Experimental measurement for absorption cross section of two-coordinated dangling OH bonds on the surface of amorphous ice at 20 K

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In cold and dense interstellar clouds, amorphous water (H_2O) is abundant and forms icy dust grains [1]. Infrared (IR) spectra of amorphous water prepared at low temperatures show two weak absorption peaks at 3696 cm^{-1} and 3720 cm^{-1} in laboratory experiments. These are assigned to "dangling OH bonds", which are the free OH stretching modes of 3-coordinated (one H doner and two H acceptors; 3dOH) and 2-coordinated (one H donor and one H acceptor; 2dOH) H_2O on the ice surface, respectively [2]. Dangling OH bonds reflect the surface structure of ice and act as a chemical reaction site on the ice surface. Recently, the James Webb Space Telescope, a high sensitivity infrared telescope in space launched in 2021, detected possible dangling OH feature for amorphous icy dust grains in an interstellar cloud, where stars and planets will form [3]. With the absorption cross section for dangling OH bonds, the number density can be calculated from the observed absorbance, which leads us to understanding the surface structure of interstellar ices [4]. In this study, we measured the number densities of 2dOH and 3dOH on amorphous ice at 20 K using infrared multiple-angle incidence resolution spectrometry (IR-MAIRS). IR-MAIRS is a technique combining oblique incidence transmit measurements and multiple variation analysis to obtain pure out-of-plane (OP) and in-plane (IP) spectra. Figure 1 shows the OP and IP spectra of amorphous water at 20 K before and after the deposition of carbon monoxide (CO). Both 2dOH and 3dOH features appeared and quenched after CO exposure at 20 K. At the same time new peaks appeared at around 2152 and 2139 cm^{-1}, which are assigned to the CO stretching vibration bands for CO molecules adsorbed at dangling OH bonds and hydrogen-bonded OH bonds [5]. Assuming that the amount of the CO molecules adsorbed at dangling OH bonds to fully quench the two peaks corresponds to the column densities of 3dOH and 2dOH, the absorption cross section for 2dOH is estimated much smaller than that for 3dOH.

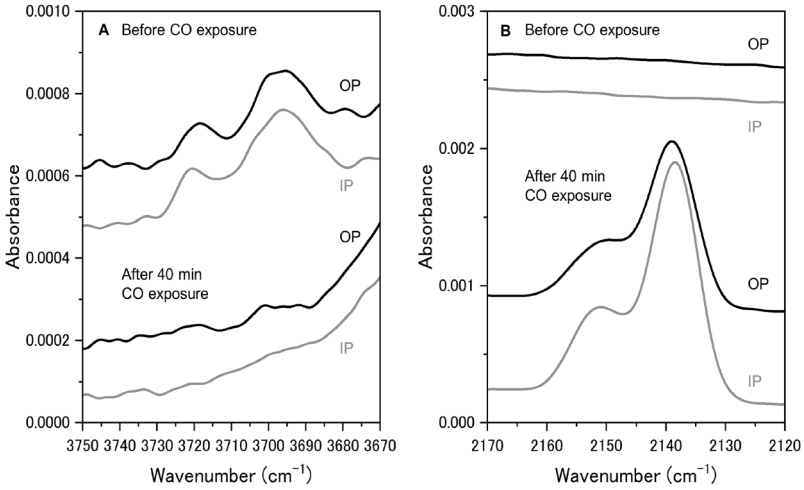

Figure 1. OP and IP spectra of amorphous ice vapor deposited at 20 K before (A) and after (B) CO exposure.

References

[1] T. Hama & N. Watanabe, Chemical Reviews 113, 8783–8839 (2013).
[2] V. Buch & J. P. Devlin, The Journal of Chemical Physics 94(5), 1, 4091-4092 (1991).
[3] M. K. McClure et al., Nature astronomy 7, 431-443 (2023).
[4] T. Nagasawa et al., The Astrophysical Journal Letters 923, L3 (8pp) (2021).
[5] S. Matsuda et al., Chemistry Letters 47(4), 468-471 (2018).