OXYGEN-ISOTOPE EFFECT ON THE NUCLEAR SPIN CONVERSION OF WATER MOLECULES

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According to the resultant spin I of two protons, water molecules are classified into two species: the ortho ($I = 1$) and para ($I = 0$) isomers. Because of the symmetry restriction, each isomer occupies specific rotational states. This coupling between the nuclear-spin and rotational states allows us to selectively monitor the isomers by rovibrational spectroscopy. The nuclear spin conversion between the isomers is extremely slow in the gas phase[1], but has been found to be much faster in condensed systems[2,3], whose mechanism is attracting interest. In the present study, we observed the conversion of H_2O trapped in solid Ar and investigated the oxygen-isotope effect.

Our experimental apparatus mainly consists of an ultrahigh-vacuum (UHV) chamber, a Fourier transform infrared spectrometer, and a HgCdTe-detector compartment. After degassing, the pressure in the UHV chamber went below 1×10^{-8} Pa. Liquid H_2O including the isotopologues of $H_2{}^{16}O$, $H_2{}^{17}O$, and $H_2{}^{18}O$ was distilled by freeze-pump-thaw cycles. The gases of Ar and H_2O were mixed in a gas handling system and were condensed on a gold substrate cooled to 10.5 K. Infrared absorption spectra were measured in the reflection configuration with the incident angle of $80°$.

The absorption band of ortho (para) H_2O appeared in the range of 1595 – 1608 (1608 – 1625) cm^{-1} in an infrared spectrum after the sample deposition. The ortho band decayed with increasing time whereas the para one grew. This time evolution originated from the nuclear spin conversion from ortho to para. In addition, each band contained three components corresponding to $H_2{}^{16}O$, $H_2{}^{17}O$, and $H_2{}^{18}O$. Performing tri-gaussian fitting, we determined the integrated intensity of each component as a function of time and conversion rates of $H_2{}^{16}O$, $H_2{}^{17}O$, and $H_2{}^{18}O$. In the presentation, we will discuss the conversion mechanism, comparing these rates.

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