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 and Gilbody [5] and with the molecular expansion calculation of Shimakura et al. [Phys. Rev. A 47, 3930 (1993)]. However, only very few experimental results are available so far.

In the 100–10 keV/amu energy range considered in this work, the dominant channels are single capture to the $1s3/2$ 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 $B^{2+}(1s)$, and all the $1s2/2$, $1s3/2$ and $1s4/2$ 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 Gardner et al. [4] and Gilbody [5], the reported cross sections differ by a factor of two at higher energies.

![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].](image-url)
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 $1s3s^1S$, $1s3s^3S$, $1s3p^1P$, and $1s3d^1D$, 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 $1s3d^3D$ 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 $^4\text{B}^+ + \text{H}$ 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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