Double differential cross sections for ion impact ionization of ammonia(NH_3) and methane (CH_4) molecules

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Synopsis We present a theoretical approach to calculate double-differential cross sections (DDCS) for single ionization of ammonia (NH_3) and methane (CH_4) molecules by the impact of proton at energies 0.25 MeV and 2 MeV respectively. The calculation are performed by the three-body formalism of three-Coulomb wave model (3C-3B). In the present formalism, the interaction of the projectile ion with the target is described by the Coulomb continuum wave functions in the initial channel. In the final channel, we have expressed the total wavefunctions as the product of pair-wise Coulomb wavefunctions among the ejected electron, projectile ion and the residual target ion, respectively.

Single ionization of atoms and molecules by bare ion impact is one of the more important challenges facing several fields of physics such as plasma physics, diagnostics for fusion in tokamaks, astro-physics, and irradiation of living matter etc. This process is also relevant to the study of the penetration of charged particles through matter. It is obvious that the interaction of heavy ions with multi-electronic molecular targets is very complex. For this reason, studies on the above mentioned processes should be such that they allow us to extract precise data without two many complications. Here, our attention is focussed on the calculation of double differential cross sections (DDCS) for the single ionization of CH_4 and NH_3 molecules by the impact proton in the framework of three body formalism of three Coulomb wave (3C-3B) model [1]. The transition matrix for single ionization may written as

$$T_{if} = \langle \psi_f^- | (V_{TP} + V_{Pe}) | \psi_i^+ \rangle$$

where ψ_i^+, the initial channel wavefunction is given by.

$$\psi_i^+ = \phi_i(\vec{r}_{Te}) \chi_i^+.$$

Here $\phi_i(\vec{r}_{Te})$ is the one-center molecular wavefunction [2] and χ_i^+ represent the Coulomb distortion. Here the initial bound state is distorted by the incoming projectile. The final state is characterised by the product of three coulomb wave function (3CW), called the BBK model [3]. We have displayed our computed results by angular distribution of DDCS for single electron ionization of NH_3 by a 250 keV proton in figure 1 at selective electron emission energies of 20, 50, 200 and 500 eV respectively.

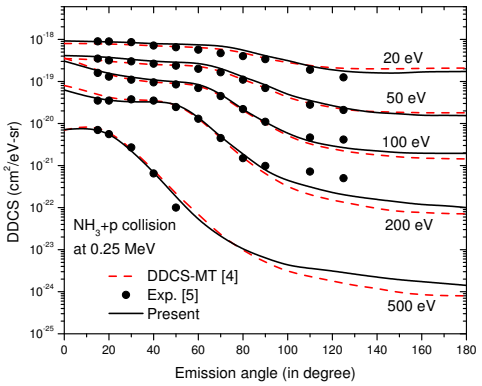

Figure 1. p-NH_3 collision at 0.25 MeV

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References

[1] A Mondal, T K Ghosh, C R Mandal and M Purkait 2016 *J. Phys.B: At.Mol. Opt. Phys.* ***49***, 245203

[2] C Champion, J Hassen and P A Hervieux 2004, *J. Chem. Phys.* ***121***, 9423

[3] M Brauner, J S Briggs and H Klar 1989, *J. Phys.B: At.Mol. Opt. Phys.* ***22***, 2265

[4] B Senger 1988, *Z. Phys. D* ***9***, 79

[5] D J Lynch et al 1976, *J. Chem. Phys.* ***64***, 2616

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