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アモルファス氷からの水分子の真空紫外光脱離機構

Vacuum ultraviolet photodesorption mechanism of water molecules from amorphous solid water (ASW)

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1. Introduction

In interstellar molecular clouds, dust grains are coated with an amorphous solid water (ASW) ice. Photodesorption has been proposed as an important process from ices in protoplanetary disks and other astrophysical regions characterized by dense clumps of material and excess vacuum ultraviolet photons. It is often invoked to account for the high gas-phase abundances of less volatile molecules, such as water, that are observed under conditions where complete freeze-out onto dust grains might otherwise be expected. To reveal details of the photodesorption mechanism, we have measured the translational and rotational energies of H_2O (v = 0) molecules that are photodesorbed from ASW at 90 K using a 157 nm laser to the first absorption band.

2. Experimental

The experiments have been performed in a high vacuum chamber equipped with a pulsed molecular beam source, an excimer laser and a dye laser. ASW films were prepared by back-filled deposition of water vapor onto the Au substrate at 90 K.

An excimer laser at 157 nm (< 0.1 mJ cm^{-2} $pulse^{-1}$) were used. Photodesorbed H_2O were subsequently ionized at a distance of 2 mm from the Au substrate by (2+1) resonance enhanced multiphoton ionization (REMPI) technique on the H_2O C(000)-X(000) transition. The measured time-of-flight (TOF) spectra were fitted to the flux weighted Maxwell-Boltzmann distribution defined by a translational temperature, T_{trans}.

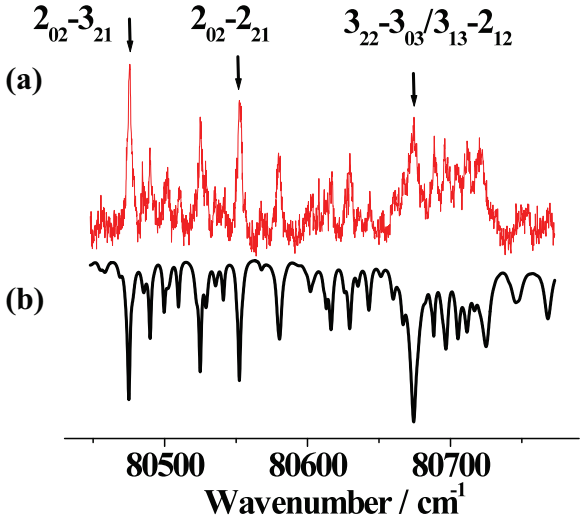

Fig 1. (a) REMPI spectrum of H_2O(v=0) following 157 nm photoirradiation of water ice at 90 K. Time-of-flight = 2.5 μs. (b) A simulated spectrum assuming a Boltzmann distribution with T_{rot}=300 K.

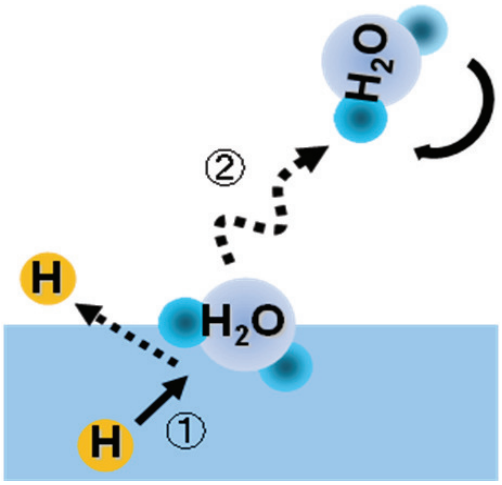

Fig 2. "kick-out" mechanism of H_2O from the ice by an energetic H atom released by VUV dissociation of water ice.

3. Results and Discussion

Figure 1(a) shows a (2+1) REMPI spectrum of photodesorbed H_2O (v=0) at the peak of TOF profile. Figure 1(b) shows a spectral simulation characterized by a Boltzmann distribution with a rotational temperature T_{rot} = 300 ± 100K.

TOF spectra of H_2O (v=0) were measured when exciting the 2_{02}-3_{21} line of the REMPI spectrum. The TOF spectrum is well reproduced by a Maxwell-Boltzmann distribution with T_{trans} (v=0) = 1800 ± 500 K. TOF spectra of other transition, *e.g.*, the 2_{02}-2_{21} or 3_{22}-3_{03}/3_{13}-2_{12} line are essentially the same.

The time evolution of the H_2O signal at the 2_{02}-3_{21} line as a function of the 157 nm irradiation time was also measured. The signal was promptly appeared, which suggests that the H_2O signal directly comes from the water ice and not from the secondary photoproducts that might be accumulating on the surface.

The main photodesorption mechanism is the "kick-out" of an H_2O molecule in the ice by an energetic H atom released by photodissociation.

$$H_2O(s) + 157\ nm \rightarrow \textit{hot}\ H + OH$$

$$H_2O(i) + \textit{hot}\ H \rightarrow H_2O(g) + H$$

where i stands for "interfacial". The average translational and rotational energies are well accord with predictions by classical molecular dynamics calculations for the "kick-out" of an H_2O molecule in the ice by an energetic H atom, suggesting that this process would be the dominant desorption mechanism.

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