MIXED QUANTUM/CLASSICAL APPROACH TO PHOTODISSOCIATION OF H_2O AND $Ar - H_2O$

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Recently, experimental studies of the vibrationally mediated photodissociation of H_2O in $Ar - H_2O$ 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 H_2O at the same photolysis wavelengths.[a] Much warmer OH rotational distributions were obtained from photolysis of the $Ar - H_2O$ clusters. In order to understand the physical origins of these results we have simulated the photodissociation of H_2O and $Ar - H_2O$ 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.

[a] Votava, O.; Plusquellic, D. F.; Myers, T. L.; Nesbitt, D. J. *J. Chem. Phys.* 112, 7449 (2002).