Elastic Rate Coefficients of Li + H_2 collisions in the calibration of a Cold Atom Vacuum Sensor

Constantinos Makrides[a] and Eite Tiesinga[a,b]

[a] *Joint Quantum Institute,* [b] *National Institute of Standards and Technology*
eite.tiesinga@nist.gov

Ongoing efforts at the National Institute of Standards and Technology in creating a cold-atom vacuum standard device have prompted theoretical investigations of atom-molecule collision processes that characterize its operation [1]. Such a device will operate as a primary standard for the ultrahigh-vacuum and extreme-high-vacuum regimes. This device operates by relating loss of ultracold lithium atoms from a conservative trap by collisions with ambient atoms and molecules to the background density and thus pressure through the ideal gas law. The predominant background constituent in these environments is molecular hydrogen H_2. We have computed the relevant Li+H_2 Born-Oppenheimer potential energy surface (PES), paying special attention to its uncertainty. With increasing accuracy we constructed potentials labeled TZ, QZ, 5Z, and ∞Z, respectively. Coupled-channel calculations are then used to obtain total rate coefficients, which include momentum-changing elastic and inelastic processes. We find that inelastic rotational quenching of H_2 is negligible near room temperature. For a ($T = 300$)-K gas of H_2 and 1.0-μK gas of Li atoms prepared in a single hyperfine state, the total rate coefficients are $6.0(1) \times 10^{-9}$ cm^3/s for both ^{6}Li and ^{7}Li isotopes, where the number in parentheses corresponds to a one-standard-deviation combined statistical and systematic uncertainty. We find that a 10-K increase in the H_2 temperature leads to a 1.9% increase in the rate coefficients for both isotopes. For Li temperatures up to 100 μK, changes are negligible. Finally, a semiclassical Born approximation significantly overestimates the rate coefficients. The difference is at least ten times the uncertainty of the coupled-channel result.

References

1. C. Makrides, D. S. Barker, J. A. Fedchak, J. Scherschligt, S. Eckel, and E. Tiesinga, Phys. Rev. A **99**, 042704 (2019).