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CALCULATIONS ON e^+ - N_2 IONIZATION

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ABSTRACT. Positron impact direct ionization cross sections are calculated for molecular nitrogen using two distorted wave models. The results are compared with the latest experimental and theoretical data available.

Keywords: *ionization, positron, nitrogen molecule*

INTRODUCTION

Positron collision phenomena with molecular targets have attracted much interest in the last decades. Potential improvements in applications like positron emission tomography provide an additional motivation for studying such collision phenomena. Experimental measurements for the ionization of several molecules by positrons have been carried out over the years. These molecules include simple ones like H_2 [1, 2], N_2 [3–5], O_2 [5, 6] or more complex ones like CO [5, 7], CH_4 [7] and CO_2 [7, 8]. For N_2 even differential studies are available [9].

On the theory side we studied the positron impact ionization of several molecules using distorted wave methods and a Gaussian-type multicenter molecular wavefunction [10,11]. We obtained a particularly good agreement with the experimental data for N_2 of ref. [3]. In another study [12] the Spherical Complex Optical Potential (SCOP) method was employed to calculate ionization cross section for several molecules, including N_2. These calculations also showed a good agreement with the experimental data [3].

Our present study is motivated by the publication of a new set of experimental data [4], which showed smaller cross section values than those measured in [3]. We introduce two models in order to calculate the direct ionization cross section

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for N_2 in collision with positron projectiles and compare the new results with the existent experimental and theoretical data.

THEORY

The ionization cross section of a molecular target can be calculated by integrating the triple-differential cross section

$$\frac{d^3\sigma}{d\boldsymbol{k_f} d\boldsymbol{k_e} dE_e} = \sum_n \frac{(2\pi)^4}{E_i} |f^n|^2 \quad (1)$$

which is a function of several physical quantities, like the projectile energy E_i, the energy of the ejected electron E_e and the scattering angles of the momenta of the outgoing particles. The sum in the above equation is performed over all occupied molecular orbitals. The scattering amplitude, f^n may be written as

$$f^n = \langle \phi_f(\boldsymbol{r_1})\phi_e(\boldsymbol{r_2})|V(r_{12})|\phi_i(\boldsymbol{r_1})\phi_b^n(\boldsymbol{r_2})\rangle \quad (2)$$

In equation (2), ϕ_i, ϕ_e and ϕ_f stand for the wavefunctions of the incident, ejected and scattered particles, while ϕ_b^n describes the bound state of the active electron represented as a Gaussian-type multicenter wavefunction [10]. The position vector of the active electron is $\boldsymbol{r_2}$, while $\boldsymbol{r_1}$ is the corresponding vector for the projectile. $V(r_{12})$ is the interaction potential between the projectile and the active electron. In order to separate the radial and angular part of the multicenter bound state, we expand it in terms of the Legendre polynomials for σ orbitals:

$$\phi_b^n(\boldsymbol{r_2}) = \sum_{l_b} y_{l_b}^n (r_2, R) P_{l_b}(\cos\omega_2) \quad (3)$$

where the expansion coefficient can be calculated as

$$y_{l_b}^n(r_2, R) = \frac{2l_b+1}{2} \int_{-1}^{1} d(\cos\omega_2) P_{l_b}(\cos\omega_2) \phi_b^n(\boldsymbol{r_2}) \quad (4)$$

Here, l_b stands for the orbital angular momentum quantum number of the bound state electron and R is the internuclear separation, while ω_2 is the angle between $\boldsymbol{R}$ and $\boldsymbol{r_2}$. The expansion cannot be applied directly to $\boldsymbol{\pi}$ orbitals due to the dependence on the $\boldsymbol{\varphi}$ angle of such states, hence a transformation to the centre of mass coordinates is applied before the expansion. Further, we apply a transformation

from the molecular frame to the laboratory frame. These transformations are all detailed in [10]. The wavefunctions of the free particles were expanded into partial wave series. Performing all these calculations the triple-differential cross section may be written as a sum of cross sections characterized by a certain angular momentum of the initial state with quantum numbers l_b and m_b:

$$\frac{d^3\sigma}{d\boldsymbol{k_f} d\boldsymbol{k_e} dE_e} = \sum_n \sum_{l_b m_b} \frac{(2\pi)^4}{E_i} \left| f^n_{l_b m_b} \right|^2 \tag{5}$$

where $f^n_{l_b m_b}$ is the partial scattering amplitude for orbital n. In the laboratory frame the molecule can have an arbitrary orientation, therefore we must average the cross section (5) over all possible orientations of $\boldsymbol{R}$. In order to obtain the total ionization cross section the differential cross section is integrated over the angles of the outgoing particles and the energy of the ejected electron.

In order to calculate the ionization cross section, we use two different approaches to the wavefunctions of the particles involved in the process. The first model, employs Coulomb waves for describing the outgoing particles, while the incoming projectile is described by a plane wave. This can be formalized in terms of the potentials 'seen' by the particles as follows:

$$\begin{cases} V_i = 0 \\ V_e = -\frac{1}{r} \\ V_f = \frac{1}{r} \end{cases} \tag{6}$$

Here, V_i, V_e and V_f are the potential energies for the incoming, ejected and scattered particles. We call the above ensamble of potentials the CCA (Coulomb-Coulomb Approximation) model, which refers to the Coulomb wave functions describing the outgoing particles, calculated by solving the radial Schrödinger equation for these potentials. The CCA model was first introduced for the description of the positron impact ionization of the helium atom [13]. In a second model, called TSS (Total Screening - Symmetric) we have calculated the wave functions of the free particles by employing the potentials detailed below:

$$\begin{cases} V_i = V_{nuclei} - V_{electrons} \\ V_e = -V_{nuclei} - V^-_{electrons} \\ V_f = V_{nuclei} - V^-_{electrons} \end{cases} \tag{7}$$

where V_{nuclei} , $V_{electrons}$ and $V^-_{electrons}$ are the spherically averaged potentials of the nuclei, electrons and residual electrons, respectively. These potentials provided distorted waves for the description of the continuum states by solving the radial Schrödinger equation. The averaging of these potentials was detailed in [11].

RESULTS

Figure 1 shows our CCA and TSS results compared with two of the existing experimental sets of data and with our previous theoretical cross sections and the theoretical calculations of [12]. The data of Bluhme et al [3] were obtained by normalizing the relative experimental cross sections to the theoretical cross sections of Krishnakumar et al [14], while the data of Cooke et al [4] were obtained by normalizing their relative cross sections to the electron impact cross sections measured with the same apparatus. We also show in Figure 1 the experimental data of Marler and Surko [5], which include contributions from dissociative ionization too, hence the large disagreement with the Cooke et al [4] experiment. Our models CPE, ES and TS were employed to calculate positron impact ionization cross sections for several molecules including N_2 [11]. All these models take into account the screening of the residual ion by the slower particle. If the scattered projectile is faster than the ejected electron, the model assumes that the ejected electron moves in the spherically averaged potential field of the nuclei and residual electrons, while the projectile is essentially described by a plane wave. For an ejected electron faster than the scattered positron, the electron moves in the averaged field of the nuclei-positron and the averaged field of the residual electrons, while the positron is described by a Coulomb wave. The difference between the 3 models is in the way they include the screening. ES (Electron Screening) considers the screening only for the ejected electron, TS (Total Screening) considers screening for all free particles, while CPE uses only Coulomb and plane waves. Figure 1 shows that the our ES and the SCOP calculations of [12] are in very good agreement with the experimental data of Bluhme et al [3]. In the CCA and TSS models both outgoing particles move in the field of the residual ion independent of their energies. In the CCA model the wavefunctions of the outgoing particles are Coulomb waves calculated by employing the potential of the residual ion, while in the TSS model both outgoing particles move in the spherically averaged potential of the nuclei and residual electrons. In ref. [13] model CCA was shown to produce ionization cross sections significantly lower than the CPE model. The same is seen in Figure 1. Both the CCA and TSS model provide cross sections which are lower than those of the CPE, ES and TS models. The height of the peak in the CCA and TSS curves is similar to the height of the peak in the experimental data of Cooke et al [4], but the theoretical peaks appear at an impact energy of 200 eV, while the experimental peak at 80-100 eV. This shift is probably the consequence of the simplification we employed in our models, that both particles move in the field of the residual ion, regardless of their energy.

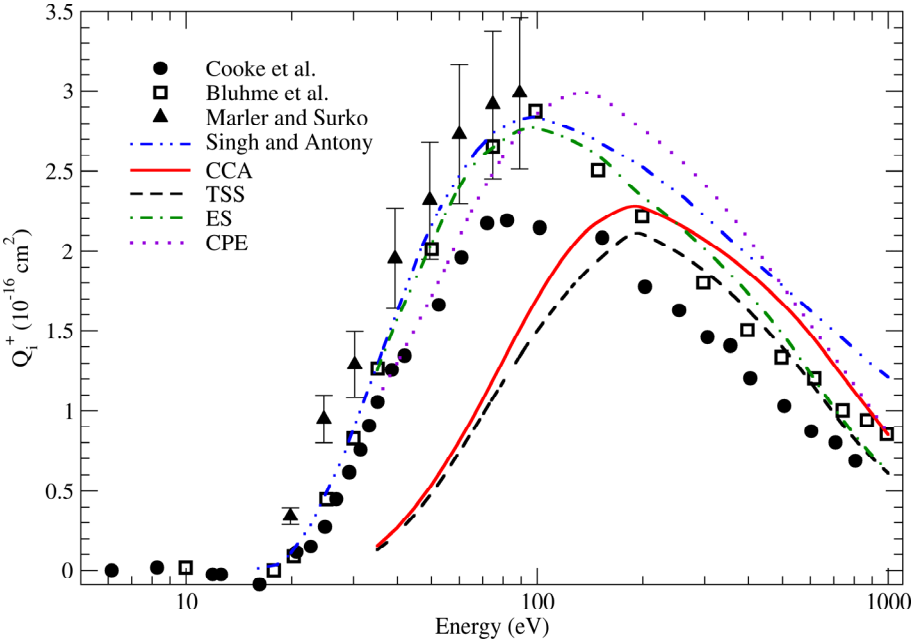

Fig. 1. Direct ionization cross sections for the N_2 molecule as a function of the impact energy of the positron. Our present results are provided by the CCA and TSS models, compared with the experimental data of [3] and [4] and the theoretical calculations of [12]. Our previously calculated results are also shown for the CPE, ES and TS models [11].

CONCLUSIONS

We have calculated direct ionization cross sections for the ionization of N_2 by positron projectiles using two distorted wave models and we compared them with the existent experimental data and theoretical calculations. This work was motivated by the discrepancy between the experimental cross sections of Cooke et al [4] and Bluhme et al [3]. Our current theoretical results, obtained by employing the CCA and TSS models, showed similar values for the ionization cross section as the data of Cooke et al [4], but the theoretical peaks were shifted relative to the experimental peak to higher impact energies. The best agreement between theory and experiment was obtained in the case of model ES and the experimental data of Bluhme et al [3].

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