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Resolving vibration in H^++H_2 charge transfer collisions

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Synopsis We measure the vibrational distribution of H_2^+ ions issued from charge transfer in H^+ + H_2 collisions to probe the details of the electron transfer mechanism from low to high impact energies. The experiments are accompanied by theoretical calculations. This joint experimental-theoretical study allows us to elicit the adequacy and accuracy of widely used assumptions in the description of molecular collisions.

H^+ + H_2 collisions are the benchmark of ion-molecule collisions. In spite of this, refined measurements of state-selective cross sections are still lacking in a large impact energy range so that one can not gauge the degree of accuracy of the theoretical descriptions of molecular collisions. In this work we study the charge transfer (CT) reaction:

$$H^+ + H_2(^1\Sigma_g^+, \nu = 0) \rightarrow H(1s) + H_2^+(^2\Sigma_g^+, \nu')$$

and especially focus on the vibrational distribution. At high impact energies E, the Franck-Condon (FC) approximation, which assumes that the target nuclei remain fixed during the collision, can safely be applied. The partial cross sections for populating the vibrational states $\chi_{\nu'}$ are then proportional to the FC factors $| < \chi_{\nu'} | \chi_0 > |^2$. Niedner *et al.* [1] suggested that, at $E = 30$ eV, the CT reaction takes place through an alternative two-step mechanism involving the intermediate vibrational excited state $H_2(\nu = 4)$ + H^+, quasi-degenerate with H + $H_2^+(\nu' = 0)$. This mechanism has been corroborated by vibronic close-coupling (VCC) calculations [2] and ascertained by semi-classical calculations including nuclear rearrangement channels [3].

Here we measure vibrationally resolved cross sections in the wide energy range E =15-5000 eV. In the experimental setup, the protons are extracted from a duoplasmatron ion source, accelerated and decelerated to enter the collision cell hosting neutral molecules from an effusive jet. The daughter molecular ions are extracted sideways and accelerated to 2 keV before crossing an effusive potassium jet where they undergo resonant dissociative CT. The positions and flight time difference of the two resulting H atoms give access to the vibrational distribution of the CT products. Concurrently with experiments, we perform quantal VCC calculations. An excellent agreement is found between calculations and experiments, as illustrated in Fig. 1. As E decreases, the maximum of the vibrational distribution shifts from $\nu = 1$ to 0, which signs the departure from the FC behaviour.

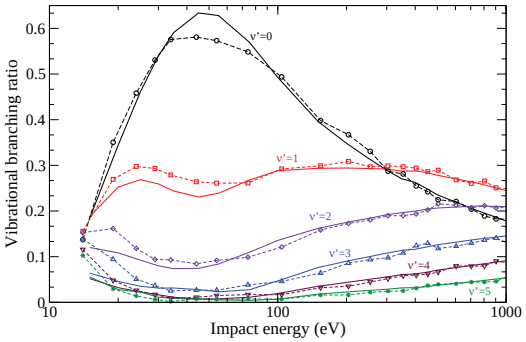

Figure 1. Comparison of the experimental (symbols) and theoretical (lines) H_2^+ vibrational branching ratios for CT in H^++H_2 collisions.

Details on the experimental setup and calculations will be given at the Conference. The isotopic systems D^++H_2, H^++D_2, as well as H_2^++H_2, will also be presented.

References

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