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Single-center technique for rearrangement processes[1] ALISHER KADYROV, ILKHOM ABDURAKHMANOV, IGOR BRAY, Curtin Univ of Technology — Recently, we developed a two-center convergent close-coupling (CCC) approach to ion-atom collisions. The approach requires large computing power since the rearrangement matrix elements describing the electron-capture channels demand more computational recourses. This fact somewhat limits the applicability of the two-center formalism to more complex targets. For such targets the formalism requires calculations of many different types of direct and rearrangement matrix elements and, as a result, becomes very challenging. Therefore, complex collision systems require the development of simpler but at the same time robust numerical methods. We present a simple approach to rearrangement collisions based on the computationally more convenient one-center formalism. To calculate electron-capture cross sections, we start from the exact definition of the electron-capture amplitude in terms of the total scattering wave function. However, we approximate the total scattering wave function with the one obtained from the one-center CCC approach. This way the total and state-resolved electron-capture cross sections can be calculated. Then the total ionization cross section can be obtained by subtracting the total electron-capture cross section from the total electron-loss cross section.

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