Total and state-selective electron capture cross sections for $B^{4+}+H$ collisions

H. C. Tseng[1] and C. D. Lin[2]
[1]*Department of Physics, Chung Yuan Christian University, Chung Li, 32023 Taiwan*
[2]*Department of Physics, Kansas State University, Manhattan, Kansas 66506*

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Electron capture cross sections for $B^{4+}+H$ collisions are calculated using a two-center atomic orbital close coupling expansion method. Total electron capture cross sections are shown to compare well with the recent experimental data of Pieksma *et al.* [Phys. Rev. A **57**, 1892 (1998)] and with the molecular expansion calculation of Shimakura *et al.* [Phys. Rev. A **47**, 3930 (1993)], but not with the molecular calculation of Fraija *et al.* [Phys. Rev. A **49**, 272 (1994)]. Subshell electron capture cross sections are also compared.

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Current interest in the B^{4+}-H charge changing collision system stems from its relevance to processes near the wall in a magnetic fusion plasma [1]. Only very few experimental and theoretical studies have been carried out in the last decades for this system and the results are controversial. The most recent data are from the merged-beam experiment of Pieksma *et al.* [2] for collision energies between 60 and 1200 eV/amu. Earlier data for collisions above 1 keV/amu have been obtained by three experimental groups: Crandall *et al.* [3], Gardner *et al.* [4], and Gilbody [5], but the results vary widely and the reported cross sections differ by a factor of two at higher energies.

From the theoretical side, close-coupling calculations based on the molecular orbital expansion method have been carried out by Shimakura *et al.* [6] and by Fraija *et al.* [7]. The molecular basis functions used in the two calculations are rather similar even though they were calculated using different primitive basis sets. They also used somewhat different electron translational factors. The resulting total electron capture cross sections reported by Fraija *et al.* [7], however, are about 40% higher than those of Shimakura *et al.* [6]. In comparing with experiments, the results of Shimakura *et al.* agree better with the recent data of Pieksma *et al.* [2], while the results of Fraija *et al.* appear to agree better with the earlier data of Gardner *et al.* [4]. Despite of the general agreement between the data of Pieksma *et al.* [2] and the calculations of Shimakura *et al.* [6], the theoretical results are still about 20 to 30 % larger than the experimental data.

In view of the above conflicts we have undertaken an independent study of the present collision system within the semiclassical close coupling method by expanding the electron wave function in terms of atomic orbitals (AO) at the two atomic centers [8]. 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 treat B^{4+}-H as a two-electron collision system employing the same code which has been used previously for other systems [9]. We also obtained state-selective electron capture cross sections to distinct singlet and triplet final states to compare with the results of Shimakura *et al.* [6]. No experimental subshell electron capture cross sections for this system has been reported so far.

In the 100–10 keV/amu energy range considered in this work, the dominant channels are single capture to the $1s3\ell$ states of B^{3+}. Separate calculations for total spin singlet and spin triplet symmetries were carried out. The basic atomic states included are the initial state where one electron is in H($1s$) and the other in $B^{4+}(1s)$, and all the $1s2\ell$, $1s3\ell$ and $1s4\ell$ states of B^{3+}. The primitive basis orbitals are varied to make sure that these atomic states are well represented to give correct binding energies. We also kept a few pseudostates which were obtained from diagonalizing the atomic Hamiltonian with the primitive basis set. In the final calculation, 36 atomic states for singlet calculations and 40 atomic states for triplet calculations were used. In the scattering calculation, straight-line trajectories were used for all impact parameters and energies.

In Fig. 1 we compare the present total electron capture cross sections with the existing experimental data and other theoretical calculations. Comparing to the two MO calculations, it is clear that our results are much closer to those of Shimakura *et al.* and we may conclude that the results of Fraija *et al.* are questionable. In comparing with the data of

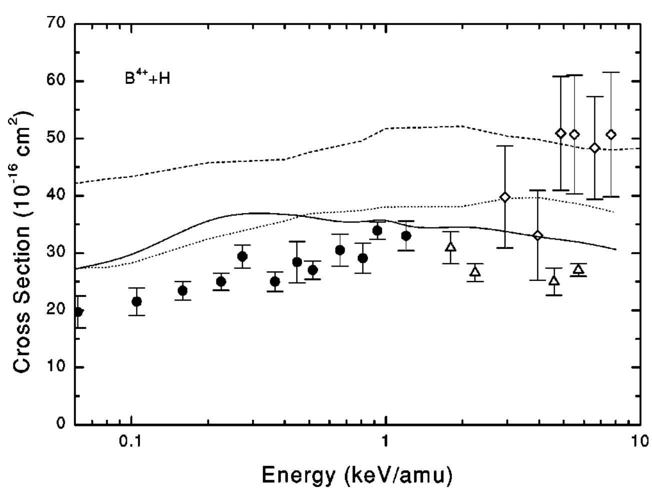

FIG. 1. Present total capture cross section results for $B^{4+}+H$ compared with other theories and with experiments. Theoretical results: solid line, present work; dashed line, Fraija *et al.* [7]; dotted line, Shimakura *et al.* [6]. Experimental results: solid circles, Pieksma *et al.* [2]; open up triangle, Crandall *et al.* [3]; open squares, Gardner *et al.* [4].

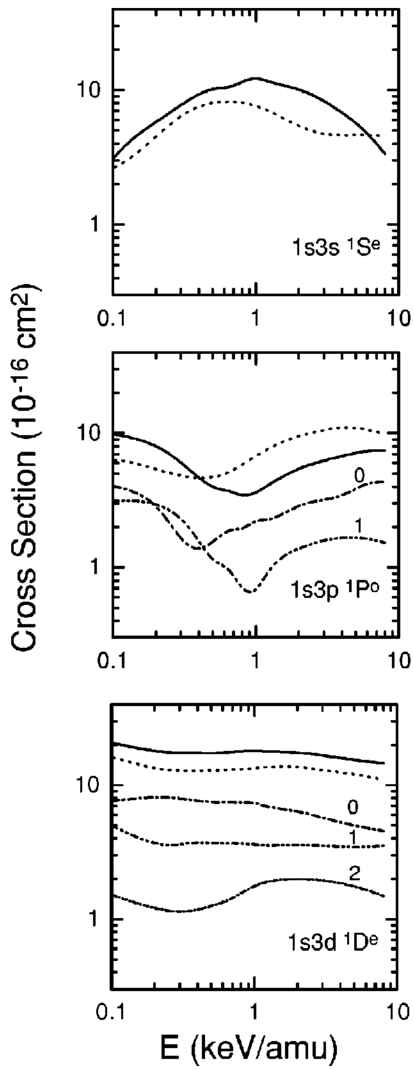

FIG. 2. Comparison of theoretical results for subshell electron capture cross sections to $1s3\ell$ singlet states for $B^{4+}+H$ collisions. Solid line, present work; dotted line, Shimakura *et al.* [6]. The magnetic subshell cross sections from the present calculations are also shown using dash-dotted lines with the magnetic quantum numbers indicated.

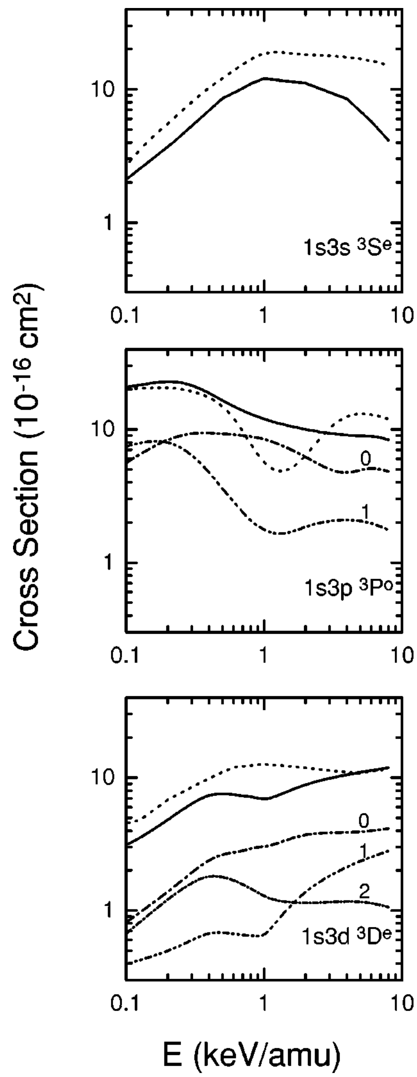

FIG. 3. Same as Fig. 2 but for triplet states.

Pieksma *et al.*, our results as well as those of Shimakura *et al.*, tend to overestimate, although the theoretical results are within the absolute errors of the experiment. For energies above 1 keV/amu, our total cross sections are smaller than those of Shimakura *et al.* and agree better with the experiments.

The experimental total electron capture cross sections do not provide a clear discrimination of the theoretical results between ours and those of Shimakura *et al.* It would be desirable to have subshell electron capture cross sections for comparison since the two calculations predict somewhat different subshell cross sections for a number of states. In Figs. 2 and 3 we compare the electron capture cross sections to $1s3s$, $1s3p$, and $1s3d$, for singlet states and triplet states, respectively. For $1s3s^1S$, the overall agreement between the two calculations is quite good. For $1s3p^1P$, the two calculations do not agree well. Each calculation shows a minimum, but the minima are at different locations. It turns out that the minimum exists in each magnetic substate cross section as well, as shown in the figure. (Note that the cross sections for M and $-M$ magnetic substates are identical.) The rapid variation of the M-subshell cross sections with energies implies that the polarization of the light emitted in the decay of the state will change rapidly in the 200–2000 eV/amu region. For capture to $1s3d^1D$ the results from the two calculations agree quite well and the M-subshell cross sections do not show strong energy dependence.

For the triplet states, our results for $1s3s^3S$ agree with those of Shimakura *et al.* below 1 keV/amu. Above this energy, ours is smaller. For electron capture to $1s3p^3P$, we have significant discrepancy with the results of Shimakura *et al.* where their cross section varies rapidly with collision energies while ours have a smoother energy dependence. On the other hand, we do show that the M-subshell cross sections vary more rapidly with energies. For capture to the $1s3d^3D$ state, our results show a kink. The kink is traced to the energy dependence of the M-subshell cross sections which are also shown in the figure.

In summary, we reported electron capture cross sections for the $B^{4+}+H$ collisions using the close-coupling method with atomic orbitals as basis functions. The goal initially was to resolve the discrepancy between the two molecular orbital calculations. Our results tend to support the calculations of Shimakura *et al.* By examining the MO curves and the coupling terms between the two molecular calculations, it appears that the dominant radial coupling terms from the calculation of Fraija *et al.* are larger than those from the work of Shimakura *et al.* for the triplet states. Unfortunately Fraija *et al.* did not report partial cross sections which would provide insight on the origin of the discrepancy. Comparing with the recent experimental data of Pieksma *et al.* the present results and those of Shimakura *et al.* are still about 20 to 30 % higher, but they are within the absolute errors of the data. Although the total cross sections vary slowly with energies, the subshell cross sections do show faster energy dependence where the present calculations and the results of Shimakura *et al.* differ for some of the states. We further notice that the magnetic substate cross sections exhibit even more pronounced energy dependence. Thus one can expect that measurement of the polarization of the emitted radiations from the decay of these states will have strong energy dependence as well. There are no subshell cross section measurements nor any photon spectroscopy experiments for this system to date.

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