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Total and state-selective electron capture cross sections for C^{3+} + H collisions

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Abstract. Electron capture cross sections in collisions of C^{3+} ions with atomic hydrogen have been studied using the close-coupling two-centre atomic orbital (AO) expansion method by treating the collision system in a quasi-two-electron model. Total electron capture cross sections to the dominant individual singlet and triplet excited states are calculated over the energy range 0.1–50 keV amu^{-1}. The results are compared with existing experimental data and with theoretical calculations based on the molecular orbital (MO) expansion method. It is found that our AO results are in general agreement with the MO results of Errea *et al* (1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 4061) and with experiments but that discrepancies still exist in the details.

1. Introduction

Apart from its fundamental importance, current interest in the C^{3+}–H charge changing collision system stems from its possible application in plasma diagnostics and modelling and astrophysics [1]. Several experimental and theoretical studies have been carried out in the last two decades over a broad range of collision energies for this system. The total electron transfer cross section has been measured by Ćirić *et al* [2] at collision energies of 0.92, 1.39 and 1.85 keV amu^{-1}, by Gardner *et al* [3] at 2.0 keV amu^{-1}, and by Crandall *et al* [4] at 2.8 keV amu^{-1}. More extensive measurements have been performed by Phaneuf *et al* [5] in the 5–112 keV amu^{-1} region, by Phaneuf *et al* [6] in the low-energy range of 10–110 eV amu^{-1} and more recently by Havener *et al* [7] in the 0.3–3000 eV amu^{-1} range using the merged-beam technique. State-selective cross sections have been carried out by both translational energy spectroscopy in the 50–1500 eV amu^{-1} range [8] and by photon-emission spectroscopy in the 0.7-4.6 keV amu^{-1} range [2].

Theoretically, an early calculation of Bienstock *et al* [9] was based on the full quantal quasimolecular orbital description of the collision but without the inclusion of electron translational motion. They considered cross sections from strong adiabatic coupling to triplet product states $C^{2+}(1s^22s3s)\,^3S$, $C^{2+}(1s^22s3p)\,^3P$ and to singlet product states $C^{2+}(1s^22p^2)\,^1S$, $C^{2+}(1s^22p^2)\,^1D$. Later, Opradolce *et al* [10] also performed a molecular model calculation by including the translation effect but their results are significantly different from the results of Bienstock *et al* [9]. Both of these calculations include only a limited number of states. In a much more elaborate calculation, Errea *et al* [11] employed 22 molecular states where each state was modified by a common translation factor. Their results are found to be in better general agreement with most of the existing experimental data. However, the large spread of

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experimental total and partial cross sections makes it difficult to draw conclusions on whether the detailed cross sections for this collision system are fully settled.

In view of the above situation, we have undertaken an independent study of the present collision system within the semiclassical close-coupling method by expanding the time-dependent electronic wavefunction in terms of atomic orbitals (AO) at the two nuclear centres [12]. Since transitions to the dominant electron capture channels occur mostly at large impact parameters, the AO expansion method is expected to be adequate down to relatively low energies. In the present calculation, we model C^{3+}–H as a two-electron collision system, thus allowing us to obtain state-selective electron capture cross sections to distinct final singlet and triplet states. We used a basis set of about 40–50 atomic states and the main emphasis is to compare our results with the 22-state MO calculations of Errea *et al* [11]. In the energy range of interest here, straight-line trajectories were used. In section 2, we document the parameters used in the present calculation. The results and the comparison with experiments and other theoretical calculations are reported in section 3. A short summary and conclusion is given in section 4.

2. The theoretical model

We first model C^{3+}–H as a two-electron system consisting initially of an electron with the C^{4+} core and an electron with the proton. The time-dependent wavefunction for these two electrons is expanded in terms of travelling two-electron atomic eigenstates, consisting of configurations where one electron is on the target and the other on the projectile to describe elastic as well as single excitations of either the target or the projectile or both, and of configurations where both electrons are on the projectile for final states populated by the single-electron capture process. The present calculation is carried out using the general two-electron code which has been used previously to study ion–atom collisions [12–14]. For the C^{4+} core potential we take the screened hydrogenic potential as proposed by Garvey *et al* [15] with a slightly adjusted thickness parameter of $1/\xi = 0.201$ au and $\eta = 4.58$ in order to fit the initial experimental C^{3+}(2s) binding energy. From the model potential one-electron C^{3+} states and two-electron C^{2+} states are calculated, the latter using a standard configuration–interaction approach where the two-electron eigenstates are expanded in terms of antisymmetrized products of wavefunctions of two electrons. The dominant electron capture channels considered are (2s3s) ^{3}S , (2s3p) ^{3}P, (2s3d) ^{3}D for triplet states and (2s3s) ^{1}S, ($2p^2$) ^{1}S, (2s3p) ^{1}P, ($2p^2$) ^{1}D, (2s3d) ^{1}D for singlet states. We compare in table 1 the calculated energies of these states from the model potential with the experimental values.

In performing the close-coupling calculation the total spin is conserved, thus calculations were carried out separately for spin singlet and spin triplet symmetries. In each calculation, the two-electron states on the projectile consist of those listed above, together with a number of pseudostates generated from the basis functions. The products of one-electron states on each centre consist of the initial state, the single excitation of the target to 2s or 2p, and the single excitation of the projectile from 2s to 2p. The total number of atomic states included in the close-coupling calculations is 36 for singlet symmetry and 40 for triplet symmetry, but in test calculations the number has been raised to about 50 by including more pseudostates to check the convergence. With the basis functions chosen, the standard procedure for performing close-coupling calculations is used to obtain scattering cross sections to individual final states. We considered straight-line trajectories only in the calculations. We stopped our calculations at 100 eV amu^{-1} since at lower energies the Coulomb repulsion between C^{4+} and H^+ is no longer negligible. Thus the present calculation is a genuine AO calculation within the basis set and the model potential chosen.

Table 1. Comparison of energy levels in atomic units for the C^{2+} ion from the present model potential calculations and the experimental data [18]. Energies are given relative to the C^{4+} ion.

Two-electron state	Present work	Experimental value
$2s^2\ {}^1S^e$	−4.13	−4.13
$2p^2\ {}^1S^e$	−3.27	−3.30
$2s3s\ {}^{1(3)}S^e$	−2.96(−3.04)	−3.00(−3.04)
$2p3p\ {}^{1(3)}S^e$	−2.55(−2.64)	−2.56(−2.64)
$2s2p\ {}^{1(3)}P^e$	−3.60(−3.88)	−3.67(−3.89)
$2s3p\ {}^{1(3)}P^e$	−2.94(−2.94)	−2.95(−2.95)
$2p3s\ {}^{1(3)}P^e$	−2.65(−2.72)	−2.72(−2.73)
$2p3d\ {}^{1(3)}P^e$	−2.54(−2.56)	−2.55(−2.58)
$2p3d\ {}^{1(3)}P^e$	−2.54(−2.56)	−2.55(−2.58)
$2p^2\ {}^1D^e$	−3.46	−3.47
$2s3d\ {}^{1(3)}D^e$	−2.86(−2.89)	−2.87(−2.90)
$2s4d\ {}^3D^e$	−2.66	−2.67
$2p3p\ {}^{1(3)}D^e$	−2.61(−2.64)	−2.61(−2.66)

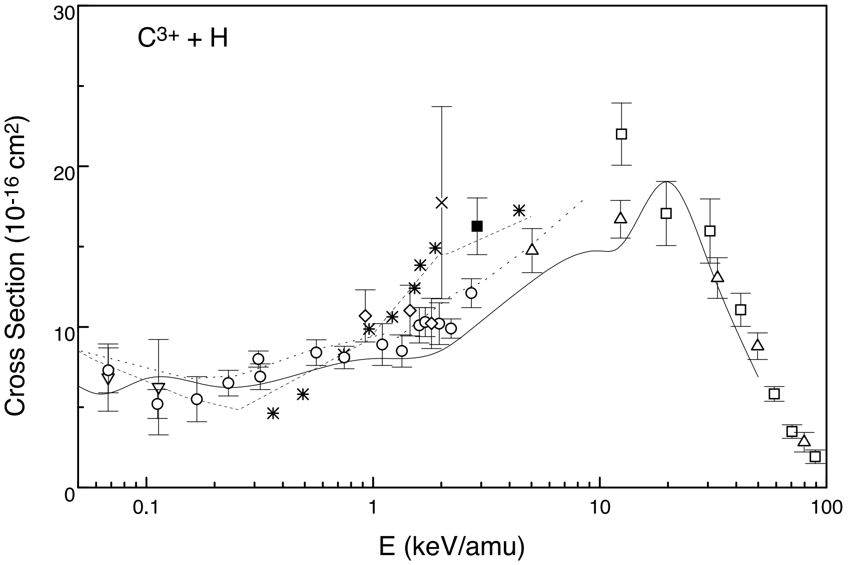

Figure 1. Present total electron capture cross section results for C^{3+} + H compared with other theoretical and experimental data. Theoretical results: solid curve, present work; dashed curve, Bienstock *et al* [9]; dotted curve, Errea *et al* [11]. Experimental results: open circles, Havener *et al* [7]; open up triangle, Phaneuf *et al* [5]; open down triangle, Phaneuf *et al* [6]; open squares, Goffe *et al* [17]; solid squares, Crandall *et al* [4]; stars, Yousif and Geddes [16]; crosses, Gardner *et al* [3]; open diamond, Ćirić *et al* [2].

3. Results and discussion

In figure 1 we compare the available experimental and theoretical total electron capture cross sections in the energy range of 50 eV amu^{-1} to 100 keV amu^{-1}. Within the error bars of the experiments there is an overall global agreement. Our results have good agreement with the experimental data from 100 eV amu^{-1} to 100 keV amu^{-1}, except that we tend to underestimate the experimental data by about 20% in the energy region of 1–5 keV amu^{-1}.

In this energy region the calculations of Errea *et al* have the better overall agreement with experiments. Within 400–4000 eV amu^{-1} the data of Yousif and Geddes [16] appear to deviate from other experiments but they are in good agreement with the calculation of Bienstock *et al* [9]. However, the latter calculations were carried out with a small basis set and thus we believe that both of these two results should be taken less seriously. If we also remove the two singular measured points, as indicated by the cross and by the solid square, and the lowest energy point indicated by the open square, then we can conclude that the total charge transfer cross section for the present system is known to within about 20%. Between the two extensive calculations, the results of Errea *et al* are consistently 10–20% higher than the present results.

For the present system there are two measurements of the state-selective electron capture cross sections, one from the translational energy spectroscopy measurements of Wilkie *et al* and the other from the photon-emission spectroscopy measurement of Ćirić *et al*. We compare the theoretical results with these two measurements for energies between 100–10 000 eV amu^{-1} in figures 2 and 3. We note that in this energy region the dominant electron capture is to the (2s3s) ^{3}S state. We show the comparison of the results for this state in figure 2(*a*). The calculations of Errea *et al* agree quite well with the data of Ćirić *et al* in the energy region where they overlap. Interestingly, the calculations of Bienstock *et al* are in good agreement with the data of Wilkie *et al*. However, these two MO calculations do not agree with each other. Our AO results are in better agreement with the MO results of Errea *et al* in terms of the energy dependence, but we are consistently about 20% lower than theirs in terms of absolute cross sections.

We next check the weaker channels. In figure 2(*b*) the cross sections for electron capture to the (2p^2) ^{1}S state are shown. Our results are in good agreement with Errea *et al* for the whole energy range displayed but both calculations are higher than the experimental data of Ćirić *et al* at higher energies. Similarly for capture to the (2p^2) ^{1}D state, as shown in figure 2(*c*), our calculations are closer to the results of Errea *et al* and agree well with the experiments of Wilkie *et al*, but we are consistently higher than the data of Ćirić *et al*.

In figures 3(*a*)–(*e*), we compare the theoretical calculations with the experimental data of Ćirić *et al*. The overall agreement is satisfactory in view of the fact that these are the weaker channels. Our predicted state-selective cross sections are, in general, quite close to the calculations of Errea *et al* except for the case of the (2s3s) ^{1}S state, especially at low energies. This may be due to the fact that we did not achieve a good fit of the experimental energy for this state (see table 1). We comment that in most cases the results of Errea *et al* appear to be in better agreement with the data of Ćirić *et al*.

Returning to figure 2(*a*), it is surprising to find that there is a consistent discrepancy between the present calculation and the MO result of Errea *et al* for electron capture to the dominant (2s3s) ^{3}S state, especially in the 1–10 keV amu^{-1} region. It is noted that from the MO picture transition to this state occurs primarily through the avoided crossing near $R = 11.7$ au. At this distance the two MO states are essentially atomic in nature and thus the AO expansion method is expected to be as good as the MO method. In figure 4 we show the comparison of the electron capture probabilities calculated by Errea *et al* and from the present AO calculation at 2.25 keV amu^{-1}. While the shapes of the electron capture probabilities appear to be quite similar, the MO calculation clearly has larger probabilities at larger impact parameters and at smaller impact parameters. While the discrepancy at smaller impact parameters can be expected because of the nature of the basis functions used in the two calculations, the discrepancy at larger impact parameters is less clear since the basis functions in the two calculations are essentially identical, the only difference is in the form of electron translational factors. We also checked the difference of the model potentials used in the two calculations, and there is no significant distinction between the two. However, it is noted that a

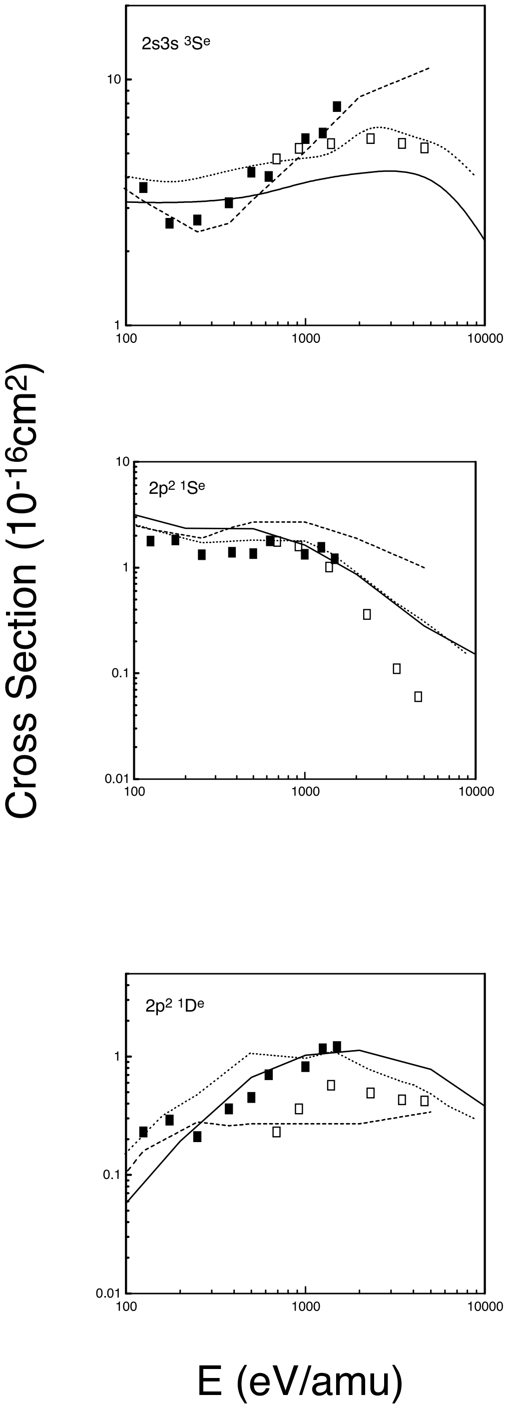

Figure 2. Comparison of theoretical results and experimental data for state-selective electron capture cross sections. Solid curve, present work; dashed curve, Bienstock *et al* [9]; dotted curve, Errea *et al* [11]. Experiments: solid squares, Wilkie *et al* [8]; open squares, Ćirić *et al* [2].

non-local Phillips–Kleinmann pseudopotential was used to shift all virtual MO (or core) states to higher energies to avoid possible spurious curve crossing in the calculation of Errea *et al*.

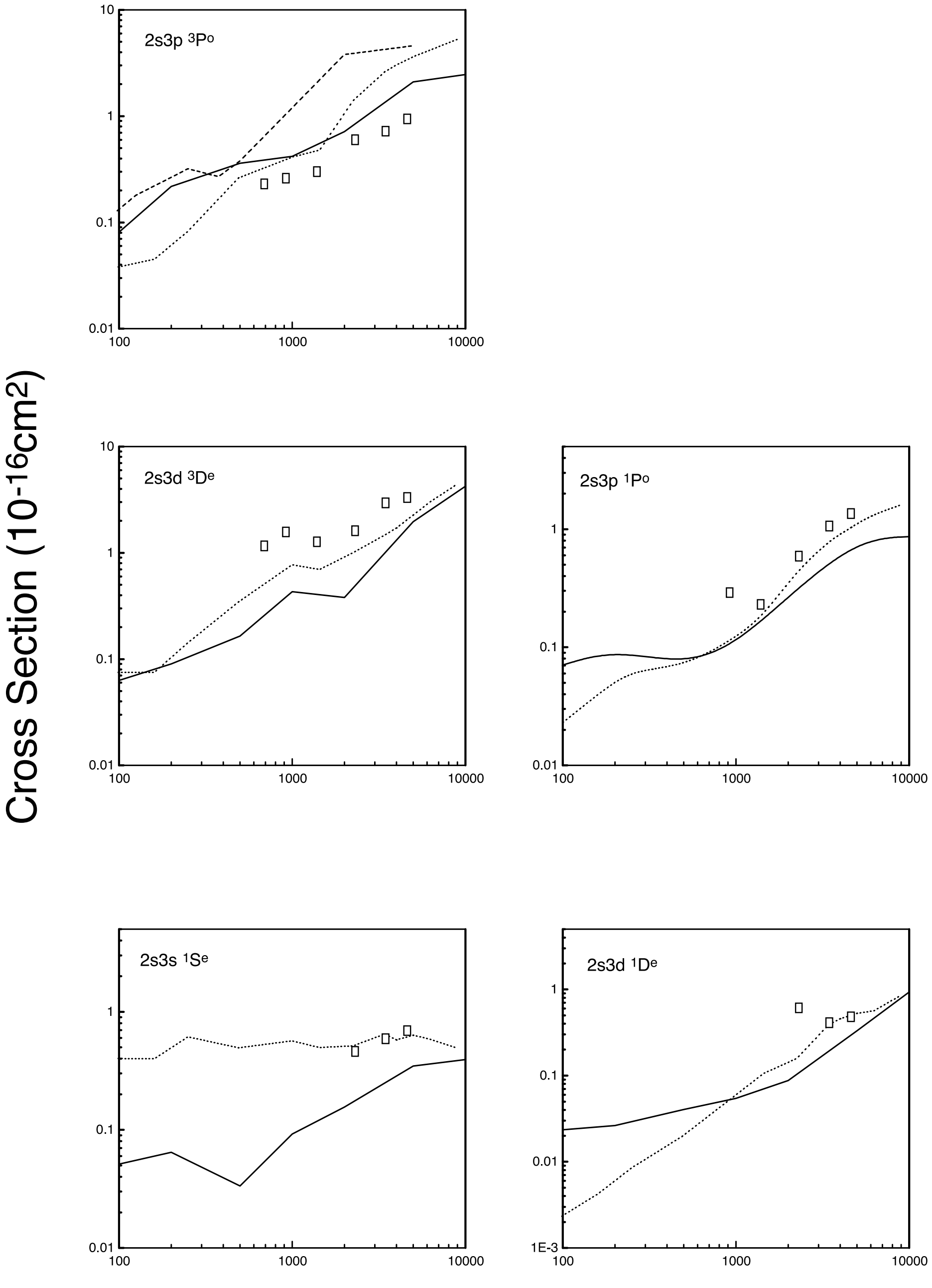

Figure 3. Comparison of theoretical results and experimental data for state-selective electron capture cross sections. Solid curve, present work; dashed curve, Bienstock *et al* [9]; dotted curve, Errea *et al* [11]; open squares, experimental data of Ćirić *et al* [2].

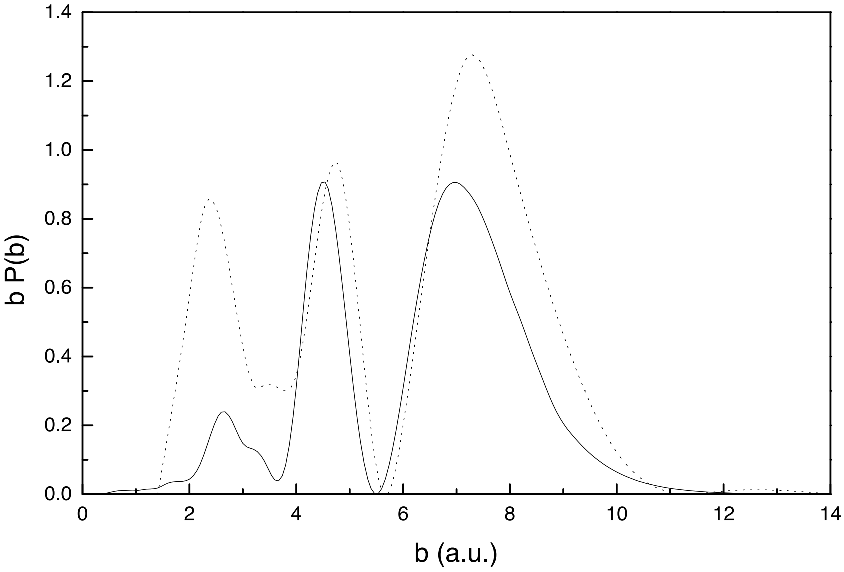

Figure 4. Impact parameter dependence of electron capture probability $P(b)$ to the (2s3s) ^{3}S state times impact parameter b at 2.25 keV amu^{-1}. Solid curve, present work; dotted curve, Errea *et al* [11].

4. Summary and conclusion

In this paper we report the total and state-selective single-electron capture cross sections for C^{3+} on H collisions over the energy range of 100–100 000 eV amu^{-1} using the close-coupling expansion method in terms of two-electron atomic basis functions. In this energy region the trajectory effect is negligible and thus the present calculation is a genuine AO calculation without any corrections. In terms of the total electron capture cross sections, there is a general agreement among the experiments and the more advanced theoretical calculations. Our results are shown to be in best overall agreement with the 22-state MO calculations of Errea *et al*. For the state-selective electron capture cross sections the agreement between the two calculations is also satisfactory. However, there still exists a 10–20% discrepancy in the total cross sections which probably can be resolved by a much more dedicated experimental and theoretical effort in the future.

Acknowledgments

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