Abstract Submitted
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Non-universal behavior in the ultracold Li + LiNa $\rightarrow$ Li_2 + Na reaction BRIAN KENDRICK, Los Alamos National Laboratory, JAMES CROFT, NADUVALATH BALAKRISHNAN, University of Nevada Las Vegas, MING LI, HUI LI, SVETLANA KOTOCHIGOVA, Temple University — Quantum reactive scattering calculations for the ultracold Li + LiNa $\rightarrow$ Li_2 + 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 deep potential well that is energetically accessible even in the ultracold regime for Li + 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. The non-adiabatic and geometric phase effects associated with the energetically accessible conical intersection between the two electronic states are shown to produce non-universal behavior in the ultracold rate coefficient. The non-adiabatic ultracold rate coefficient is approximately 1.6 times larger than the universal value computed using a single ground state electronic potential energy surface. A significant enhancement or suppression of up to two orders of magnitude is also observed in many of the rotationally resolved rate coefficients due to constructive or destructive quantum interference.

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