Abstract Submitted
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Ultracold chemistry with alkali-metal–rare-earth molecules[1] CONSTANTINOS MAKRIDES, Department of Physics, Temple University, JISHA HAZRA, GAGAN PRADHAN, Department of Chemistry, University of Nevada Las Vegas, BRIAN KENDRICK, Theoretical Division (T-1, MS B221), Los Alamos National Laboratory, THOMÁS GONZÁLEZ-LEZANA, Instituto de Física Fundamental, IFF-CSIC, BALAKRISHNAN NADUVALATH, Department of Chemistry, University of Nevada Las Vegas, ALEXANDER PETROV, SVETLANA KOTOCHIGOVA, Department of Physics, Temple University — A first principles study of the dynamics of ^{6}Li(^2S)+^{6}Li^{174}Yb($^2\Sigma^+$) $\rightarrow$^{6}Li$_2$($^1\Sigma^+$)+^{174}Yb(^1S) reaction is presented at cold and ultracold temperatures. The computations involve determination and analytic fitting of a three-dimensional potential energy surface for the Li_2Yb system and quantum dynamics calculations of varying complexities, ranging from exact quantum dynamics within the close-coupling scheme, to statistical quantum treatment, and universal models. It is demonstrated that the two simplified methods yield zero-temperature limiting reaction rate coefficients in reasonable agreement with the full close-coupling calculations. The effect of the three-body term in the interaction potential is explored by comparing quantum dynamics results from a pairwise potential that neglects the three-body term to that derived from the full interaction potential. Inclusion of the three-body term in the close-coupling calculations was found to reduce the limiting rate coefficients by a factor of two.

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