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**Theoretical studies of reaction rates for the Rb-NH system**[1]
DANIEL HAXTON, STEVEN WRATHMALL, HEATHER LEWANDOWSKI, CHRIS GREENE, JILA and the University of Colorado, Boulder — We present the results of ab initio calculations on the Rb-NH system. We are interested both in ultracold collisions of Rb and NH and in higher-energy collisions more typical of chemical reactive scattering. We have constructed a set of sixteen unique two-dimensional potential energy surfaces, including the spin-orbit interaction, using the COLUMBUS quantum chemistry package. For the moment we fix the NH bond distance. The sixteen surfaces include the charge-transfer state $Rb^+ + NH^-$, which becomes the ground state at small Rb-NH separations, and also the channel Rb ($^2S$) + NH ($^1\Delta$), which enjoys a near degeneracy with the spin-orbit split components of Rb ($^2P$) + NH (X $^3\Sigma^-$). A property-based diabatization is employed, after which we perform reactive scattering calculations using the R-matrix propagator method. Our results indicate that transitions between the nearly degenerate channels are indeed highly favored.

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