Vibrationally-resolved electron-impact excitation of molecular hydrogen

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Molecular hydrogen and its isotopologues are present in a range of vibrationally excited states in fusion, atmospheric, and interstellar plasmas. Electron-impact excitation cross sections resolved in both final and initial vibrational levels of the target are required for modeling the properties and dynamics, and controlling the conditions of many low-temperature plasmas [1]. Measurements of excitations in H_2 by electron impact are typically limited to scattering on the ground vibrational state, and hence there is significant demand for accurate theoretical calculations of scattering on excited states. The majority of the available data have been obtained using the adiabatic-nuclei (AN) impact parameter (IP) method [2], and are resolved in the initial, but not final, vibrational levels. At low to intermediate energies, the IP results are up to a factor of two higher than the available experimental data for scattering on the ground vibrational state, and are likely to be similarly inaccurate for scattering on excited levels. To our knowledge, there have been no previous efforts towards compiling a database of electron-impact electronic excitation cross sections for H_2 resolved in both the initial and final vibrational levels.

Recently, the convergent close-coupling (CCC) method has been utilized in the fixed-nuclei (FN) approximation to provide a comprehensive set of accurate cross sections for electrons scattering on H_2 in the ground (electronic and vibrational) state [3]. The CCC method has also been applied in the AN approximation to study collisions with the H_2^+ and H_2 molecules in the ground vibrational state [4, 5, 6], yielding good agreement with experiment in each case. Here we extend the CCC method to generate a complete set of cross sections resolved in all initial and final vibrational levels for electronic excitations from the $X\ ^1\Sigma_g^+$ state to a number of low-lying singlet and triplet electronic states. These calculations have been performed for H_2 as well as each of its isotopologues (D_2, T_2, HD, HT, and DT). In Fig. 1 we present examples of the present calculations for excitation of the $B\ ^1\Sigma_u^+$ and $D\ ^1\Pi_u$ states.

We expect that the present calculations will be of considerable interest for modeling fusion plasmas, where H_2 and its isotopologues are present in a range of excited vibrational states. Temperature-dependent collision rates can be used to infer the populations of vibrational levels, while the calculation of vibrationally-resolved cross sections will allow for an accurate study of molecular break-up through individual dissociation channels.

Acknowledgements
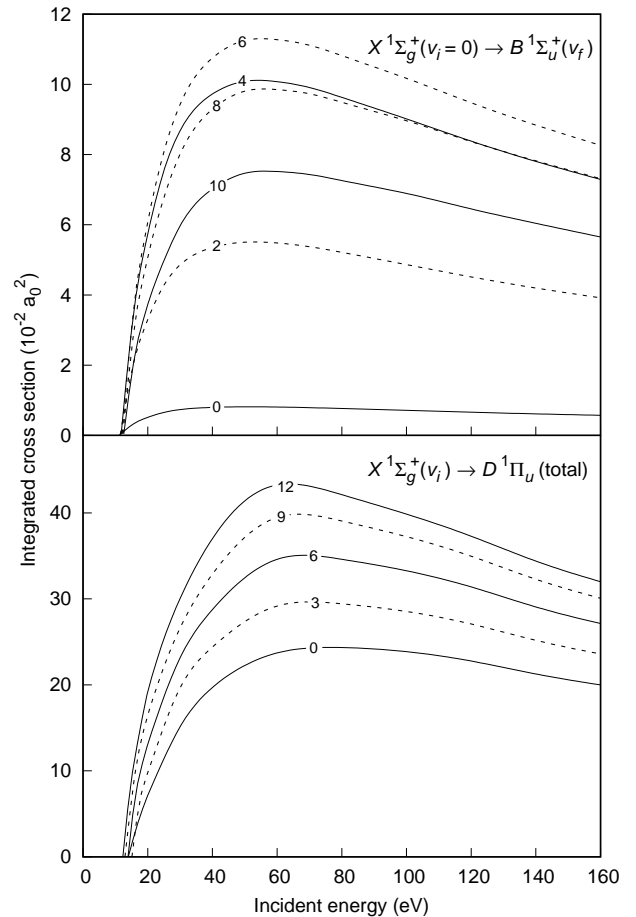
Figure 1: **Cross sections for excitation of vibrational levels in the $B\ ^1\Sigma_u^+$ from the $X\ ^1\Sigma_g^+(v_i = 0)$ state, and total excitation of the $D\ ^1\Pi_u$ state from levels of the $X\ ^1\Sigma_g^+$ state of H_2.**

References

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