

Classical and semiclassical calculation of cross sections of $\text{Be}^{4+} + \text{H}(1s)$ and $\text{H}(2s)$ collisions at 20, 100 and 500 keV/u

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A computational study of $\text{Be}^{4+} + \text{H}(1s)$ and $\text{H}(2s)$ collisions has been carried out. Two computational models have been employed: The Classical Trajectory Monte Carlo (CTMC) method and the numerical solution of the Time-Dependent Schrödinger Equation (GTDSE). The integral n and nl partial cross sections for H excitation and electron capture, obtained with both methods, will be compared for both systems.

In the case of $\text{H}(2s)$, we will compare our results at two energies: 20 and 100 keV/u. It will be shown that the CTMC, with an improved hydrogenic initial distribution, provides excitation cross sections in good agreement with the numerical calculation for excitation to $\text{H}(n)$ with $n > 3$. The agreement between the corresponding nl partial cross sections from both methods is less satisfactory at 100 keV/u. The electron capture cross sections calculated with the CTMC method do not depend on the initial distribution and show a reasonable agreement with the GTDSE ones, which supports the use of the CTMC method to calculate electron capture cross sections into highly excited levels and total cross sections.

Similarly, integral n and nl partial cross sections obtained with both methods for the case of $\text{Be}^{4+} + \text{H}(1s)$ will be shown. Classical total ionization cross sections will be also presented for both systems.