

Photodissociation of a water molecule in ice: a molecular dynamics study

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Abstract. UV irradiation of ice may be important for dust grain chemistry in dense clouds through (i) the photolysis of molecules in the icy mantles releasing reactive species that can react with each other or other species present in the ice, (ii) desorption of atoms and molecules into the gas phase, and (iii) phase transformation of the ice. There have been a number of experiments studying the effects of UV irradiation of water ice. Ghormley and Hochanadel (1971) studied flash photolysis of crystalline hexagonal ice at 263 K and could detect OH radicals in the ice. In a study of different UV doses on the chemical composition of a number of pure ices at 10 K, Gerakines *et al.* (1996), OH, H₂O₂, and HO₂ were detected after UV irradiation of amorphous ice. In their work on UV irradiation of amorphous D₂O ice, Watanabe *et al.* (2000) found that D₂ was efficiently formed upon irradiation of 9.8 eV photons, while Yabushita *et al.* (2004) detected H atoms desorbing from amorphous ice that had been irradiated by 6.4 eV photons. The amorphization of crystalline cubic ice at 16 K was shown to be quite efficient through Ly- α irradiation (Leto & Baratta (2003)).

In the work presented here the photodissociation dynamics of a water molecule in crystalline and amorphous pure water ices is studied computationally using classical molecular dynamics (Andersson *et al.* in press, Andersson *et al.* in prep). Photodissociation in the first bilayer of crystalline ice leads mainly to H atoms desorbing, while in the third bilayer trapping of H and OH dominates. Results for amorphous ice shows a similar depth dependence for the outcome of photodissociation. The probability of H atom desorption is however somewhat higher for the upper layers of amorphous ice compared to the corresponding layers in crystalline ice. The kinetic energy distribution of the desorbing H atoms is much broader than that for the corresponding gas-phase photodissociation due to loss of energy through collisional encounters with the ice water molecules. H atom desorption from amorphous ice shows a hotter kinetic energy distribution than the one for crystalline ice. The H atoms on average move about 10 Å before becoming trapped, while OH radicals typically move 2 Å, their motion through the ice being more restricted. OH formed from photodissociation at the surface has in some cases however been found to move more than 50 Å over the surface before being readsorbed. In accordance with experiments a blueshift of the absorption spectrum is obtained relative to gas-phase water.

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