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POSITRON IMPACT IONIZATION OF ALKALI ATOMS

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ABSTRACT. The models CPE and CPE4, which were successfully used in positron impact ionization studies, are applied to positron impact ionization of Li, Na and K. This work produces total cross sections which are in agreement with the existing theoretical papers and shows the necessity for experimental measurements of these processes.

Keywords: *Positron collisions; Ionization of Atoms*

1. Introduction

Recent theoretical work on positron impact ionization of atoms and molecules was based on the use of several simple models related to CPE (Coulomb plus plane waves with full energy range). In these models the initial state of the atoms was represented in the Hartree-Fock approximation, while the incident and scattered positron and the ejected electron were described by plane waves and Coulomb waves. We found that a significant improvement in the performance of these distorted wave models was obtained by the inclusion in the final state representation of the electrostatic interaction between the ejected electron and scattered positron. The resulting CPE4 model was shown in [1] to produce good agreement with experiment for hydrogen and all the noble gases. For these targets the model CPE gives results which are not too different from the model CPE4 [2].

For positron impact ionization of alkali atoms there are no experimental data. However for Na and K there are measurements of the total cross sections [3,4], which combined with close coupling calculations of elastic, positronium formation and excitation cross sections [5,6] could in principle suggest the size of the ionization cross sections.

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In this paper we shall use the models CPE and CPE4 for positron impact ionization of alkali atoms. Our cross sections will be compared with other theoretical data available in the literature for lithium [7, 8, 9] and for sodium [10].

2. Theory

Using the partial-wave expansion and performing the angular integrations the electron impact ionization total cross section can be written as:

$$Q(Ei) = \frac{16}{\pi E_i}\int_0^{E/2} dEe \sum_{lilelf} \quad (2L+1) I(lilelf) \tag{1}$$

Here l_i, l_e, l_f represent the orbital angular momentum quantum numbers of the incident, ejected and scattered electrons respectively, E_i is the energy of the incident positron, E_e the energy of the ejected electron, and $E = E_i - I = E_e + E_f$ is the total energy of the scattered positron and ejected electron, where I is the ionization energy. $I\ (l_i\ l_e\ l_f)$ is given by Bransden *et al* [11] as a function of the direct scattering amplitude F:

$$I\ (l_i\ l_{ef}) = |F|^2 \tag{2}$$

The CPE model considers that both the ejected electron and scattered positron see the residual atomic ion as a positive single charge:

$$V_i = 0,\ V_e = -1/r \text{ and } V_f = 0 \text{ for } E_f > E_e \tag{3a}$$
$$V_i = 0,\ V_e = -2/r \text{ and } V_f = 1/r \text{ for } E_f < E_e \tag{3b}$$

The CPE4 model includes the attraction between the ejected electron and scattered positron:

$$Ve = -\frac{1 - Ee/Eef}{r} \text{ for } E_f > E_e \tag{4}$$

where E_{ef} is given by:

$$E_{ef} = E_e + E_f - 2\,(E_e\,E_f)^{1/2} \tag{5}$$

Thus in both models the incident positron is represented as a plane wave, while the ejected electron and scattered positron are represented as Coulomb or plane waves.

Details of the numerical work were presented in a previous paper [12], which dealt with positron impact ionization of He.

3. Results and discussion

Tables 1 presents total cross sections for positron impact ionization of the 2s shell of lithium. For the incident energies considered in this paper the contributions from the ionization of the inner shells is insignificant. In addition to our model CPE and CPE4 data we also show the results obtained with models DCPE and EDEC2 by Acacia *et al* [9] and by Mukherjee *et al* [8].

In the paper by Acacia *et al* [9] the model DCPE differs from our model CPE only in the incident channel where it considers the static potential of the target, while their model EDEC2 uses effective charges similarly to our model CPE4. The models used in the distorted wave calculations of Basu *et al* [7] and Mukherjee *et al* [8] are similar to our CPE model. The data of Refs. [7, 8] are available for impact energies equal and lower than 20 eV.

Our CPE data agree with the DCPE data of Ref. [9] and with the data of Refs. [7, 8], while our CPE4 cross sections agree with the EDEC2 data of Ref.[9].

It is interesting to note that for positron impact ionization of Li, Na and K the CPE4 cross sections are significantly larger than the CPE cross sections. This was not the case for other targets such as the noble gases atoms, where the difference was relatively small.

Table 1. Positron-lithium ionization cross sections (in $\pi\ a_0^2$)

E_i (eV)	CPE	CPE4	DCPE	EDEC2	Refs. [7,8]
20	5.63	11.90	5.0	12.5	5.8
30	5.30	9.41	4.2	11.4	
50	3.67	6.13	3.2	7.1	
70	2.40	3.41	2.2	5.2	
100	2.06	2.55	1.6	3.0	

Table 2 presents total cross sections for the positron impact ionization of the 3s shell of sodium. Our data is compared with the distorted wave calculation of Mukherjee *et al* [10], which describes each channel with static and polarization potentials. Our cross sections are significantly larger than those of Ref. [10].

Table 2. Positron - sodium ionization cross sections (in πa_0^2)

E_i (eV)	CPE	CPE4	Ref. [10]
15	8.51	18.14	5.6
20	9.37	19.64	5.4
30	8.16	15.56	4.6
50	5.74	8.29	
70	4.26	5.27	
100	33.05	3.56	

The paper by Hewitt *et al* [6] compares the experimental total cross sections for positron sodium scattering of ref. [3] with the close coupling calculation of elastic + positron formation and excitation cross sections. The agreement is very good but the experimental data are underestimated because in the experiment of ref.[3] it was not possible to discriminate between unscattered positrons and those elastically scattered through small angles in the forward direction. This is why this approach cannot help us to decide the correct size of the positron-Na ionization cross sections.

Table 3 presents total cross sections for the positron impact ionization of the 4s shell of pothasium. There are no other theoretical calculations for this process. As for Li and Na the CPE4 data are larger than the CPE data but the shape of the variation with the impact energy is similar.

Table 3. Positron - pothasium ionization cross sections (in πa_0^2)

E_i (eV)	CPE	CPE4
10	9.37	22.53
20	10.56	24.36
25	11.12	20.55
30	10.77	16.42
40	9.54	12.17
50	8.07	9.41
70	6.12	6.64
100	4.38	5.08

The paper by Hewitt *et al* [6] does the comparison of experiment and close-coupling theory also for the positron – pothasium system. The experimental points in this case are clearly above the theoretical curve particularly at impact energies smaller than 30 eV. Unfortunately from this paper we cannot have the exact suggested ionization cross sections but our data shown in Table 3 agree with the observation of Hewitt *el al* [6] that the ionization cross sections increase significantly at very low impact energies.

4. Conclusions

This work demonstrates that our models CPE and CPE4 produce positron impact ionization cross sections for lithium in agreement with the existing calculations. For all targets the ionization cross sections decrease for increased impact energies, with the CPE4 data being significantly higher than the CPE data.

Our ionization cross sections for sodium are larger than the ionization cross sections of Mukherjee *et al* [10]. For sodium and pothasium there are total cross section measurements and by eliminating the theoretical elastic, positronium formation and excitation estimates one could in principle obtain the size of the ionization cross sections. However the existing experimental cross sections are underestimated and therefore this avenue of experimental verification of our data is only partially useful. For pothasium this method leads to the observation that the ionization cross sections should increase at energies smaller than 30 eV, which agrees with our findings in Table 3.

Our work shows the necessity for experimental measurements of cross sections for the positron impact ionization of the alkali atoms.

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