The three-center parameterized continuum wave function and Dyson orbitals for the determination of the triply differential cross section of the simple ionization of CO_2 by electron impact

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The three-center parameterized continuum wave function and Dyson orbitals for the determination of the triply differential cross section of the simple ionization of CO_2 by electron impact

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Synopsis (e,2e) ionization of the linear three center CO_2 molecules by fast electron impact.

The triple differential cross section of the simple (e, 2e) ionization of CO2 is determined [1]. Its variation with the direction of the ejected electron is studied and compared to existing experimental [2] and a theoretical [3] results. The first-order perturbative Born procedure is applied where three-center Dyson type $1\pi_g$ orbital are employed for the bound electron. This orbital is obtained from coupled cluster results [4] by calculating the overlap between the N state of the target and the (N-1) state of the singly ionized ion [5] and constructed by linear combinations of Gaussian type orbitals. The ejected electron is described by a three-center continuum (ThCC) solution of the Schrödinger equation for a specific wave vector k satisfying the correct asymptotic boundary condition. This model given in the following form

$$\chi(\mathbf{k},\mathbf{r},\boldsymbol{\rho}) = \frac{\exp(\imath\mathbf{kr})}{(2\pi)^{3/2}} M_a\, {}_1F_1(\imath\alpha_a, 1, -\imath[kr_a + \mathbf{kr}_a]) \times M_b\, {}_1F_1(\imath\alpha_b, 1, -\imath[kr_b + \mathbf{kr}_b]) M_c\, {}_1F_1(\imath\alpha_c, 1, -\imath[kr_c + \mathbf{kr}_c]), \quad (1)$$

is an extension of the two-center continuum model developed in the past [6, 7], and lately applied to the ionization of CO_2 [3]. Here

$$M_j = \exp\left(-\pi\frac{\alpha_j}{2}\right)\Gamma(1-\imath\alpha_j), \quad j = a, c, b. \quad (2)$$

and $\alpha_j = -Z_j/k$ is the Sommerfeld parameter. Empirical values for the screening of the three nuclei of the target and for the Sommerfeld parameters of the three-center Coulomb continuum function are introduced.

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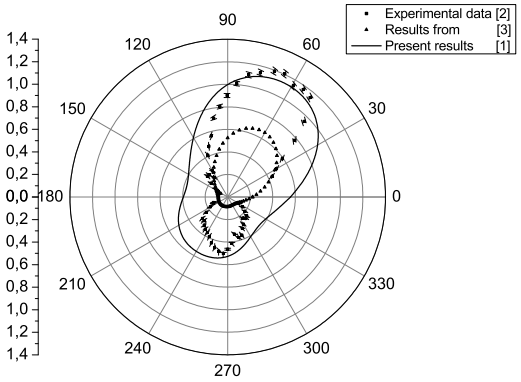

Figure 1. The variation, in polar representation, of the TDCS in terms of the ejection angle θ_e of the ionization of the $1\pi_g$ level of CO_2 for the empirical parameter $Z_a = 0.3$ for the final state. The energy of the scattered electron $E_s = 500eV$, detected at an angle $\theta_s = -6°$. The energy of the ejected electron $E_e = 37eV$.

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