Atomic and Molecular Processes in Astrophysics

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Collisions play a vital role in establishing the internal state distributions, particle velocity distributions, particle abundances, and ionization balance in gaseous and plasma environments from the terrestrial laboratory to the onset of chemistry in the beginning of the Universe. State-to-state rate coefficients for chemical reactions and molecular rotational/vibrational transfer over a broad range of temperatures and initial conditions are needed for non-LTE (NLTE) modeling of astrophysical media and early universe chemistry. Collisions of H, H_2, and He with trace species, both neutral and ionic, are among the most important ingredients for NLTE modeling but the computations become challenging for heavier diatomics and polyatomic molecules.

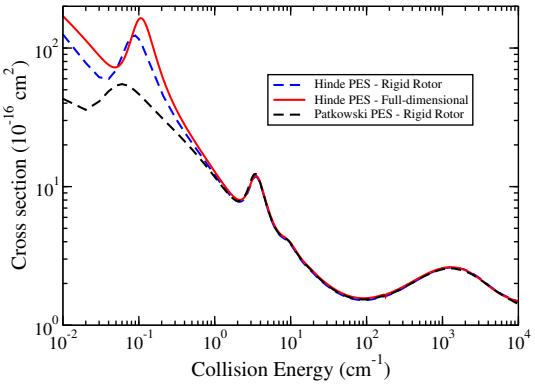

Figure 1: Cross sections for $v_1 = 0, j_1 = 1 \rightarrow v_1' = 0, j_1' = 0$ transition in HD induced by collisions with ground state para-H_2 as a function of the collision energy.

The reliability of collisional data is tied to both the accuracy of the interaction potential and the accuracy of the scattering calculations. For small molecule systems, both can be performed with high accuracy. As an example, Figure 1 shows a comparison of cross sections for the $j = 1 \rightarrow 0$ rotational transition in the $v = 0$ vibrational level of HD induced by collisions with para-H_2 as a function of the collision energy from a full-dimensional quantum calculation with those from a rigid rotor approximation on two different interaction potentials. It is seen that the 4-dimensional rigid rotor calculations on the Hinde [1] and Patkowski et al. [2] potentials yield similar results and they agree near quantitatively with the full 6-dimensional results on the Hinde potential for energies above 1.0 cm^{-1}. The discrepancies at energies below 1.0 cm^{-1} are due to the increased sensitivity to the interaction potential but less important for astrophysical applications. See Ref. [3] for more details. Recent progress in quantum scattering calculations of rate coefficients for non-LTE modeling of astrophysical environments will be discussed.

[1] Hinde R J 2008 *J. Chem. Phys.* **128** 154308
[2] Patkowski K *et al* 2008 *J. Chem. Phys.* **129** 094304
[3] Balakrishnan N *et al* 2018 *Astrophys. J.* **866** 95