B.5.8. Charge Transfer in D^++H(1s) and in μ^++H(1s) Reactions at Low Energies-- *A. Igarashi,* Z.X. Zhao and C.D. Lin*

We have used the hyperspherical close-coupling method to calculate the charge transfer reaction cross sections for the above two systems from threshold up to about 2 eV. These two systems serve as the prototype elementary ion-atom collisions, but they also belong to the general three-body Coulomb systems that are amenable to the hyperspherical approach [1].

Ion-atom collisions at low energies are generally formulated using the perturbed stationary state (PSS) approximation. The PSS model is known to have many practical limitations since the theory does not satisfy the asymptotic boundary conditions [2]. In the higher energy region where semiclassical theory is used, the problems in the asymptotic region can be corrected by employing the electron translational factors [3], but such factors are inappropriate in the low energy region where classical velocity has no meaning.

In principle, the hyperspherical close coupling code developed for any three-body Coulomb systems [1] can be applied to the specific examples here. In applying to D^++H(1s) and to μ^++H(1s) reactions, however, it would take hundreds of partial waves to obtain converged cross sections even for collisions at subthermal energies. Since in hyperspherical calculations, the adiabatic potentials and coupling terms have to be obtained for each partial wave J, the straightforward application of the hyperspherical close-coupling method to ion-atom collisions would impose a heavy load on the computational needs. However, in our recent Publication #103, we have shown that in actual applications the problem can be simplified significantly. In fact, the potential curves and the coupling terms need to be calculated only once, just like in the PSS model. The only difference is that the calculations should be carried out in hyperspherical coordinates that give correct asymptotic boundary conditions.

In Publication #103, we have shown that in order to obtain cross sections at a given collision energy E for partial wave $J\neq0$, one needs only to modify each hyperspherical potential curve for J=0 by adding to each curve a centrifugal potential term $J(J+1)/(2\mu\rho^2)$, here ρ is the hyperradius and μ is the reduced mass of the two heavy particles. One can retain the same nonadiabatic coupling terms. With this prescription, one solves the hyperradial equation repeatedly for each partial wave J until the total cross section is converged. We called this approximation the rotor model. Note that within this rotor model, the procedure is entirely equivalent to the standard PSS approach for ion-atom collisions at low energies, but without the

inherent errors of the latter since the hyperspherical approach does give the correct asymptotic boundary conditions.

We have shown that the partial cross sections obtained from the rotor model for J≠0 agree well with those from actual hyperspherical calculations.

By performing the hyperspherical close-coupling calculations with the rotor model, we have obtained the charge transfer reaction cross sections for $D^+ + H(1s) \rightarrow D(1s) + H^+$ and $\mu^+ + H(1s) \rightarrow \mu(1s) + H^+$ collisions from the threshold to about 2 eV. The results are shown in Fig. 1. Note that the results for $D^+ + H(1s) \rightarrow D(1s) + H^+$ have been published (Publication #103). For $\mu^+ + H(1s) \rightarrow \mu(1s) + H^+$, the full report will be finished soon.

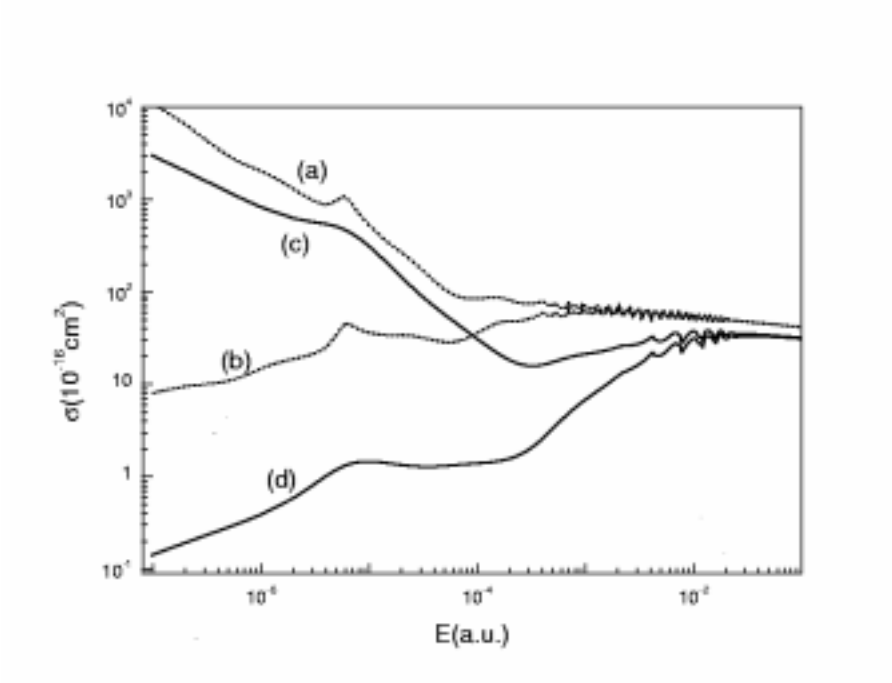

Figure 1. Comparison of the total charge transfer cross sections for: (a) $D^+ + H(1s) \rightarrow D(1s) + H^+$; (b) the reverse of (a); (c) $\mu^+ + H(1s) \rightarrow \mu(1s) + H^+$; (d) the reverse of (c). The collision energy is measured from the threshold of each reaction. Only the two lowest hyperspherical channels are included in the close-coupling calculations.

The goal of the present calculations is to establish benchmark results for such elementary reactions, and to compare how the reaction cross sections depend on the masses of the three charged particles. Since the energy difference between H(1s) and D(1s) is 3.7 meV, while the energy difference between H(1s) and μ(1s) is 58 meV, the cross sections clearly are larger if the energy difference between the initial and final states is smaller, see Fig. 1. As the collision

energy is increased, the cross section does not decrease monotonically. The minor structures at the lower energies reflect the contributions of a limited number of partial waves to the total cross section. The bump near 10^{-5} a.u. is due to the J=4 partial wave contribution. Note also the oscillatory structures at energies near 10^{-2} a.u. These structures partly come from the shape resonances that occur at energies near the top of the effective potential barriers for the higher partial waves. However, one cannot identify individual peaks as due to individual shape resonances.

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References

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