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Ultracold chemistry with alkali-metal-rare-earth molecules CON-STANTINOS 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 KO-TOCHIGOVA, Department of Physics, Temple University — A first principles study of the dynamics of ${}^6\text{Li}({}^2S) + {}^6\text{Li}{}^{174}\text{Yb}({}^2\Sigma^+) \rightarrow {}^6\text{Li}_2({}^1\Sigma^+) + {}^{174}\text{Yb}({}^1S)$ reaction is presented at cold and ultracold temperatures. The computations involve determination and analytic fitting of a three-dimensional potential energy surface for the Li₂Yb 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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