

Dissociative electron attachment to water

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Abstract

Dissociative electron attachment (DA) to H_2O is of direct importance for both biological and technological systems. The calculations on H_2O and H_2S presented comprise the first *ab initio* treatment of DA to a polyatomic molecule employing the full dimensionality of nuclear motion. Calculations of the DA cross section via the ${}^2\text{B}_1$ state of H_2O^- agree well with experiment, reproducing the high degree of vibrational excitation of the OH fragment. Several interesting features of the A' manifold of resonances for H_2O have been discovered, including a conical intersection between the ${}^2\text{A}_1$ and ${}^2\text{B}_2$ Feshbach resonances and a branch-point degeneracy between the ${}^2\text{B}_2$ shape and Feshbach resonances. This latter feature has no direct analogue in bound-state theory, although the theory of “hidden crossings” represents an interesting parallel. The two-seam structure of the ${}^2\text{A}_1 / {}^2\text{B}_2$ conical intersection is probed. Preliminary calculations on the Renner-Teller coupled ${}^2\text{A}_1$ and ${}^2\text{B}_1$ surfaces, and on electronically coupled diabatic ${}^2\text{A}_1$ and ${}^2\text{B}_2$ surfaces, will be presented.

In addition, the angular dependence of the $\text{H}^- + \text{OH}$ channel for the ${}^2\text{B}_1$ state of H_2O and that of the analogous channel and state of H_2S have been calculated by incorporating the mixing of different partial waves into the entrance amplitude, and for H_2S , the variation of this mixing with geometry. The fact that the H_2S entrance amplitude is not factorable into a part dependent upon the internal coordinates and one dependent upon the relative orientation of the molecule and the incident electron beam is the most probable cause of the final-state-specific angular dependences observed in experiment.