

MIXED QUANTUM/CLASSICAL APPROACH TO PHOTODISSOCIATION OF H₂O AND Ar – H₂O

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Recently, experimental studies of the vibrationally mediated photodissociation of H₂O in Ar – H₂O van der Waal complexes have been reported. In these studies, the OH rotational distributions were measured and compared with the ones that resulted from the photodissociation of H₂O at the same photolysis wavelengths.^a Much warmer OH rotational distributions were obtained from photolysis of the Ar – H₂O clusters. In order to understand the physical origins of these results we have simulated the photodissociation of H₂O and Ar – H₂O using a multiple configuration mixed quantum/classical approach. By comparing the rotational distribution of the OH products that are obtained from photodissociation of the complexed and uncomplexed water molecules, we find that the Ar atom has a strong effect on the rotational distribution of the OH fragment in intracluster collisions. The simulations provide insights to the dynamics of photodissociation in clusters.

^aVotava, O.; Plusquellic, D. F.; Myers, T. L.; Nesbitt, D. J. *J. Chem. Phys.* 112, 7449 (2002).