Molecular-state treatment of electron capture in slow collisions of C^{4+} with H: Alignment and orientation effects

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Total and state-selective charge-transfer cross sections for C^{4+}-H collisions have been calculated in the energy range 0.02–1.0 keV/amu by employing the semiclassical, impact-parameter, close-coupling method based on a molecular-state description of the CH^{4+} system and including plane-wave translation factors. The calculated cross sections are in good agreement with the quantum calculations as well as with the experimental findings. The integral alignment (A_{20}) parameter for the $C^{3+}(3p)$ state is also presented.

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Charge-exchange processes involving collisions between highly (partially as well as fully ionized) charged ions and atomic targets are of considerable interest not only in energy balance and fusion plasmas diagnostics [1], but also in astrophysics [2]. The charge-transfer mechanism dominates all other types of inelastic collisions in low-temperature plasmas, particularly when the electron temperature remains below 15 keV [3]. A detailed knowledge of the state-selective cross sections is essential in creating a population inversion for achieving lasing effects [4].

Low-energy ($E \ll 1$ keV/amu) collisions of multiply charged ions with neutral atoms have received considerable attention both theoretically [3,5] and experimentally [6,7] in recent years. Theoretically, collisions involving bare ions and atomic hydrogen are attractive because computationally, one-electron systems lend themselves to rigorous treatments. The ion C^{4+}, which has a spherically symmetric ground-state $1s^2$ core, is a much studied projectile. The earliest semiclassical study of this system was reported by Olson, Shipsey, and Browne [8] using a seven-state close-coupling calculation without incorporating the effects of the electron translation factors (ETF).

McCarroll and co-workers [9–11] have investigated the same problem by treating the collision dynamics quantum mechanically. In their first calculation, Gargaud *et al.* [9] approximated the interaction between the ionic core and the active electron by a model potential of the Hellman type [12]. Bottcher and Heil [13] also calculated total cross sections for the same system quantum mechanically. Both of the above quantum calculations have retained only four molecular orbital Σ states (MO4) and neglected the effect of the rotational coupling as well as the ETF. The neglect of the coupling to Π states, however, posed questions regarding the reliability of the partial cross sections.

Using the local l-independent model potential [10], Hanssen *et al.* [14] calculated cross sections semiclassically, employing straight-line trajectories and a common translation factor (CTF) [15], and concluded that the better agreement between the results of Gargaud *et al.* (MO4) and the experiment [16] is fortuitous. For $2 < E < 25$ keV/amu the total cross sections of Hanssen *et al.* agree with measured values [16]. However, for $E < 2$ keV/amu their cross sections are larger than other close-coupling results [9,10] and the experimental findings [16] by as much as 50%.

Fritsch and Lin [17] have investigated the same problem in the energy range $E = 0.1$–20 keV/amu using a modified two-center atomic-orbital (AO^+) expansion. They employed the local model potential of Gargaud *et al.* (MO4) and retained all orders in the projectile velocity v in the plane-wave ETF [18]. They have used bare Coulombic trajectories (with $Z_1 = 4$ and $Z_2 = 1$) for $E < 1$ keV/amu and classical straight-line trajectories for $E > 1$ keV/amu. Above $E = 0.3$ keV/amu they obtained fairly good agreement with the experimental total cross sections. However, at lower energies there are discrepancies with the experimental findings [16] and also with the quantal MO4 results.

In their study of the role of the rotational coupling Gargaud, McCarroll, and Valiron [11] used a different l-independent model potential to obtain a more accurate energy separation of the degenerate $3p$ and $3d$ levels of the C^{3+} atom. In their seven-state (MO7) close-coupling calculation, the effects of the ETF were included via the CTF procedure [15].

Recent measurements [19] of C^{4+} colliding with H and H_2 in the energy range $0.048 \leq E \leq 1.333$ keV/amu have renewed interest in this quasi-one-electron system. In addition to the total cross section (σ_T), they have also reported l-subshell cross sections. The information on the final-state distribution of the captured electrons provides a more stringent test of the theoretical calculations. It is important to note that the branching ratios of Hoekstra *et al.* are quite different from those of Baptist *et al.* [20]; in contrast to their findings, the results of Baptist *et al.* below 0.1 keV/amu show a decrease in the cross sections for the $3p$ transitions, while for $3d$ excitation there is a strong enhancement.

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The theoretical approach used in this study is the semiclassical, impact-parameter, coupled-states method, where the time-dependent wave function of the system is expanded in terms of electronic states, represented by molecular orbits [21]. The molecular orbitals and the corresponding electronic energy curves were calculated by a standard variational procedure, in which the ionic core is represented by a pseudopotential [22]. In the expansion of the system's wave function, the coefficients satisfy a set of linear first-order coupled differential equations, with initial conditions that satisfy a particular initial state; their asymptotic values represent transition amplitudes for various final states. These equations are solved numerically for a sufficiently large number of impact parameters b to ensure convergence, and cross sections are calculated by integrating the respective square of the transition amplitudes over b.

The adiabatic potential-energy curves are displayed in Fig. 1. We show only those states that make the most significant contributions at the low energies we are considering. The figure shows that a network of multiple avoided crossings dominates the charge-transfer process, leading to capture into the ($1s^2,3l;l=0$, 1, and 2) states of the C^{3+} atom. There are two distinct avoided crossings between the entrance channel (denoted as 4Σ) and the $3d\Sigma$ channel; the inner one is around ($R_1=$) $4.46a_0$ and the outer one is around ($R_2=$) $7.90a_0$. The corresponding energy defects ΔE's are $\Delta E_1=0.0034$ a.u. and $\Delta E_2=0.0032$ a.u., respectively. The $3d\Sigma$ and $3p\Sigma$ states show an avoided crossing around $R_3=7.38a_0$, while that for the $3p\Sigma$ and $3s\Sigma$ states is at $R_4=7.14a_0$. Our potential-energy curves are in good agreement with those of Gargaud and McCarroll [10]; it is important to note that Gargaud and McCarroll have included only the Σ states in their calculation. The energy of the $3d\Pi$ states is indistinguishable on the present scale from that of the entrance channel at $4.46<R<7.9a_0$. In this region, ΔE between the $3d\Sigma$ and $3p\Pi$ is very small.

Figure 2 compares our calculated total cross sections for capture into all $n=3$ states of C^{3+} with other

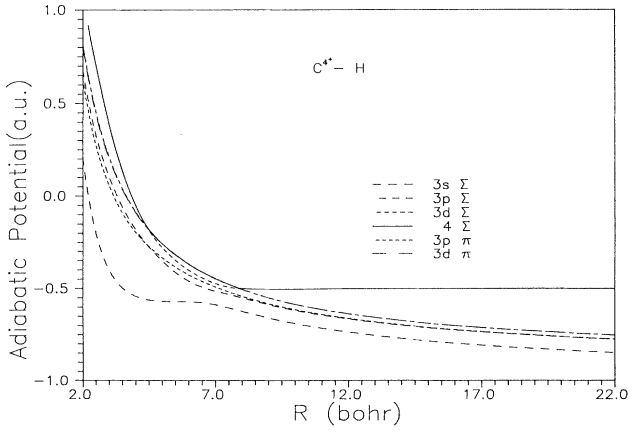

FIG. 1. Adiabatic potential energies for $3s\Sigma$, $3p\Sigma$, $3p\Pi$, $3d\Sigma$, and $3d\Pi$ states of a CH^{4+} system. The entrance channel is denoted by 4Σ. In the separated atom limit $3s$, $3p$, and $3d$ refer to the atomic states.

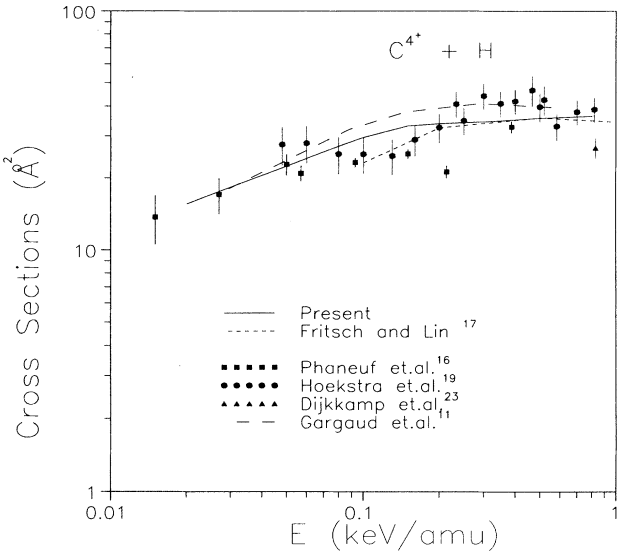

FIG. 2. Comparison of the total electron-capture cross sections with experiments and other coupled-state calculations for the formation of C^{3+} ($n=3$) in $C^{4+}+H$ collisions.

theoretical close-coupling results and with experimental measurements [16,19,23]. Our results agree very well with the low-energy measurements of Phaneuf *et al.* [16] and reasonably well with the MO7 results of Gargaud, McCarroll, and Valiron [11]. However, at intermediate energies ($0.5<E<1$ keV/amu) our results are lower than the results of Gargaud, McCarroll, and Valiron [11] because our coupling matrix elements and the core potentials are not identical to theirs. At lower energies, the energy dependence of the AO^+ cross sections [17] are different from our results, as well as from the MO7 results of Gargaud, McCarroll, and Valiron [11]. The use of Coulomb trajectories at such low velocities may cause this discrepancy. The variation of the cross sections with the projectile velocity is relatively very slow. However, the cross sections for specific atomic states show a considerable velocity dependence. To illustrate this, we show the branching ratios using $\sigma_{\rm rel}(3l)=[\sigma(3l)/\sum_l\sigma(3l)]$ in Figs. 3, 4, and 5, respectively, for $3s$, $3p$, and $3d$ states of the C^{3+} along with various measurements [16,19,20,23] and calculations [11,17].

It is evident from Fig. 3 that our results for transfer to the $3s$ state are in very good accord not only with the experimental values of Hoekstra *et al.* but also with those of Baptist *et al.* Below 0.1 keV/amu the agreement between the MO7 results and our results is very good. Above 0.8 keV/amu both the AO^+ and the MO7 cross sections predict an increase, but our calculated cross sections show constant behavior and remain within the experimental limits. Below $E\leq 0.4$ keV/amu the rate of fall of AO^+ results is faster than either of the MO results.

In the case of capture into the $3p$ state, depicted in Fig. 4, the present cross sections follow closely the quantum MO7 results of Gargaud *et al.* and agree reasonably well with the measurements [19]. From 0.3 to 0.7 keV/amu our results are slightly larger than the MO7 predictions. This may be due to (i) different pseudopotentials generat-

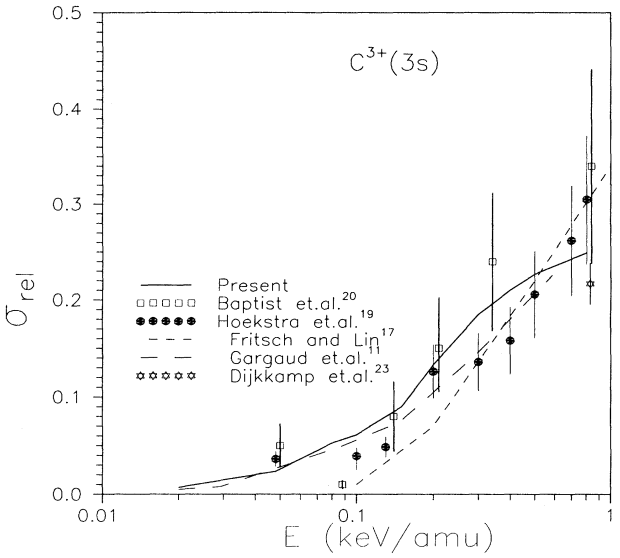

FIG. 3. Comparison of the state-selective cross sections for C^{3+} ($3s$) with experiments and other calculations.

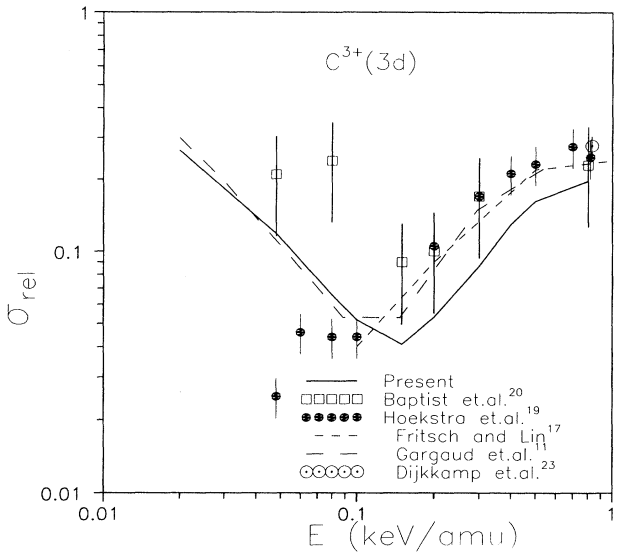

FIG. 5. Comparison of the state-selective cross sections for C^{3+} ($3d$) with experiments and other calculations.

ing different molecular properties; (ii) different ETF effects causing altogether different coupling matrix elements; and (iii), most importantly, the different ways of treating the collision dynamics; semiclassical vs quantum mechanical. At higher energies ($E \geq 0.4$ keV/amu) our results are slightly larger than both AO^+ and MO7 values. The $3p$ states remain the dominant capture channels throughout the energy range considered, and the effect of rotational coupling is very significant. Indeed, in the energy region $0.8 \leq E \leq 1.0$ keV/amu, the contribution due to the $3p\Pi$ state is much larger than that due to the $3p\Sigma$. Below 0.1 keV/amu, our results show a downward trend in conformity with the earlier MO7 calculations. The experimental values, however, in this velocity regime remain more or less constant.

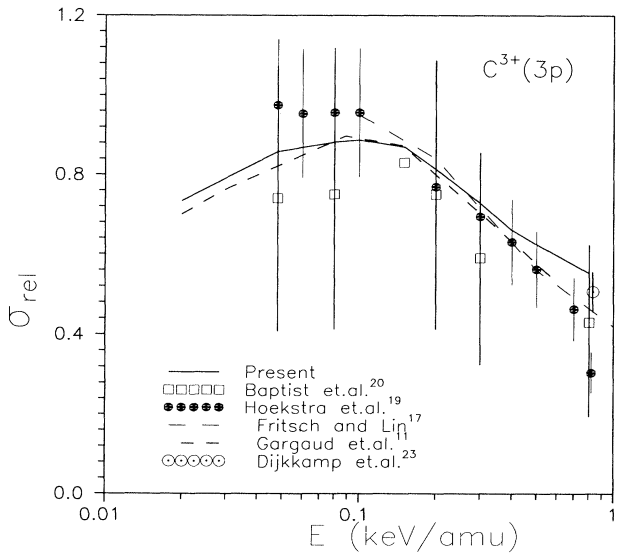

FIG. 4. Comparison of the state-selective cross sections for C^{3+} ($3p$) with experiments and other calculations.

The relative subshell electron-capture cross sections for the $3d$ states displayed in Fig. 5 are in good qualitative agreement with the quantum-mechanical MO7 results. At low energies, the semiclassical and quantum-mechanical MO calculations predict an increase in the cross sections. The results of Baptist *et al.* [20] show this enhancement and are in excellent agreement with our values. However, the measurements of Hoekstra *et al.* have not shown this behavior. To understand the physical effects causing this interesting feature in the cross sections, we have evaluated the transition probabilities using the Landau-Zener approximation and have found that the outer crossing (R_2) (see also Fig. 1) between the entrance channel and the $3d\Sigma$ states becomes more and more diabatic with increasing energy. At lower velocities this crossing remains adiabatic and becomes the main gateway to transfer probability to the $3d\Sigma$ and $3d\Pi$ states; this in turn may produce larger amplitudes, causing the larger cross sections.

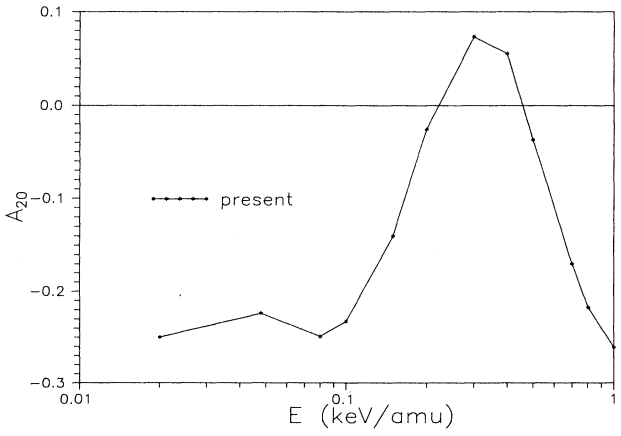

FIG. 6. Integral (over impact-parameter b) alignment A_{20} as a function of impact energy E.

Using the calculated partial cross sections σ_{nlm} the integral alignment A_{20} can be evaluated using the relation [24]

$$A_{20}=(\sigma_1-\sigma_0)/(\sigma_0+2\sigma_1)\ ,$$

where σ_0 and σ_1 represent the integral cross sections for the magnetic quantum number $m=0$ and $m=1$, respectively. In Fig. 6 we plot the alignment parameter A_{20} for the $C^{3+}(3p)$ states as a function of energy. The negative values observed for A_{20} indicate that capture to the $3p_0$ level is the overwhelming dominant process. In the region $0.2 \leq E \leq 0.25$ keV/amu the rotational couplings become very important in promoting flux mixing and give rise to an increased probability population of the $3p_{\pm 1}$ sublevel of the C^{3+} atoms. At higher energies ($E \geq 0.3$ keV/amu), the overwhelmingly dominant contributions from the $m=0$ sublevel may be due to the fact that the angular momentum vector becomes more and more perpendicular to the quantization axis.

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