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Non-Adiabatic Dynamics of B + H_2 DAVID WEEKS, LACHLAN BELCHER, Air Force Institute of Technology — A description of the non-adiabatic molecular dynamics of B + H_2 requires knowledge of the derivative coupling terms usually ignored in the standard Born-Oppenheimer approximation. These coupling terms are functions of the nuclear degrees of freedom, and for three body dynamics calculations, Jacobi coordinates are often employed because they separate the asymptotic Hamiltonian. On the other hand, code we use to compute derivative coupling terms produces output in Cartesian coordinates. The derivative coupling terms must therefore be transformed to Jacobi coordinates using the Jacobian matrix of the Jacobi to Cartesian transformation equations. This procedure is somewhat complicated by an ambiguity in the choice of the overall rotation coordinate in the plane containing the B and H_2 nuclei. This ambiguity is exacerbated by the fact that many choices of overall rotation angle will yield the same derivative coupling term with respect to the overall rotation coordinate, while at the same time producing disparate results for the derivative coupling term with respect to the Jacobi angle between the H_2 bond and the line between the B atom and H_2 center of mass. We discuss this ambiguity and its resolution using a collinear two body problem, and apply the resolution to the B + H_2 system to obtain derivative coupling terms and associated diabatic surfaces suitable for dynamics calculations.

David Weeks
Air Force Institute of Technology

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