SPECTROSCOPY AND DYNAMICS OF H_2OH

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There has been much recent interest on the spectroscopy and dynamics of weakly-bound clusters formed between radicals and other atoms or molecules. The weakly-bound dimer H_2OH is of special interest as H_2 and OH have the potential to react to produce H_2O+H. This talk will present recent calculations we have performed on the vibrational predissociation (VP) dynamics of H_2OH. The VP lifetimes and rotational product distributions for initial excitation of both the OH and H_2 vibrations have been calculated. A time-dependent wavepacket method has been used in which all nine coupled degrees of freedom are treated. The potential energy surface is obtained from high-quality ab initio calculations [1]. The results compare quite favourably with time-resolved measurements made recently by M. I. Lester and co-workers. Comparison will also be made with similar calculations on the related weakly-bound molecule H_2HF. In addition, the possibility of inducing reaction by vibrationally exciting H_2OH to produce H_2O+H reactive products will be discussed.

[1] S. M. Miller, D. C. Clary, A. Kliesch and H.-J.Werner, Molec. Phys.,83, 405 (1994).