Abstract Submitted
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The Adiabatic-to-Diabatic Mixing Angle for the Inelastic Collision $\mathbf{B(^2P_{1/2}) + H_2}(j,n) \leftrightarrow \mathbf{B(^2P_{3/2}) + H_2}(j\text{'}, n\text{'})$ DAVID WEEKS, MATTHEW GARVIN, 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. A line integral along various contours through the vector field defined by the derivative coupling matrix elements is used to compute the adiabatic-to-diabatic mixing angle. In particular, we investigate the path independence of this coupling angle for the inelastic collision $B(^2P_{1/2}) + H_2(j) \leftrightarrow B(^2P_{3/2}) + H_2(j')$ collision (1). (1) D.E. Weeks, T.A. Niday, and S.H. Yang, J. Chem. Phys, 125, 164301 (2006).

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