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2012 J. Phys.: Conf. Ser. 388 052078

(http://iopscience.iop.org/1742-6596/388/5/052078)

Journal of Physics: Conference Series **388** (2012) 052078 doi:10.1088/1742-6596/388/5/052078

Theoretical study of the simple (e,2e) ionization of the $1\pi_g$ molecular level of CO_2 by the introduction of a three-center continuum wave function

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Synopsis An appropriate closed analytical description of the state of an ejected electron from a linear three-center molecular target is presented resulting from the approximate solution of the Schrödinger equation for an unbound electron in the Coulomb field of three fixed charged nuclei.

We determine the multiply differential cross section (MDCS) of the (e,2e) simple ionization of the three-center collinear molecule CO_2 [1], where the ejected and scattered electrons are detected in coincidence, we employ, as in [2], a first order Born series perturbation procedure. The MDCS of a general out-of-plane detection of the scattered and ejected electrons in the case of an oriented linear CO_2 target is fourfold given by:

$$\sigma^{(3)}(\boldsymbol{\rho}) = \frac{k_s k_e}{2k_i} \int d\Omega_\rho (|T_{fi}^{m=-1}|^2 + |T_{fi}^{m=1}|^2),$$

where ρ is the internuclear axis, k_i, k_s and k_e represent respectively the moduli of the wave vectors of the incident, scattered and ejected electrons. m is the electronic magnetic quantum number corresponding the level from which the electron will be ejected. In the limits of the "frozen-core" model of the electronic structure of the target, the T matrix element $T_{fi}^m(\lambda_i^m, \lambda_f)$ involves only two electrons, the fast incident (scattered) and the bound (slow ejected) electrons. Here $\lambda_i^m(\mathbf{r}, \boldsymbol{\rho})$ is the wave function of the bound electron in the initial state in the body fixed system of reference for which we have used an extended three center basis set constructed on Slater type $1s$, $2s$, $2p$ and $3d$ orbitals [1]. $\lambda_f(\mathbf{r}, \boldsymbol{\rho})$ represents the wave function of the ejected electron in the final state:

$$\lambda_f(\mathbf{r}, \boldsymbol{\rho}) = \exp(\imath \mathbf{k}_e \mathbf{r})(2\pi)^{-3/2} M \times \prod_{j=O_1,C,O_2} {}_1F_1(-\imath \frac{Z_j}{k_e}, 1, -\imath[k_e r_j + \mathbf{k}_e \mathbf{r}_j]).$$

Recently experiments were performed [3] for the measurement of the TDCS of the simple (e,2e) ionization of the valence $1\pi_g$ level with fast electrons. We have thus performed our calculations for the same conditions as these experiments, namely, the detection of the fast $E_s = 500$ eV scattered electron at an angle $\theta_s = -6°$ with respect to the incidence direction in coincidence with the ejected electron of $E_e = 37$ eV. We observe that, the expected binary peak around the direction of the momentum transfer $\mathbf{K} = \mathbf{k}_i - \mathbf{k}_s$, i.e. $\theta_e = \theta_K$ is obtained only by our new extended basis [1]. The disagreement between experimental in the direction of the recoil peak was attributed in the past in the case of the ionization of N_2 [4] to the magnitude of the impact energy ($\sim$ 600 eV). In this regime, non-first-Born effects, which are not taken into account in our procedure are expected to start playing a role.

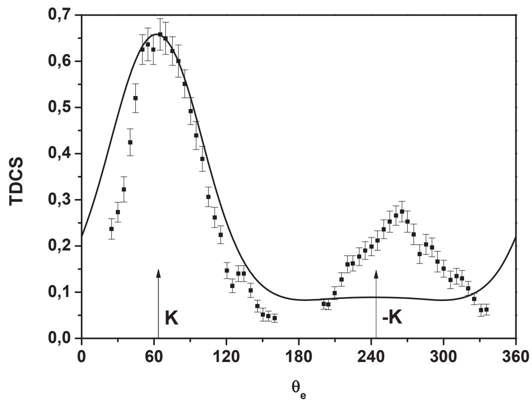

Figure 1. The variation of the TDCS in terms of the ejection angle θ_e. The experimental cross-section normalized on the binary pick of the theoretical cross-section with extended basis set.

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