Non-resonant vibrational excitation of HOD and selective bond breaking

This paper reports a time-dependent quantum mechanical wave packet study for bond-selective excitation and dissociation of HOD into the H + OD and D + OH channels in the first absorption band. Prior to excitation, the HOD molecule is randomly oriented with respect to a linearly polarized laser field and accurate static dipole moment and polarizability surfaces are included in the interaction potential. Vibrational excitation is obtained with intense, non-resonant 800 nm few-cycle excitation using dynamic Stark effect/impulsive Raman scattering. Dissociation is accomplished by another ultrashort vacuum ultraviolet-laser excitation. A laser control scheme is designed with a train of simple, non-resonant laser pulses in order to enhance the selectivity between the fragmentation channels. The effect of the carrier-envelope-phase of the ultrashort laser pulses is also investigated.

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