Translational and rotational energy measurements of vacuum-ultraviolet photodesorped water molecules in their vibrational ground state from amorphous solid water

A. Yabushita,[1] T. Hama,[2] M. Yokoyama,[1] M. Kawasaki,[3] S. Andersson,[4] C. M. Western,[5] M. N. R. Ashfold,[5] R. N. Dixon,[5] and N. Watanabe[2]

[1]*Department of Molecular Engineering, Kyoto University, Japan*
[2]*Institute of Low Temperature Science, Hokkaido University, Japan*
[3]*Research Institute for Humanity and Nature, Japan*
[4]*SINTEF Materials and Chemistry, Norway and Department of Chemistry, Physical Chemistry, University of Gothenburg, Sweden*
[5]*School of Chemistry, University of Bristol, United Kingdom*

For large grains in the cosmic space, the most important desorption mechanism at the edge of molecular clouds is photodesorption. To reveal the details of photodesorption mechanism, we have experimentally measured the average translational and rotational energies for photodesorbed H_2O (v=0) from amorphous solid water (ASW) and polycrystalline ice (PCI) at 90 K using 157 nm laser. The experimental findings are compared with the results of classical molecular dynamics (MD) calculations performed for photodesorption from ASW.
The rotational temperature $T_{rot}(v=0)$ is estimated to be 300 ± 100 K by spectral simulation. Time-of-flight spectrum of H_2O (v=0) measured for the (2_{02}-3_{21}) line of the REMPI spectrum was measured, which is well reproduced by a M-B distribution with $T_{trans}(v=0)$ = 1800±500 K. The main mechanisms for this photodesorption is a "kick-out" of an H_2O molecule on the ice surface by the energetic H atom released from photodissociation of $H_2O + h\nu \rightarrow H + OH$.(Fig. 1) The experimentally observed average translational and rotational energies are in good accord with predictions by classical molecular dynamics calculations for the "kick-out" mechanism. H_2O molecules desorbed from ASW might be expected to lose energy in interactions with cold ice surface. Hence, a slow TOF component might be expected. The absence of any such slow TOF component suggests that H_2O only on the ice surface can desorb and not from bulk phase.

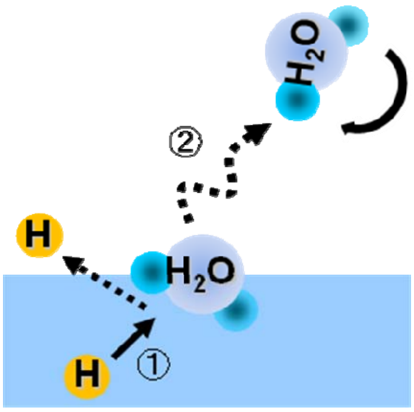

Figure 1 Schematic illustrations of a "kick-out" of another H_2O molecule in the ice by the energetic H atom released from VUV irradiation of amorphous water ice. The numbers dedicate for sequence of the reaction.

References

[1] A. Yabushita, T. Hama, M. Yokoyama, M. Kawasaki, S. Andersson, C. M. Western, M. N. R. Ashfold, R. N. Dixon, & N. Watanabe, 2009, ApJ 699, L80.

[2] T. Hama, M. Yokoyama, A. Yabushita, M. Kawasaki, S. Andersson, R. N. Dixon, M. N. R. Ashfold, & N. Watanabe, 2010, J. Chem. Phys. 132, 164508.