Theoretical Study of Molecular Collisional Excitation for Modeling FIR/Submm Observations

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Abstract.
Molecular collisional rate coefficients are required, for a range of temperatures, to interpret spectra of molecular gas not in local thermodynamic equilibrium (LTE). While the rate coefficients describing such processes can often be calculated, enhancements in the spectral line resolution and sensitivity expected from ALMA, SOFIA, Herschel, and other FIR/submm telescopes, place unquenchable demands on the collisional data. Further, collisional rate coefficients usually pose the largest source of uncertainty of the molecular data input to a radiative transfer analysis, in most cases simply due to the lack of such data. Despite some progress in state-to-state collision rate coefficient measurements over the last decade, limited results have been obtained for systems of astrophysical interest. Astrophyical models therefore rely heavily on theoretical estimates due to the difficulty of direct measurements of collisional rate coefficients. Theoretical predictions of rate coefficients involve both molecular structure and scattering components. State of the art calculations typically utilize *ab initio* electronic potential energy surface (PES) calculations and the close-coupled solution of the nuclear scattering equations on these surfaces. Both of these components involve significant computational effort. We review these issues and present recent work on computations of PESs and rotational and vibrational excitation of H_2, HF, HCl, CO, CO_2 due to He and H_2 collisions. The role of collisional excitation in the modeling of various astrophysical environments as well as on-going and future work will be discussed.

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