydrogen Order in Ice XIII

Christina M. Tonaauer, Eva-Maria Köck, Raphael Henn, Christoph Kappacher, Christian W. Huck, and Thomas Loerting

Phys. Rev. Lett. **135**, 018002 (2025) - Published 2 July, 2025

Infrared spectroscopy performed on high-pressure ice phases demonstrates a possible technique for studying ice on other planets or moons.

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We identify hydrogen ordering in  $\text{H}_2\text{O}$  ices spectroscopically in the near-infrared (NIR) range ( $10\,000\text{--}4\,000\text{ cm}^{-1}/1\text{--}2.5\text{ }\mu\text{m}$ ) based on the example of ices V/XIII. Previously it was thought that hydrogen ordering can only be revealed on the basis of lattice phonons, i.e., intermolecular vibrations. Here we show differences in the overtone spectrum of the intramolecular OH-stretching vibration. This makes NIR spectroscopy the first remote sensing method that is sensitive to different orientations of the water dipoles within ice. As such it will allow for future observations of the hydrogen order of ices in space by the James-Webb Space Telescope or the JUICE mission.

