

Abstract Submitted  
for the MAR10 Meeting of  
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**Effective potential energy surfaces for the Inelastic Collision**  
 $\text{B}(^2\text{P}_{1/2}) + \text{H}_2(j, n) \leftrightarrow \text{B}(^2\text{P}_{3/2}) + \text{H}_2(j', n')$  DAVID WEEKS, LUKE  
BARGER, Air Force Institute of Technology — The Born-Oppenheimer approxima-  
tion 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  
 $\text{B}(^2\text{P}_{1/2}) + \text{H}_2(j, n) \leftrightarrow \text{B}(^2\text{P}_{3/2}) + \text{H}_2(j', n')$  collision (1). (1) D.E. Weeks, T.A.  
Niday, and S.H. Yang, J. Chem. Phys, 125, 164301 (2006).

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