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Scattering matrix elements for the nonadiabatic B + H_2 collision
DAVID WEEKS, LUKE BARGER, Air Force Institute of Technology — The 1^2A', 2^2A', and 1^2A" adiabatic potential energy surfaces together with derivative coupling terms between the 1^2A' and 2^2A' electronic states are calculated at the multi-reference configuration-interaction level for the B+H_2 system. These surfaces and couplings are used to compute a set of effective potential energy surfaces that govern the dynamics of atomic boron and molecular hydrogen as they collide. Scattering matrix elements are calculated by propagating reactant wave packets on these surfaces with the split-operator method. The correlation function between the evolving reactant wave packets and stationary product wave packets is computed. A Fourier transformation of the correlation function is then used to calculate the scattering matrix elements using the channel packet method. These scattering matrix elements yield the probability that the B+H2 system will undergo fine structure, rotational, and vibrational transitions as a function of energy.

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