VIBRATIONALLY RESOLVED INELASTIC TRANSITIONS IN SLOW H_3^+ COLLISION SYSTEMS

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It is widely recognized in the fusion community that the divertor region is of crucial importance for the successful engineering, design, and operation of tokamak fusion reactors, while the atomic collision data needed to model and diagnose this region are often unknown or only poorly considered in the extant literature. The high density, low temperature divertor plasma is characterized by similar densities of ions and neutrals, consisting predominantly of hydrogen atoms, ions and molecules in various isotopic combinations.

In addition, formation of the divertor plasma detachment layer might critically depend on Molecule Assisted Recombination (MAR), which involves ion conversion via electron capture by a proton from a vibrationally and rotationally excited hydrogen molecule, followed by dissociative recombination of the molecular ion with plasma electrons. Such collisions require accurate data for the relevant processes, particularly for vibrationally resolved charge transfer from H_2 to H^+. Only one comprehensive data set exists for the charge transfer from excited vibrational states of H_2, calculated by the Trajectory Surface Hopping (TSH) method [1]. Due to the classical nature of the TSH method, this approach might not give reliable data in the eV energy range.

We report on a comprehensive study of scattering of hydrogen ions on vibrationally excited hydrogen molecules as well as of hydrogen atoms on vibrationally excited hydrogen molecular ions in the range of center of mass energies 0.5 - 10 eV. Total and partial, initial and final vibrational state resolved cross sections for excitation, charge transfer, dissociation (including dissociative energy spectra), and association have been calculated "on the same footing" using a fully-quantal, coupled-channel approach. An extensive vibrational basis set of several hundred states, including discretized dissociative continua in a large configuration space (to include nuclear particle arrangements) was employed, while the rotational dynamics of H_2 and H_2^+ were treated within the Infinite Order Sudden Approximation (IOSA) [2-4]. Concerning the details of the treatment of the reactive dynamics, the data summarized here are an improvement over these previously published [5]. In addition to a limited number of bound vibrational states (totaling 35 on both H_2 and H_2^+), several hundred continuum states were needed (including the closed channels) to achieve convergence of the cross sections in the energy range considered.

Fig. 1 shows cross sections for excitation by proton impact of the ground state of H_2 to all bound vibrational states. The results are compared with cross sections from the literature. The role of the particle rearrangements in the excitation process is of particular importance at the lowest energies. The previous quantum calculations shown in Fig. 1, do not include the rearrangements, underestimating the cross sections at lowest energies. Our data contain coherent sums over the direct and rearrangement channels.

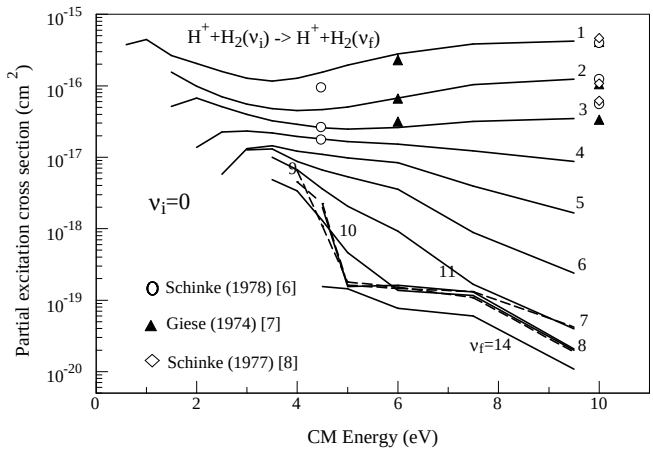

Figure 1. Vibrational excitation cross sections for collisions of protons with H_2 in the ground state. Solid and dashed lines: present calculation.

The charge transfer (CT) cross sections (summed over final vibrational states) from initially excited vibrational states of H_2 in collisions with protons are shown in Fig 2. Comparison with experimental data of Holiday [6] and Linder [7] shows good agreement at lowest energies, but lies between these two data sets at the higher energies. Among all the cross sections shown, charge transfer from the first three excited states constitutes a separate group. The reason is that CT from the higher excited states is dominantly exoergic and often quasi-resonant with the vibrational states of H_2^+. The corresponding cross sections therefore are large even at the lowest energies. Comparison of our data with the TSH ones of Ichihara [1] shows good agreement for the higher initial vibrational states, as could be expected from the correspondence principle. It is interesting to note that our quantum and the TSH calculations show similarly large contributions of the particle re-arrangement channels at low energies.

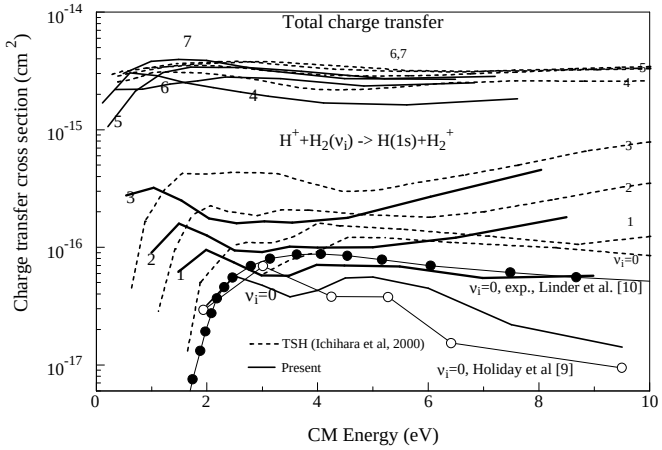

Figure 2. Charge transfer to H^+ from vibrationally excited states of H_2.

As a contrast to Fig. 2, Fig. 3 shows charge transfer cross sections from excited states of H_2^+ in collisions with H. Since this process is exoergic from all vibrational states (including the ground one), the characteristic increase of the cross section toward lower energies is expected, and is not strongly dependent on the initial state. The cross sections from high vibrational states are suppressed due to depletion of these states to the vibrational continuum (dissociation).

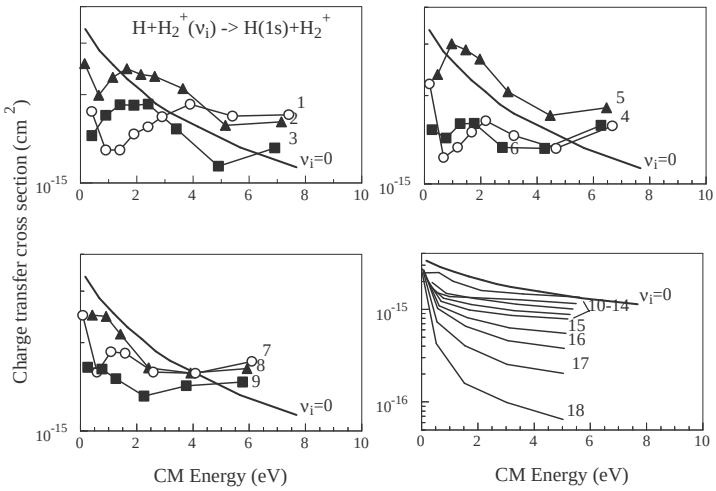

Figure 3. Charge transfer from H on vibrationally excited states of H_2^+. All lines and symbols are show present calculation, alternated for better visibility.

Figure 4 presents the dissociation cross sections, for all initial vibrational states of H_2. Comparison with the TSH calculations shows a good agreement for higher vibrational states at the higher end of the collision energy range. We note that this process includes both direct dissociation (DD) into the dissociative continuum of H_2, as well as charge transfer dissociation (CTD) into the continuum of H_2^+. These two channels are of the same order of magnitude. Concerning the energy spectra (Fig. 6) of the dissociating fragments, these have the characteristic cusp at the continuum edge, which is more pronounced for the lower collision energies.

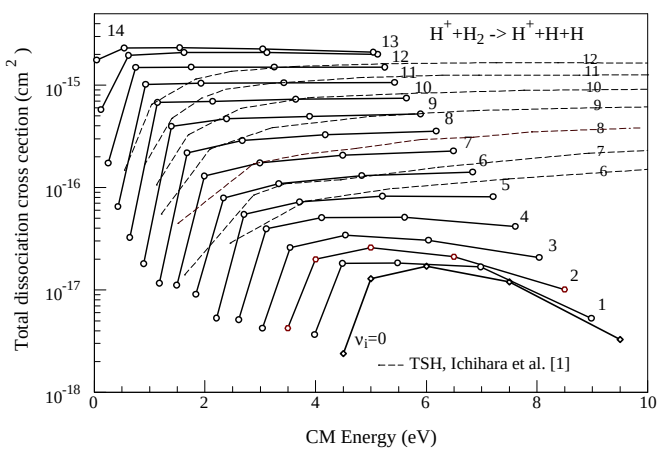

Figure 4. Cross section for dissociation from various excited states of H_2 in collisions with H. Solid lines: present calculation.

The database produced can be found at *www-cfadc.phy.ornl.gov* and contains all the processes mentioned above for the $H+H_2^+$ and H^++H_2 collision systems in the form of partial

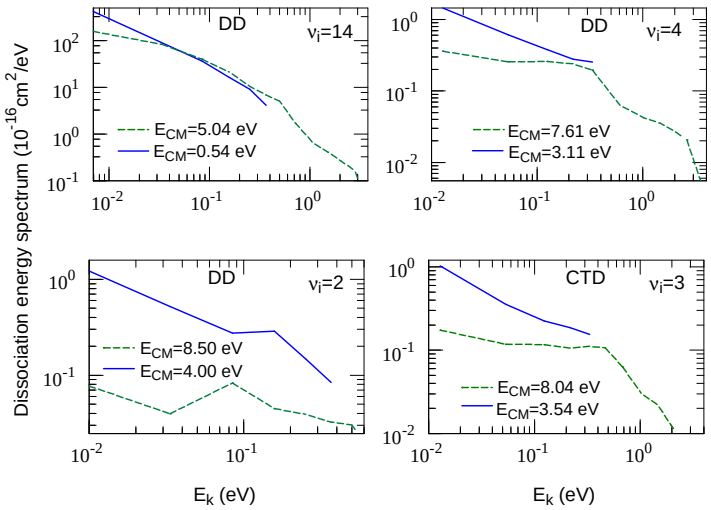

Figure 5. Energy spectra of dissociated fragments of H_2 for various collision energies E_{CM} of the proton projectile.

and total, initial- and final-vibrational-state-resolved cross sections. This represents currently the most comprehensive set of quantum-mechanically obtained inelastic data for collisions that involve hydrogen atoms, ions and molecules. Still, in order to study rovibrationally resolved processes at low collision energies with various isotopic combinations of H and with resolved particle rearrangement channels, the rotational dynamics have to be fully accounted for. This will be the subject of our future work.

ACKNOWLEDGEMENT

We acknowledge support from the US Department of Energy, Office of Fusion Energy Sciences, through Oak Ridge National Laboratory, managed by UT-Battelle, LLC under contract DE-AC05-00OR22725.

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