Electron Impact Ionization of CH_4 for Different Momentum Transfers

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Synopsis The electron impact single ionization of the outer valence orbital $1t_2$ of methane is investigated theoretically using an expansion on Generalized Sturmian Functions. Triple differential cross sections, calculated for several coplanar asymmetric geometries, are compared with other theoretical models and with two sets of relative experimental data (incident energy of 500 eV and 250 eV). An analysis with respect to the momentum transfer is presented. A double peak structure in the cross section binary region, a clear signature of the p-nature of the molecular orbital, is predicted for given kinematical conditions.

We study the electron impact ionization of CH_4 from the outer valence orbital $1t_2$. We calculate triple differential cross sections (TDCSs) for coplanar asymmetric geometries, and compare them with those obtained with other theoretical results (in an absolute scale), and with the relative scale measurements reported in Refs. [1] and [2], The binary to recoil ratio is analyzed as a function of the momentum transfer. Some of our results were already presented in Ref. [3].

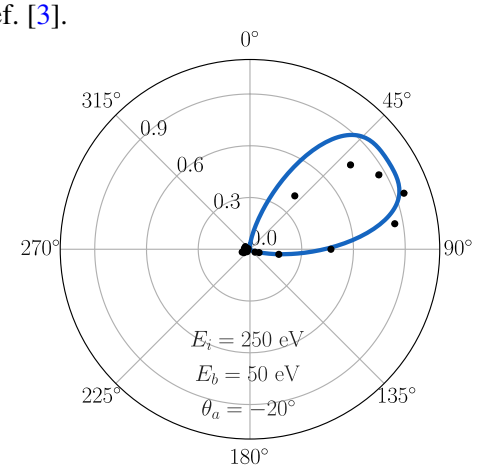

Figure 1. TDCS for $CH_4\left(1t_2^{-1}\right)$. Kinematic conditions: incident electron energy $E_i = 250$ eV, ejected electron energy $E_b = 50$ eV. Scattered electron detected at $\theta_a = -20°$. Experimental data from Ref. [2].

The TDCSs are obtained using a Sturmian approach with generalized Sturmian functions (GSFs) [4]. Such approach has been used to study, among others, single photoionization of atoms and small molecules [5]. In order to simplify the scattering problem, we use as molecular potential the one described through a static exchange approximation [7], make the one-center expansion, and take the initial state wave function from Ref. [6]. In a first Born approximation, the scattering wave function describing the ejected electron is expanded in a set of GSFs with appropriate Coulomb asymptotic conditions; this allows us to extract the scattering amplitude directly from the expansion coefficients, without the need of calculating a transition matrix element.

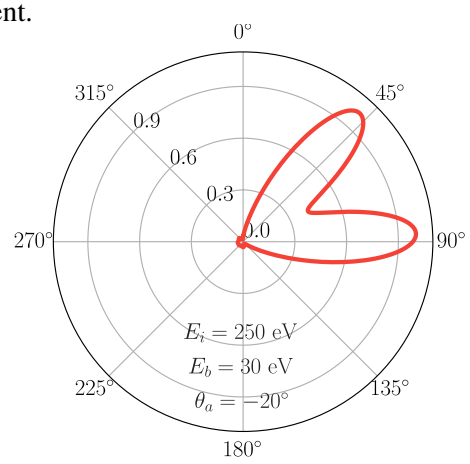

Figure 2. Same as Fig. 1, bur for ejected electron with $E_b = 30$ eV.

In Fig. 1 we present an example of one of the kinematical conditions reported in Ref. [2]. The binary peak is clearly dominant. As an extension (and a complement) to such experimental results, we consider other parameters; in the case presented in Fig. 2, for example, we predict a double peak structure in the cross section binary region, which is a clear signature of the p-nature of the molecular orbital.

References

[1] A. Lahmam–Bennani *et al.* 2009 *J. Phys. B: At. Mol. Opt. Phys.* **42** 165201

[2] Işik *et al.* 2016 *J. Phys. B: At. Mol. Opt. Phys.* **49** 065203

[3] C. M. Granados–Castro and L. U. Ancarani 2017, *Eur. J. Phys. D* in press

[4] D. M. Mitnik *et al.* 2011 *Comp. Phys. Commun.* **182** 1145; G. Gasaneo *et al.* 2013 *Adv. Quantum Chem.* **67** 153

[5] C. M. Granados–Castro *et al.* 2016 *Adv. Quantum Chem.* **73** 3

[6] R. Moccia 1964 *J. Chem. Phys.* **40** 2164

[7] L. Fernández–Menchero and S. Otranto 2010 *J. Chem. Phys.* **82** 22712

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