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Effective potential energy surfaces for the Inelastic Collision $\mathbf{B(^2P_{1/2}) + H_2}(j,n) \leftrightarrow \mathbf{B(^2P_{3/2}) + H_2}(j\mathbf{'},\ n\mathbf{'})$ DAVID WEEKS, LUKE BARGER, Air Force Institute of Technology — The Born-Oppenheimer approximation breaks down when two adiabatic potential energy surfaces become sufficiently close. Under these conditions, the nuclear dynamics are governed by a set of coupled diabatic surfaces. Derivative coupling matrix elements can be used to compute the transformation from the adiabatic to the diabatic potential energy surfaces. Diabatic surfaces governing the dynamics of the inelastic collision between atomic boron and molecular hydrogen are used to compute effective potential energy surfaces. These effective surfaces couple the rotational dynamics with the vibrational dynamics of the hydrogen molecule and with the relative dynamics of the atomic boron and the molecular center of mass. These surfaces will be used to explore the inelastic $B(^2P_{1/2}) + H_2(j,n) \leftrightarrow B(^2P_{3/2}) + H_2(j', n')$ collision (1). (1) D.E. Weeks, T.A. Niday, and S.H. Yang, J. Chem. Phys, 125, 164301 (2006).

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