Jahn-Teller effect among electronic resonant states of H_3

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The electronic bound states of H_3 are known to exhibit a Jahn-Teller conical intersection. A phenomena which has been studied extensively for bound states. Here we study the electronic resonant states of H_3 with energies above the potential energy surface of the H_3^+ ground state. These resonant states are important for dissociative recombination of H_3^+ at higher collision energies, and previous studies have indicated that these resonant states also exhibit a Jahn-Teller conical intersection.

We have performed electron scattering calculations on the lowest lying resonant states of ^{2}A' symmetry, using the Complex-Kuhn variational method to compute the potential energies and the autoionization widths of the resonant states. A local complex approximation is applied where the adiabatic resonant states are described by adding an imaginary term to the potential energy. Following the ideas of Feuerbacher et al., a complex Jahn-Teller Hamiltonian is introduced for which the parameters are extracted by a least square fit. Through this method we obtain complex adiabatic potential energy surfaces describing the system. We also calculate the non-adiabatic couplings and study the geometric phase for these resonant states.