

Abstract Submitted
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Non-adiabatic Quantum Interference Effects and Chaoticity in the Ultracold $\text{Li} + \text{LiNa} \rightarrow \text{Li}_2 + \text{Na}$ Reaction¹ BRIAN KENDRICK, Los Alamos Natl Lab, JAMES CROFT, University of Otago, NADUVALATH BALAKRISHNAN, University of Nevada Las Vegas, MING LI, HUI LI, SVETLANA KOTOCHIGOVA, Temple University — Quantum reactive scattering calculations for the ultracold $\text{Li} + \text{LiNa} \rightarrow \text{Li}_2 + \text{Na}$ reaction are presented which include both the ground and first excited doublet electronic states. In the interaction region the excited electronic state exhibits a conical intersection with the ground electronic state. This intersection is energetically accessible even in the ultracold regime for $\text{Li} + \text{LiNa}$ collisions with ground state reactants. A numerically exact full-dimensional time-independent scattering method based on hyperspherical coordinates is used to compute the total, vibrationally, and rotationally resolved non-thermal rate coefficients for collision energies between 1 nK and 0.3 K. A significant enhancement or suppression of up to two orders of magnitude is observed in many of the rotationally resolved rate coefficients. These effects are due to constructive or destructive quantum interference between the two scattering amplitudes which encircle the conical intersection. A statistical analysis of the rotational distributions shows a Poisson behavior which is indicative of the underlying classically chaotic dynamics.

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