Molecular Data for Hydrogen Plasma Modeling

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Low-temperature hydrogen plasmas are ubiquitous throughout the Universe. They exist in fusion plasmas, solar atmospheres, planetary atmospheres, primordial gas clouds, and determined much of the chemistry of the early Universe. To model these plasmas in local thermodynamic equilibrium (LTE) and non-LTE requires the constituents energy levels, transition cross sections or rate coefficients to calculate populations (for non-LTE plasmas), opacities, and emissivities.

Recently we have embarked on the projects of calculating electron- and photon-molecule data of important diatomics utilizing first-principle approaches [1-3]. Here we present a wide-variety of results required to model LTE and non-LTE plasmas containing hydrogen molecules H_2, its ions H_2^+, and the isotopologues. For example, we will present electron- and photon-molecule cross sections, the molecular emission spectra of LTE plasmas at various temperatures, and preliminary results of low-temperature hydrogen plasma equations of state [4].

To model electron-molecule collisions we have developed the molecular convergent close-coupling (MCCC) method [1,2]. Results from these studies are the first of their kind: calculating cross sections over a broad range of impact energies and explicitly demonstrating convergence of the cross sections. Generally, the results are in good agreement with experiments, however, for some important processes large discrepancies are seen with generally "accepted" and used data. Subsequent new experiments have confirmed the MCCC predictions [5].

For the photon-molecule project, we have recently developed a self-consistent approach with the goal of calculating comprehensive opacity tables that are accurate across the entire range of temperature space. We have calculated cross sections, rate coefficients and the emission spectra of H_2^+ [3] and H_2, as well as investigated isotopic effects, and the effect of including electronically excited states in the emission calculations.

References

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