

Charge exchange between H(2s) and fully stripped carbon and nitrogen ions at low-keV impact energies*

A. Salop

Molecular Physics Center, Stanford Research Institute, Menlo Park, California 94025

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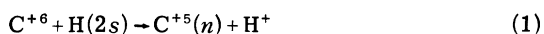
Approximate cross sections for charge transfer between H(2s) and fully stripped carbon and nitrogen ions have been obtained in the velocity range 6×10^6 – 7×10^7 cm/sec. In these systems, transfer takes place into high-lying orbitals of the final-state ion. The Landau-Zener theory modified for application to a multistate system is used to calculate the cross sections. The coupling-matrix elements are determined both from a study of the pseudocrossings observed in the relevant system of the adiabatic potential curves and by direct calculation using the appropriate asymptotic parabolic wave functions. The resulting cross sections are large, in the 10^{-14} -cm² range for both C⁺⁶ and N⁺⁷, and show the relatively flat energy dependence characteristic of systems with a number of contributing curve crossings.

I. INTRODUCTION

In a previous paper¹ (referred to as I), we reported the results of calculations using a modified Landau-Zener technique, undertaken to determine cross sections in the near-adiabatic range of velocities for electron transfer between ground-state atomic hydrogen and various fully stripped atomic ions. These studies were motivated by a more general interest in multicharged-ion interactions of concern in fields such as radiation research, controlled-thermonuclear-fusion plasma studies, and multicharged ion source development. In many of the systems under study, these ions can interact not only with ground-state atoms and molecules but also with an appreciable component of long-lived (metastable) neutrals which are expected to have particularly large cross sections. Because of the possible importance of such processes and the need for reasonable estimates of the associated cross sections, we have extended our calculational program, appropriate to one-electron, two-center systems, to include the study of charge exchange between the H(2s) metastable hydrogen atom and fully stripped carbon and nitrogen ions.

II. METHOD OF CALCULATION

We are concerned here with the charge-exchange processes typified by the exothermic reactions.



in the near-adiabatic range of velocities. For such processes, collision times ($\sim 10^{-14}$ sec) are orders-of-magnitude smaller than the radiation lifetimes of the metastable atom so that one can neglect the radiation process in calculating the collisional cross section. Here, also, as in the case of capture from ground-state atoms, the important interactions are long range, the transfer taking

place into high-lying orbitals of the final-state ion. Therefore it is possible to employ the same multistate Landau-Zener model¹⁻³ used in studying capture from ground-state hydrogen. Since the method has been described in detail in I, it suffices here to outline briefly the approach, emphasizing the modification in the computational procedures necessitated by the presence of the metastable rather than the ground-state atom as a precollision partner.

The appropriate asymptotic (separated-atom) wave functions for these one-electron systems are hydrogenic wave functions $\langle n, n_1, n_2, m |$ obtained as solutions of the Schrödinger equation in parabolic coordinates,⁴ where

$$n = n_1 + n_2 + |m| + 1 \quad (2)$$

and n_1 and n_2 are the "parabolic" quantum numbers. One can express the initial-state H(2s) wave function in terms of parabolic wave functions as

$$\varphi_{2s} = (1/\sqrt{2}) (\langle 2, 0, 1, 0 | + \langle 2, 1, 0, 0 |). \quad (3)$$

These component wave functions can be written in spherical coordinates as

$$\langle 2, 0, 1, 0 | = (1/4\sqrt{\pi}) [1 - \frac{1}{2}r_1(1 + \cos\theta_1)] \exp(-\frac{1}{2}r_1) \quad (4)$$

and

$$\langle 2, 1, 0, 0 | = (1/4\sqrt{\pi}) [1 - \frac{1}{2}r_1(1 - \cos\theta_1)] \exp(-\frac{1}{2}r_1), \quad (5)$$

where the spherical coordinate system is centered on the proton and the direction from the proton to the heavy-ion nucleus is taken as the positive z direction.

The problem resolves itself into the computation of two effectively independent cross sections Q_{2010} and Q_{2100} , corresponding to each of the above precollision parabolic separated-atom states. Thus,

in each case one considers the appropriate set of "interacting" (noncrossing) adiabatic-potential curves for the $(\text{CH})^{+6}$ and $(\text{NH})^{+7}$ systems, evaluates the appropriate crossing radii R_{cj} , coupling-matrix elements U_{ij} , Landau-Zener probabilities P_{ij} , and partial cross sections Q_j (using the same notation as in I), and then sums these to obtain the total cross section Q_{2010} or Q_{2100} . The final capture cross section is then given by

$$Q = \frac{1}{2}[Q_{2010} + Q_{2100}]. \quad (6)$$

For the Q_{2010} computation, the set of interacting terms, according to the one-electron diatomic-molecule noncrossing rule,^{4,5} are those associated with C^{+5} or N^{+6} separated-atom states $|n, 0, n-1, 0\rangle$, just as in the case of capture from $\text{H}(1s)$. For these exothermic reactions, $n < Z$, where Z is the charge on the incoming ion. Some of the relevant adiabatic-potential curves for the $\text{H}(2, 0, 1, 0)-\text{C}^{+6}$ system obtained using the OEDM computer code developed by Power^{5,6} are shown in Fig. 1. The nuclear repulsion energies have not been included in these calculations. Each curve is labeled on the right-hand side by its appropriate set of parabolic quantum numbers. The characteristic set of pseudocrossings is indicated in Fig. 1.

The coupling-matrix elements associated with

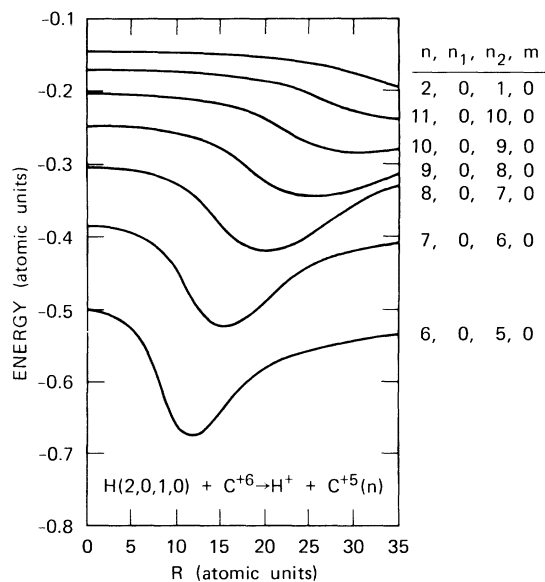


FIG. 1. Set of "interacting" adiabatic-potential curves associated with the $\text{C}^{+6}-\text{H}(2, 0, 1, 0)$ collision system. The curves are labeled on the right-hand side by the separated-atom parabolic quantum numbers. The nuclear repulsion energy has not been included in these curves or those of Fig. 2. The separated-atom limit corresponds to the $\text{H}(2s)$ level for the uppermost curve and to $\text{C}^{+5}(n)$ levels for all other curves.

each of these crossings were evaluated in two ways. They were computed directly⁷ using the procedure described in I with the initial-state asymptotic wave function given by Eq. (4) and the final-state hydrogenic heavy-ion wave function by

$$\begin{aligned} \varphi'_j &= |n, 0, n-1, 0\rangle \\ &= \frac{1}{\sqrt{\pi n}} \frac{1}{(n-1)!} \alpha^{3/2} e^{-\alpha r_j} \\ &\times \sum_{i=0}^{n-1} (-1)^i \frac{(n-1)!^2}{(n-i-1)!(i!)^2} (\alpha r_j)^i (1 + \cos\theta_j)^i. \quad (7) \end{aligned}$$

Here r_j and θ_j are spherical coordinates referred to an origin in the heavy-ion nucleus, and the direction from the heavy-ion nucleus to the proton is taken as the positive z direction. The quantity α is equal to Z/n , where Z is the charge of the incoming ion.

The matrix elements were also obtained from the adiabatic-potential curves by taking the separation between curves at the avoided crossings to be equal to $2U_{ij}$.⁸ The assumption made here is that only the two close-lying curves interact and that the influence of the other states can be neglected.

For the Q_{2100} computations, the set of interacting states are those associated with asymptotic wave functions $|n, 1, n-2, 0\rangle$. Several of the relevant molecular adiabatic-potential curves for the $\text{H}(2, 1, 0, 0)-\text{C}^{+6}$ collision system are shown in Fig. 2. Here also, the coupling-matrix elements were determined both from these curves and by direct computation; in this case using the initial-state

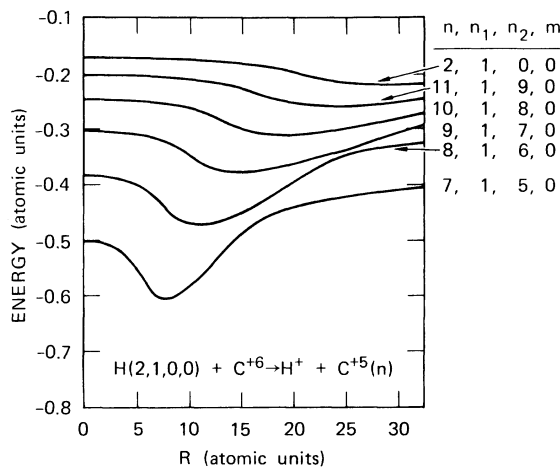


FIG. 2. Set of "interacting" adiabatic-potential curves associated with the $\text{C}^{+6}-\text{H}(2, 1, 0, 0)$ collision system. The curves are labeled on the right-hand side by the separated-atom parabolic quantum numbers. The separated-atom limit corresponds to the $\text{H}(2s)$ level for the uppermost curve and to $\text{C}^{+5}(n)$ levels for all other curves.

wave function given by Eq. (5) and the final state given by

$$\begin{aligned} \varphi_j'' &= |n, 1, n-2, 0\rangle \\ &= \frac{1}{\sqrt{\pi n}} \frac{1}{(n-2)!} \alpha^{3/2} e^{-\alpha r_j} [1 - \alpha r_j (1 - \cos\theta_j)] \\ &\quad \times \sum_{i=0}^{n-2} (-1)^i \frac{(n-2)!^2}{(n-i-2)! (i!)^2} (\alpha r_j)^i (1 + \cos\theta_j)^i. \end{aligned} \quad (8)$$

In the present problem, the initial-state long-range interaction is considerably more complex than that in the case of capture from ground-state hydrogen. For the spherically symmetric H(1s) wave function, all multipole moments vanish and the dominant interaction is a polarizability (second-order Stark) interaction. For H(2, 0, 1, 0) and H(2, 1, 0, 0), on the other hand, the multipole interactions contribute. However, terms of higher order than electric dipole are small and are neglected in this treatment.

Thus the crossing distances R_{c_j} (keeping the same notation as in I) corresponding to capture from H(2, 0, 1, 0) and H(2, 1, 0, 0) into the appropriate n levels of the final-state ion are now obtained from the relations

$$\begin{aligned} \Delta E - \frac{3Z}{R^2} - \frac{84Z^2}{R^4} - \frac{Z}{R} + \frac{\alpha^4}{16R^4} [17n^2 - 3(n-1)^2 + 19] \\ + V_{n,0,n-1,0} = 0 \end{aligned} \quad (9)$$

and

$$\begin{aligned} \Delta E + \frac{3Z}{R^2} - \frac{84Z^2}{R^4} - \frac{Z}{R} + \frac{\alpha^4}{16R^4} [17n^2 - 3(n-3)^2 + 19] \\ + V_{n,1,n-2,0} = 0, \end{aligned} \quad (10)$$

respectively. In these equations, the second and third terms are the initial-state first- and second-order Stark interactions,⁹ the fourth term is the nuclear coulomb repulsion, the fifth term is the final-state second-order Stark interaction,⁹ and the $V_{n,0,n-1,0}$ and $V_{n,1,n-2,0}$ quantities represent the long-range electrostatic interactions between the proton and the electron in the final-state ions. In practice, these quantities were decomposed into their multipole components and only the significant terms were retained. (Seven terms were found to be sufficient in all cases.) The energy defects ΔE were obtained from the simple hydrogenic expression

$$\Delta E = \frac{1}{2}(Z^2/n^2 - 0.25). \quad (11)$$

III. COMPUTATIONAL RESULTS AND DISCUSSION

Using these techniques, coupling-matrix elements and crossing separations for capture into various levels of the final-state ion C^{+5} and N^{+6} were determined both by analysis of the avoided crossings and by direct computation as discussed previously. They are listed below in Table I. Three of the relevant matrix elements and corresponding crossing radii could not be determined

TABLE I. Coupling-matrix elements and crossing separations for electron capture from H(2, 0, 1, 0) and H(2, 1, 0, 0) into various final-state levels. The unprimed quantities were obtained by direct computation. The primed quantities were derived from an analysis of the pseudocrossings observed in the adiabatic-potential curves for each system (Ref. 6). The number in parentheses following an entry is the power of 10 which multiplies it.

Final-state ion	Hydrogen parabolic state	n level	U_{1j} (a.u.)	U'_{1j} (a.u.)	R_{c_j} (a.u.)	R'_{c_j} (a.u.)
C^{+5}	H(2, 0, 1, 0)	9	3.58 (-4)	...	48.9	...
		8	2.02 (-2)	6.8 (-3)	31.1	33.1
		7	9.13 (-2)	2.08 (-2)	21.3	24.5
	H(2, 1, 0, 0)	8	1.68 (-3)	3.40 (-3)	25.5	25.2
		7	8.0 (-3)	1.96 (-2)	16.9	16.6
		6	1.13 (-2)	3.72 (-2)	12.6	11.0
N^{+6}	H(2, 0, 1, 0)	10	7.13 (-4)	...	48.5	...
		9	1.93 (-2)	7.0 (-3)	33.1	34.8
		8	7.51 (-2)	1.88 (-2)	23.9	26.8
	H(2, 1, 0, 0)	9	1.69 (-3)	...	27.3	...
		8	6.96 (-3)	1.35 (-2)	19.2	18.9
		7	1.11 (-2)	3.05 (-2)	14.5	13.2

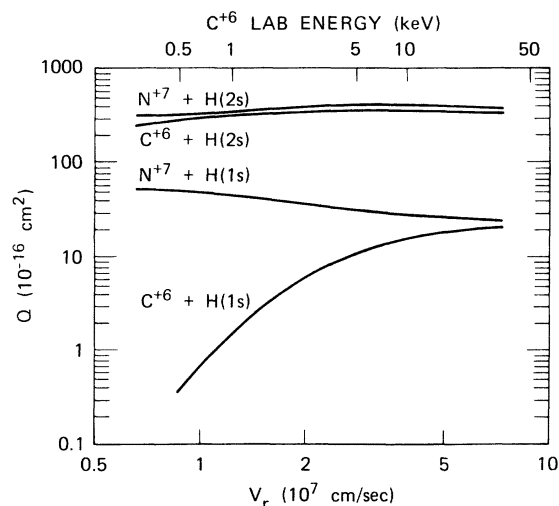


FIG. 3. Total Landau-Zener cross sections for electron transfer between H(2s) and C^{+6} and N^{+7} and between H(1s) and C^{+6} and N^{+7} .

by the potential curve method because of computational difficulties in generating the curves for the higher-lying states. The levels for which parameters are listed are those which are predominantly involved in the capture process. Thus for C^{+6} transfer from H(2, 0, 1, 0) takes place primarily into levels $n=7-9$ and from H(2, 1, 0, 0) primarily into the levels $n=6-8$. For N^{+7} , capture from H(2, 0, 1, 0) goes predominantly into the levels $n=8-10$, and from H(2, 1, 0, 0) into levels $n=7-9$. The two sets of coupling-matrix elements are in substantial disagreement, although the differences become smaller as the separations become larger. For the collisions involving H(2, 0, 1, 0), the computed values are larger than those obtained from the potential curves. For H(2, 1, 0, 0) collisions, the reverse is true. These discrepancies contrast sharply with the relatively good agreement found previously¹ in the case of capture from ground-state hydrogen. It seems clear that the asymptotic wave functions used in the matrix-element determinations are inadequate for these systems except possibly at the more distant crossings. We therefore chose for the cross-section computations, the matrix elements (and crossing radii) derived from the molecular-potential curves. In the three cases

where they could not be determined in this way, the crossings are so distant that it was reasonable to assume that the matrix elements computed from the asymptotic wave functions were valid.

Total cross sections for electron transfer from H(2s) to C^{+6} and N^{+7} in the range of velocities from 6×10^6 to 7×10^7 cm/sec were then computed and are plotted in Fig. 3. Also shown for each ion are the previously determined Landau-Zener cross sections for capture from H(1s). The upper limit of the velocity range is chosen to be small enough relative to the hydrogenic orbital velocity so that near-adiabatic conditions are assumed to exist. The lower limit is set by the condition that the relative energy is always considerably greater than any of the relevant coupling-matrix elements, which is a constraint for applying the Landau-Zener model.

The H(2s) cross sections for both ions are large, being in the 10^{-14} -cm² range for the velocities considered and usually at least an order of magnitude larger than those for the corresponding ground-state reactions. The curves are relatively flat over the entire velocity range. This lack of structure in the cross-section curve can be attributed to the smearing-out effect of a number of crossings contributing significantly over a range of energies.

IV. CONCLUDING REMARKS

These calculations are basically exploratory in nature, designed as an initial approach to the solution of this highly complex class of collision problems. Rotational coupling effects which may contribute significantly in some of these systems have been neglected. Despite this omission and the well known limitations of the Landau-Zener theory,¹⁰⁻¹⁴ we believe this approach is extremely useful in its function of pinpointing the important charge-exchange channels and giving cross sections with an estimated factor-of-2 accuracy at a minimum of computational expense.

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