Energy partitioning in H_2 formation by photolysis of amorphous water ice

A. Yabushita, T. Hama, M. Yokoyama, and M. Kawasaki

Department of Molecular Engineering, Kyoto University, Kyoto 615-8510, Japan

In molecular clouds at temperatures below approximately 130 K, dust grains are covered with amorphous water ice mantles and thus photolysis of water ice plays an important role in grain chemistry. The formation of H_2 from water ice is a process of fundamental importance in molecular clouds and the outer solar system. H_2 formation from hot H atoms produced by photolysis of water ice involves two distinct mechanisms: endothermic hydrogen abstraction (HAB) and highly exothermic hydrogen recombination (HR).

HAB:	$H + HOH \rightarrow H_2 + OH$	$\Delta H = 0.6$ eV	(1)
HR:	$H + H \rightarrow H_2$	$\Delta H = -4.5$ eV	(2)

Since these routes result in very different rovibrational distributions of the H_2 product, measurements of the H_2 state distributions point directly to the respective formation mechanism.

Formation of H_2 molecules from amorphous solid water has been investigated at 100 K using pulsed 157 nm laser radiation. We report the simultaneous measurement of kinetic and rovibrational energy distributions of the H_2 photoproduct. Two distinct mechanisms can be identified as shown in reaction (1) and (2): Endothermic abstraction of a hydrogen atom from H_2O by a photolytically produced H-atom yields vibrationally cold H_2 products, whereas exothermic recombination of two H-atom photoproducts yields H_2 molecules with a highly excited vibrational distribution, non-Boltzmann rotational population distributions, and kinetic energies that decrease according to their depth of formation beneath the ice-vacuum interface.

Table 1: Energy partitioning and relative population distribution in H_2 from the photolysis of amorphous water ice at 100 K. The tabulated data show the relative populations of products with v = 2, 3 and 4, and their variation with J. HAB and HR denote endothermic hydrogen abstraction and highly exothermic hydrogen recombination, respectively.

$H_2(v)$	Relative vibrational population	Vibrational energy (eV)	Translational energy (eV)	Rotational energy (eV)	Energy absorbed by ice (eV)	Dominant Mechanism
0	-	0	0.028	0.013	-	HAB
2	0.58	1.00 (22%)	0.032(0.7%)	0.65(14%)	2.82(63%)	HR
3	1	1.48(33%)	0.028(0.6%)	0.54(12%)	2.45(54%)	HR
4	1.34	1.88(42%)	0.044(0.1%)	0.33(7%)	2.25(50%)	HR

References

[1] Yabushita, A.; Hama, T.; Iida, D.; Kawanaka, N.; Kawasaki, M.; Watanabe, N.; Ashfold, M. N. R.; Loock, H.-P. *Astrophys. J.* **682**, L69 (2008)

[2] Yabushita, A.; Hama, T.; Iida, D.; Kawanaka, N.; Kawasaki, M.; Watanabe, N.; Ashfold, M. N. R.; Loock, H.-P. *J. Chem. Phys.* **129**, 044501 (2008)