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8 March 1999

PHYSICS LETTERS A

Physics Letters A 252 (1999) 321-327

Ionization–excitation of helium into the np ($n = 2$–5) states

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Received 29 October 1998; revised manuscript received 21 December 1998; accepted for publication 24 December 1998
Communicated by B. Fricke

Abstract

Cross sections for the simultaneous ionization and excitation to the np states ($n = 2$–5) of the helium atom by fast proton and antiproton impact have been calculated. We have applied the impact parameter method and have used second-order perturbation approximation. Electron correlation has been taken into account in the initial state but has been neglected in the final state. Our cross sections are compared to the experimental data. © 1999 Published by Elsevier Science B.V.

PACS: 34.50.Fa
Keywords: Multi-electron transitions; Ion-atom collisions; Ionization–excitation; Helium atom

1. Introduction

Over the last years several theoretical results [1–8] and experimental data [9–17] have been published on different two-electron processes in helium induced by charged particle impact. It has been made clear that taking into account the electron correlation is essential for a correct theoretical description of these transitions [18].

The less studied two-electron transition is the ionization–excitation. Only a few experimental data are available. The theoretical calculations are made mostly for electrons [2–5], and, except for the results of Kuplyauskene and Maknitskas [3], are much below the experimental data.

The experiments of Pedersen and Folkmann [11], Schartner et al. [12], Fülling et al. [13] and of Bailey et al. [14] for the ionization and excitation of helium to the np states revealed that cross sections got with electron projectiles are about a factor of two higher than those obtained with protons, for projectile velocities between 4 and 10 a.u. This difference cannot be reproduced neither by first-order calculations, neither in the independent-electron approximation.

We have previously published theoretical results for the simultaneous ionization and excitation to the $2p$ state of helium by fast proton and antiproton impact [19]. In that second-order perturbation approximation the initial and final states have been described by a properly symmetrized product of two one-electron wavefunctions. Electron–electron interaction has been taken into account only through the screening effects. The obtained results (similar to the other theoretical calculations [2,4,5]) were below the experimental data. We have obtained higher cross sections for negative projectiles than for equivelocity positive projectiles, but only by 5–8%, instead of the factor-of-two difference in experimental data.

PII S0375-9601(98)00963-3

Now we have completed these previous calculations by including electron correlation in the initial state. Beside the $2p$ final state of the helium ion we have considered the excitation to the $3p$, $4p$ and $5p$ states too.

2. Theory

The framework of our calculation is the impact parameter method. In this model the projectile moves on a classical straight-line trajectory. This method is suitable for proton and antiproton projectiles above 1 a.u. velocity (25 keV), but for electrons, because of their lower mass, this approximation gives reliable results only, if the energy of the projectile is much higher than the energy transfer. The average energy transfer in case of the ionization–excitation of helium is around 100 eV. The impact parameter approximation can be taken to be valid for electrons with velocities above 5 a.u. (350 eV). This is the reason why direct comparison with other theoretical results for electrons below 350 eV energy is not possible.

For the study of the evolution of the two-electron system we have applied second-order time-dependent perturbation theory. The method we use has been described in detail elsewhere [20,21] and has been applied for the double ionization [21] and double excitation [22] of helium.

The first-order probability amplitude for the transition of the electrons can be written as

$$a^{(1)} = -\mathrm{i}\int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f - E_i)t}\langle f|[V_1(t) + V_2(t)]|i\rangle. \tag{1}$$

Here $|i\rangle$ and $|f\rangle$ are the initial respectively the final two-electron states, E_i and E_f the energies of these states, while $V_1(t)$ and $V_2(t)$ stand for the two time-dependent projectile–electron interactions.

The second-order amplitude is obtained to be

$$a^{(2)} = -\sum_k \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f - E_k)t}\langle f|V_1(t)|k\rangle \int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{\mathrm{i}(E_k - E_i)t'}\langle k|V_2(t')|i\rangle$$
$$-\sum_k \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f - E_k)t}\langle f|V_2(t)|k\rangle \int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{\mathrm{i}(E_k - E_i)t'}\langle k|V_1(t')|i\rangle. \tag{2}$$

Here we have to sum up over the intermediate states $|k\rangle$ with energies E_k, the infinite number of eigenstates of the two-electron unperturbed Hamiltonian.

For the description of the initial state we have used configuration–interaction (CI) wavefunctions [23], which are written as a sum of products of one-electron orbitals

$$|i\rangle = \sum_l c_l |i_1^l\rangle |i_2^l\rangle. \tag{3}$$

The final state is described by a properly symmetrized product of two one-electron wavefunctions

$$|f\rangle = \frac{1}{\sqrt{2}}(|f_c'(1)\rangle|f_e'(2)\rangle + |f_e'(1)\rangle|f_c'(2)\rangle). \tag{4}$$

Here $|f_c'\rangle$ stands for the state of the ejected electron, while $|f_e'\rangle$ represents the excited state of the electron in the residual ion. The wavefunction of the bound electron is calculated neglecting the effect of the ejected electron, but the wavefunction of the free electron is calculated taking into account the screening potential created by the other electron.

Introducing the initial and final-state wavefunctions into the first-order amplitude (1), one gets a sum of products of overlap integrals and one-electron transition amplitudes

$$
\begin{aligned}
a^{(1)} = -\mathrm{i}\frac{1}{\sqrt{2}}\sum_l c_l \Bigg(& \langle f'_e(2)|i'_2\rangle \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f-E_i)t}\langle f'_c(1)|V_1(t)|i'_1\rangle \\
& + \langle f'_e(1)|i'_1\rangle \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f-E_i)t}\langle f'_c(2)|V_2(t)|i'_2\rangle + \langle f'_c(2)|i'_2\rangle \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f-E_i)t}\langle f'_e(1)|V_1(t)|i'_1\rangle \\
& + \langle f'_c(1)|i'_1\rangle \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f-E_i)t}\langle f'_e(2)|V_2(t)|i'_2\rangle \Bigg).
\end{aligned} \tag{5}
$$

The above amplitude can be associated to the generalized shake transition [18], which includes electron correlation into the asymptotic states (only into the initial state in this particular case).

In order to calculate the second-order amplitude, from the infinite number of the intermediate states we keep only the most important ones. These are assumed to be those reachable from the initial and the final state by a single-electron transition. Simplified, in the considered intermediate states one of the electrons is in its initial state, and the other one has reached the final state. Because in the case of the second-order amplitude the correlation is only a small correction (while the first-order amplitude of the two-electron transition is nonzero only because of the electron–electron interaction), in the calculation of the second-order amplitude we have taken into account only the basic, $1s^2 \equiv |i'_1\rangle|i'_2\rangle$ configuration for the description of the initial state. In this approximation one obtains for the second-order amplitude

$$
\begin{aligned}
a^{(2)} = & -\frac{1}{\sqrt{2}}\langle f'_e(2)|f_e(2)\rangle\langle i'_1|i'_1\rangle \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f-E_{ie})t}\langle f'_c(1)|V_1(t)|i'_1\rangle \int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{\mathrm{i}(E_{ie}-E_i)t'}\langle f_e(2)|V_2(t')|i'_2\rangle \\
& - \frac{1}{\sqrt{2}}\langle f'_c(2)|f_c(2)\rangle\langle i'_1|i'_1\rangle \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f-E_{ic})t}\langle f'_e(1)|V_1(t)|i'_1\rangle \int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{\mathrm{i}(E_{ic}-E_i)t'}\langle f_c(2)|V_2(t')|i'_2\rangle \\
& - \frac{1}{\sqrt{2}}\langle f'_e(1)|f_e(1)\rangle\langle i'_2|i'_2\rangle \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f-E_{ie})t}\langle f'_c(2)|V_2(t)|i'_2\rangle \int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{\mathrm{i}(E_{ie}-E_i)t'}\langle f_e(1)|V_1(t')|i'_1\rangle \\
& - \frac{1}{\sqrt{2}}\langle f'_c(1)|f_c(1)\rangle\langle i'_2|i'_2\rangle \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f-E_{ic})t}\langle f'_e(2)|V_2(t)|i'_2\rangle \int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{\mathrm{i}(E_{ic}-E_i)t'}\langle f_c(1)|V_1(t')|i'_1\rangle .
\end{aligned} \tag{6}
$$

Here E_{ie} stands for the energy of the intermediate state when one electron is in the $|i'_1\rangle$ (unscreened) initial state and the other one in the $|f_e(2)\rangle$ excited state, while E_{ic} represents the energy of the intermediate state described by the $|i'_1\rangle|f_c(2)\rangle$ configuration. The unprimed one-electron states are calculated with the other electron in the initial state, while the primed ones are calculated with the other electron in the final state, so the change in the screening (the relaxation of the orbitals [24]) is taken into account. The above expression is a simplified version of formula (22) from Ref. [21].

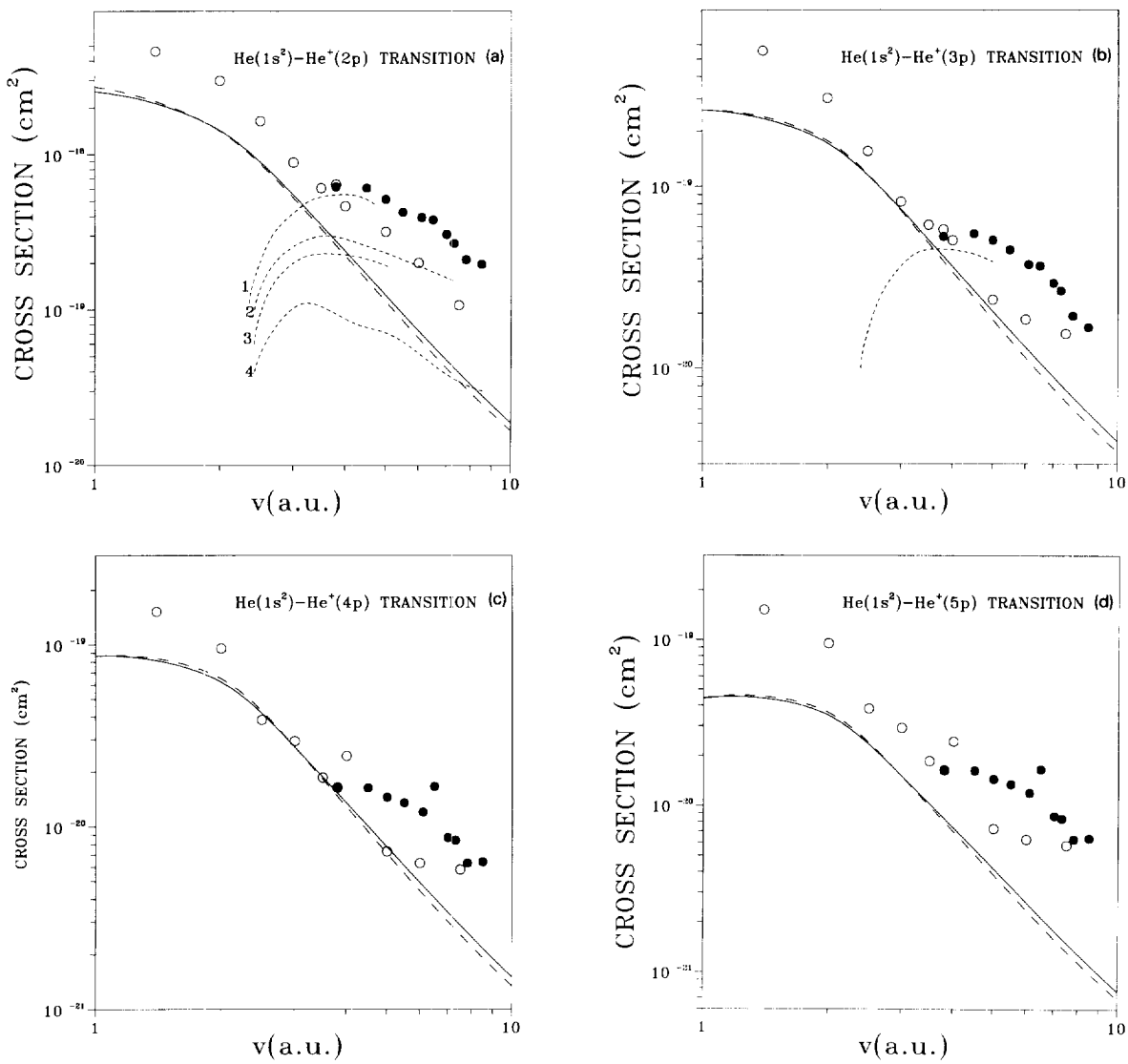

Fig. 1. Cross sections for the ionization–excitation of helium to the $2p$–$5p$ states by proton and antiproton impact as a function of the projectile energy. Solid lines stand for antiproton and long-dashed lines for proton projectiles. Short-dashed lines represent other theoretical calculations for equivelocity electrons (1: Ref. [3]; 2: Ref. [2]; 3: Ref. [4], 4: Ref. [5] in case of the excitation of the $2p$ state; and Ref. [4] for the $3p$ state). The experimental data of Bailey et al. [14] are represented by open circles (proton projectiles) and full circles (electron projectiles).

3. Results and discussion

We have performed the calculations for the ionization–excitation of helium to the $2p$, $3p$, $4p$ and $5p$ states by proton and antiproton impact. Cross sections are represented as a function of the projectile velocity in Fig. 1. Our previous results for the excitation of the $2p$ state have not been improved by the inclusion of the initial-state correlation. As Fig. 2 shows, the initial-state correlation has caused the decrease of the first-order contribution to the cross section above 2 a.u. projectile velocity. In the same figure is represented the second-

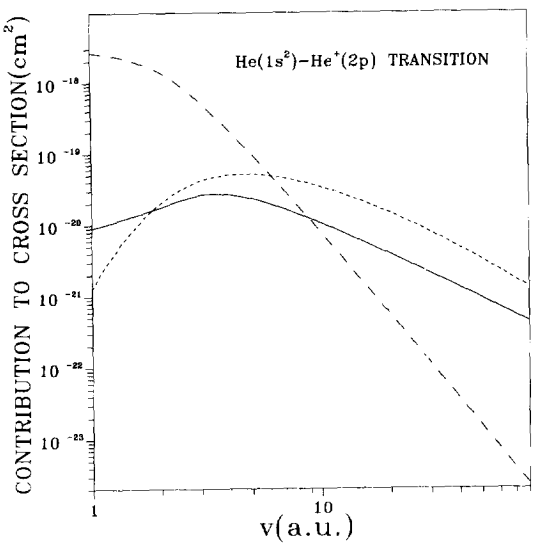

Fig. 2. The contribution of different mechanisms to the cross section of the ionization–excitation to the $2p$ state. Solid and short-dashed lines stand for the first-order contribution with and without initial-state correlation respectively, while the long-dashed line represents the second-order contribution.

order contribution to the cross section, taking into account only the basic configuration for the initial state. This contribution dominates over the first-order one up to 10 a.u. projectile velocity. Above this velocity the first-order contribution becomes more important.

As Fig. 1 shows, the interference between the first-order and second-order amplitudes leads only to a small difference between cross sections obtained with positive and negative projectiles, smaller than the experimental one [14]. We do obtain higher cross sections for antiprotons than for protons at higher velocities, in qualitative agreement with the experimental data, but at lower velocities (below 2 a.u.) the situation is reversed for every excited state. There is a similar situation in the experimental data for electron and proton impact, but this is due mainly to the lower mass of the electron. Experiments made with antiprotons could reveal if there exists a charge effect leading to lower cross sections for antiprotons than for protons below 2 a.u., as follows from our calculations.

The other theoretical results for the excitation of the $2p$ state [2–5] are only for electrons. These do not agree with each other and only the cross sections of Kuplyauskene and Maknitskas [3] are close to the experimental data. This suggests that cross sections are very sensitive to the used wavefunction, as was pointed out also by Dogan et al. [16]. In our calculations the initial state is accurately described, but the description of the final state needs improvement.

The description of the electron interactions in the final asymptotic state may be done by the use of correlated wavefunctions. Our guess is, that the static correlation in the final state is not very important, because one electron leaves the atom and the other remains bound. Probably the TS-1 mechanism, meaning a two-step on-energy shell transition (after the interaction with the projectile the first electron goes into an intermediate state, then interacting with the other both go into the final state), is more important in the case of the ionization–excitation than the final-state correlation effects in the one-step generalized shake mechanism.

Regarding the experimental data and the other theoretical results for electron impact we should note the comment of Dogan et al. [16]. In spite of the fact that the absolute cross sections obtained by different measurements lie within their combined errors, there is little agreement on the relative contributions of each np level. As for the theoretical calculations, sometimes a more complete description leads to worse results. The most sophisticated published calculation is that of Raeker et al. [4], with results much below the experimental

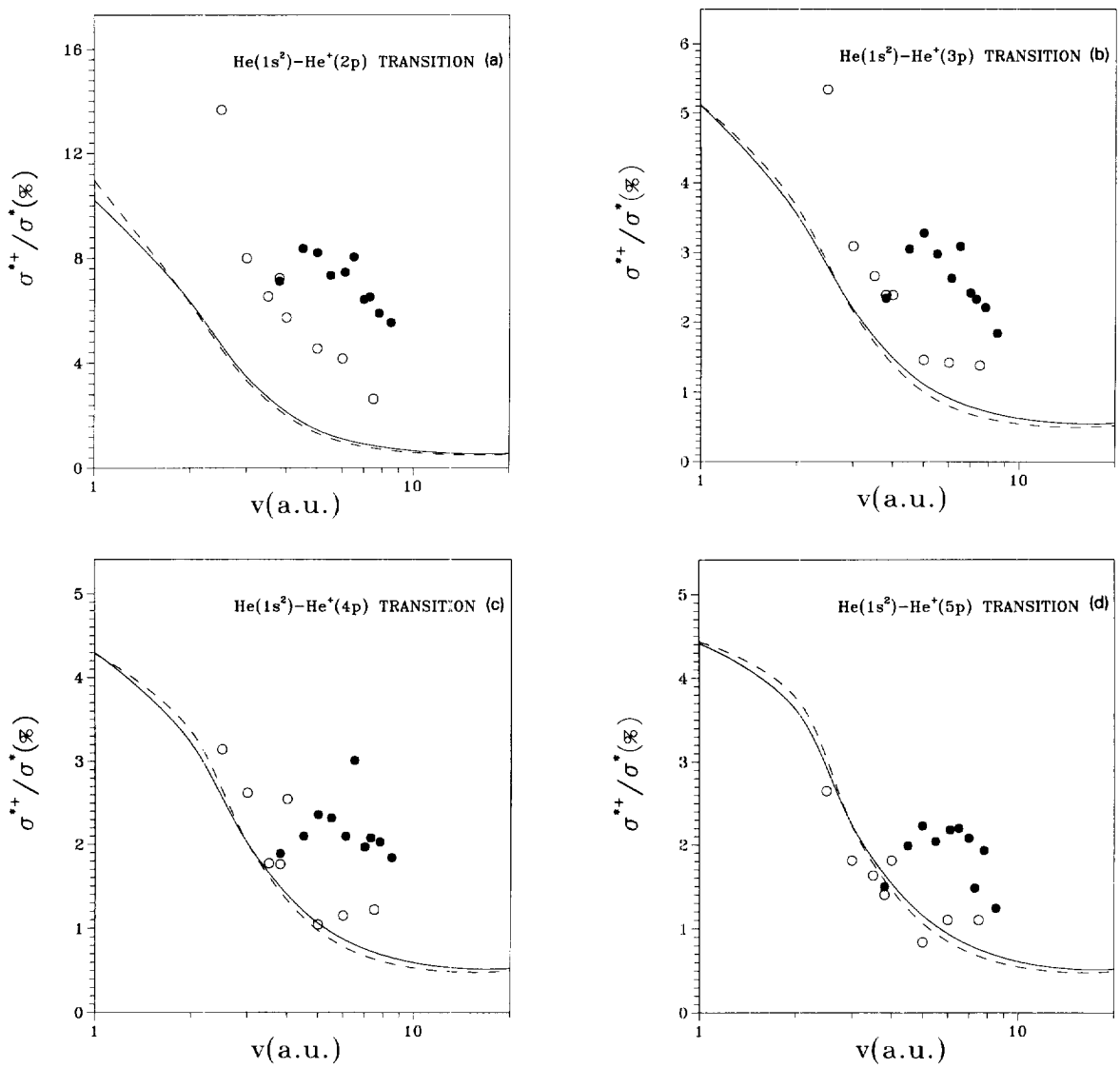

Fig. 3. The ratio of the ionization–excitation cross section to the single excitation for the $2p$–$5p$ states of helium by proton and antiproton impact as a function of the projectile velocity. Solid lines stand for antiproton and long-dashed lines for proton projectiles. The experimental data of Bailey et al. [14] are represented by open and full circles for proton and electron projectiles, respectively.

data. By a simpler description of the initial state [2], or by omitting channel coupling completely in the final state [3], the results are increased and so are closer to the experimental data.

The final-state description is poor in our calculation, too, and we do not bring light in the ionization–excitation problem by electron impact. However, our model is made mainly for heavy particle impact (or electron impact at high velocities), and for these kinds of projectiles there are no other theoretical results. Our calculation is the only one published for the ionization–excitation by proton and antiproton impact to a p state, reproducing qualitatively the difference in cross sections obtained for positive and negative projectiles.

Bailey et al. [14] have measured the ratio of the ionization–excitation to single excitation cross sections. Our

theoretical results along these experimental data are represented in Fig. 3. The transition of the second electron is due to the projectile–electron interaction (in the second-order amplitude) and electron correlation. At high projectile velocities only the latter dominates. Because of this the ratio of the ionization–excitation to single excitation cross section at high projectile velocities is a measure of the electron correlation. As can be observed in Fig. 3, the high-velocity limit of the represented ratio is about 0.5% for all the considered transitions. Unfortunately we cannot compare this value directly to the experiment, because there are experimental data only up to 8 a.u. velocity. But looking at the trend in the experimental data, the high-velocity limit of this ratio should be higher than our value.

4. Conclusions

We have calculated ionization–excitation cross sections of helium for the $2p$–$5p$ final states in case of proton and antiproton projectiles. Theoretical calculations for the excitation of $4p$ and $5p$ states are published for the first time. Our results are only in qualitative agreement with the experiment, but are the only ones reflecting the difference in cross sections obtained with positive and negative projectiles. In order to obtain more accurate results, electron correlation in the final state, and mainly the TS-1 mechanism should be included.

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