Ionization and fragmentation of methane by fast proton projectiles

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Theoretical treatment of the ionization of molecular targets by heavy charged particles is a challenging task. One of the main difficulties is the multi-centre nature of the target wave function. Previously, several perturbative and non-perturbative methods have been applied to describe the interaction of charged particles with atoms. Some of these models were adapted for collisions with molecular targets too [1, 2].

In our recent work [3] we have extended the perturbative CDW-EIS (continuum distorted wave with eikonal initial state approximation) model to describe net, single and multiple ionization of methane by fast proton projectiles. The CDW-EIS model regards the ejected electron as experiencing the combined field of the projectile and the target core-ion, thus taking into account the TCE (two centre effects), which play an important role in the differential electron emission. The initial state of the molecular orbitals were described by multi-centre Gaussian-type wave functions, using the Gaussian quantum chemistry program [4]. The continuum states of the outgoing electrons were calculated in the presence of the spherically averaged potential created by the nuclei and the target electrons. The obtained double differential and total ionization cross sections show good agreement with the experimental data. We found that these cross sections are sensitive to the value of the C-H distance, employed in the construction of the core potential of the molecule. Taking this value as 70% of the equilibrium C-H distance showed the best agreement between the theoretical and experimental data.

In our study we have also determined one-electron transition probabilities. The dependence of these quantities on the impact parameter reveals structures peculiar to a molecular target, especially in case of binary collision mechanisms. Good results have been obtained for the total ionization cross section, while in case of double ionization the calculations predict a stronger dependence on the impact velocity compared to the experimental data.

We have also considered the fragmentation of the methane molecule under the impact of proton projectiles. The cross sections for the production of the different molecular ions (CH_n^+, n = 1, 4) show a reasonable agreement with experimental measurements.

References:
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