

Experimental measurement of the absorption cross section of dangling OH bonds in water ice

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Recent astronomical observations have revealed water (H₂O) ice to be ubiquitous in space. For example, it is the most abundant solid component in interstellar molecular clouds and the outer cold part of protoplanetary disks. Its ubiquity makes it essential to clarify the physics and chemistry of ice to further our understanding of the formation of stars and planetary systems, including our solar system [1].

Key infrared (IR) features related to interstellar ice are signals at 3720 and 3696 cm⁻¹ from dangling OH bonds, which have respectively been assigned to the free OH stretch modes of two- and three-coordinated H₂O molecules at the surface of ice [2, 3]. Because dangling OH bonds reflect the porosity of ice and serve as catalytic sites for adsorption and chemical reactions, they have been intensely studied in many fields including interstellar chemistry [4, 5]. Despite much active research, the absorption cross section, a fundamental optical constant, of dangling OH bonds remains unknown. This hampers the quantification of dangling OH bonds from IR spectra of ice.

Recently, we developed an experimental setup for in situ infrared multiple-angle incidence resolution spectrometry (IR-MAIRS) in low-temperature, ultrahigh-vacuum conditions [6]. IR-MAIRS is a spectroscopic method combining oblique incidence transmission measurements and multivariate analysis to retrieve both pure in-plane (IP) and out-of-plane (OP) vibration spectra for a thin sample, which was originally developed for quantitative molecular orientation analysis of organic thin films without the use of optical parameters [6, 7]. In this study, we report our recent challenge to measure the absorption cross section of dangling OH bonds of water ice using IR-MAIRS [8].

References

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