Total cross sections for proton induced electron emission from pyrimidine, THF, and TMP in a screened independent atom model

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Synopsis We report screened-independent-atom-model calculations for the net ionization of pyrimidine, tetrahyrdofuran (THF), and trimethyl phosphate (TMP) by proton impact.

There is a growing interest in collision-induced electron emission from biomolecules, in large parts triggered by applications, e.g., in biomedicine and astrochemistry. Given the complex structure of biomolecules, this constitutes a very challenging problem for theory and simplified approaches are needed.

One such approach is the independent atom model (IAM), in which the cross section for the molecular target is obtained by summing up atomic contributions. Based on the IAM, we recently introduced a model to account for geometric screening corrections by representing the cross sections for net ionization and net capture $\sigma_{\rm mol}^{{\rm net},x}$ (with x denoting ionization or capture) in ion-molecule collisions as weighted sums

$$\sigma_{\rm mol}^{{\rm net},x} = \sum_{j=1}^{N} s_j^x \sigma_j^{{\rm net},x}$$

of atomic cross sections $\sigma_j^{{\rm net},x}$ [1]. For each atom, the screening coefficient $0 \leq s_j^x \leq 1$ is determined as that fraction of the cross sectional area of the atom which is visible when picturing the molecular cross section as a structure of overlapping atomic cross sections and looking at this structure from the perspective of the projectile ion. The effective cross sectional areas are calculated using a pixel counting method (PCM). This is done for a number of relative orientations of the molecule with respect to the projectile beam direction and orientation-independent total cross sections are obtained by averaging the pixel count.

In this contribution, we present net ionization results for proton collisions with three molecules that resemble the structure of DNA constituents: pyrimidine ($C_4H_4N_2$), tetrahydrofuran (THF: C_4H_8O), and trimethyl phosphate (TMP: $(CH_3)_3PO_4$). Our results for pyrimidine (denoted by IAM-PCM) are compared with first Born with corrected boundary conditions (CB1) calculations and with experimental data in Fig. 1. The overall agreement is very good.

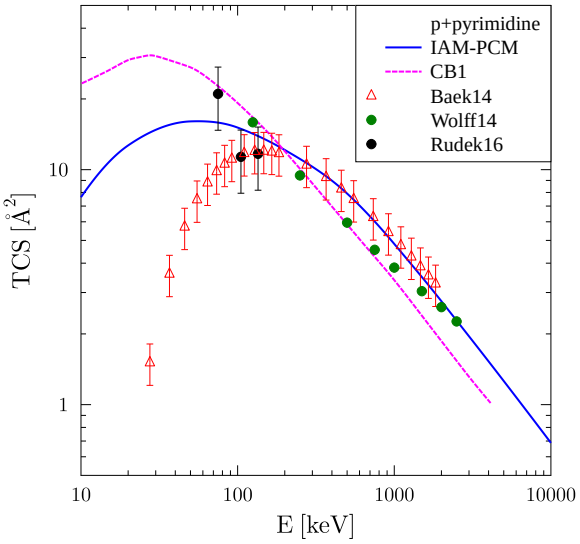

Figure 1. Total cross section for net ionization in p-$C_4H_4N_2$ (pyrimidine) collisions as a function of impact energy. Theory: IAM-PCM: present results, CB1: [2]. Experiments: Baek14 (equivelocity electron-impact cross sections): [3], Wolff14: [4], Rudek16: [2].

Similarly to what was found in Ref. [2] our cross sections for pyrimidine, THF, and TMP are approximately proportional to the number of valence electrons. A detailed analysis shows however that this apparent scaling happens in a rather subtle way for these three molecules and cannot be assumed to be true in general.

References

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