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State-selective charge exchange in ion-molecule and three-body recombination in ion-atom-atom rubidium systems at the ultracold temperatures

We study the interactions between two Rb atoms and one Rb^+ ion from a quantum chemistry perspective, considering the Rb_2+Rb^+ and Rb_2^++Rb arrangements. These interactions are relevant for the fundamental chemistry, sympathetic cooling, and three-body recombination (TBR) processes at ultra-low temperatures observed in hybrid ion-atom experiments for homo- and hetero-alkali ion-atom species, with Rb^+ (or Ba^+, Ca^+)+Rb+Rb. Formation of Rb_2^+ has recently been observed in inelastic collisions of a single cold Rb^+ in a BEC of Rb atoms [1,2]. Another experiment has reported probable formation of molecular Rb_2 in an hybrid ion-atom trap [3]. We start by calculating the electronic structure of the Rb_3^+ ion using various approaches involving both large-core and small-core effective core potentials. We find that for specific geometry configurations, state-selective charge exchange reactions would occur for the ion-molecule Rb^++Rb_2 system. We extend our investigations toward the large distance domain to elaborate on the transition from atom-molecule to three-atom configurations relevant to TBR, which could be responsible for molecular collision products Rb_2^+ and Rb_2. We show the generalization of these results for any alkali homo-nuclear three-body ion-molecule and ion-atom-atom systems.

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