Cold collisions of Li and Rb with C_2^-

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Synopsis We present a theoretical investigation of reactive and non-reactive collisions of Li and Rb atoms with C_2^- at low temperatures in the context of hybrid trap experiments. Accurate potential energy surfaces for the singlet and triplet states of the Li–C_2^- and Rb–C_2^- systems are constructed using the CASSCF/ic-MRCI+Q method. We then investigate the associative detachment reaction as well as rotationally inelastic collisions, and explore the implications for hybrid trap experiments and sympathetic cooling experiments. The results are compared to those obtained for other anionic systems such as Rb-OH^-.

Theoretical and experimental studies of low temperature reactive and non-reactive collisions involving molecular anions have gained interest due to their importance in astrochemistry as well as in the study of cold chemistry, one of the goal being to produce samples of cold molecular anions. One way of doing so is by collisions with ultracold atoms in an hybrid trap, so that understanding the collisional properties of anions at low temperature is particularly important. In the case of anions reactive collisions may lead to losses from the trap through the associative electronic detachment reaction, $AB^- + C \rightarrow ABC + e^-$, as has been observed for Rb-OH^- [1, 2].

We present results on the interaction of the molecular anion C_2^- with Li and Rb atoms based on accurate *ab initio* calculations. Potential energy surfaces for both systems in singlet and triplet states were obtained with the CASSCF/ic-MRCI+Q method. The equilibrium geometry corresponds to the T-shaped configuration with a well depth of about 2.30 eV for Li-C_2^- and 1.33 eV for Rb-C_2^-.

We also calculate the potential energy surfaces for the corresponding neutral species, and we show that the associative electronic detachment reaction should be suppressed at low temperatures. We compare these results to those obtained for other systems such as Rb-OH^-, for which the reaction proceeds with a large rate [3]. We also explore collisions involving excited electronic states of either C_2^- or Li and Rb. Based on quantum chemistry calculations, we show that for these states the reaction rates are expected to be close to the Langevin values.

Finally, we investigate the rotational (de)excitation of C_2^- in collisions with Li and Rb in order to examine the possibility of sympathetic cooling. The large inelastic rates show that C_2^- is a good candidate for producing cold anions.

References

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