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Total (complete) and ionization cross-sections of argon and krypton by positron impact from 15 to 2000 eV – Theoretical investigations

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Abstract. Considering interactions and scattering of positrons with argon (Ar) and krypton (Kr) atoms, we have calculated total cross-sections ($Q_\mathrm{T} = Q_\mathrm{el} + Q_\mathrm{inel}$) using complex spherical potentials for these systems. In positron–atom scattering it is difficult to bifurcate the ionization and cumulative excitation contained in the total inelastic cross-section. An approximate method called CSP-ic (complex scattering potential-ionization contribution) similar to electron–atom scattering has been applied to bifurcate ionization and cumulative excitation cross-sections at energies from the threshold to 2000 eV. Adequate comparisons of the present results are made, with available data.

Keywords. Positron scattering; total cross-section; complex potential.

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1. Introduction

Positron interactions with matter play important roles in many physical processes of interest. Examples include the origin of astrophysical sources of annihilation radiation, the use of positrons in medicine, the characterization of materials, and the formation of anti-hydrogen. Noble gas targets are chosen in the present investigation, because of their relatively simple atomic structure and the fact that they form mono-atomic gases. Two phenomena that can only occur for positron collisions are annihilation (appreciable only for energies much less than 1 eV) and positronium formation, which is an important factor in positron–gas scattering processes. It is interesting to compare the positron scattering from a target with the scattering of electrons, for which more extensive theoretical and experimental data are available.

Total cross-sections (TCS) for the scattering of positrons by argon (Ar) were measured by Canter *et al* [1], Kauppila *et al* [2], Coleman *et al* [3], Brenton *et al* [4], Griffith *et al* [5]. Dababneh *et al* [6,7] measured total cross-sections for positron-krypton (Kr) scattering. Karwasz *et al* [8] have measured total cross-sections for both Ar and Kr targets. Theoretical calculations were done by Baluja and Jain [9] using variable phase approach, and also by Reid and Wadehra [10] along the lines of their method for electron–atom/molecule scattering. Bluhme *et al* [11] have measured the total ionization cross-sections of positron impact with Ar and Kr. Mori and Sueoka [12] measured ionization and excitation cross-sections for helium, neon and argon targets. The single ionization cross-sections of Ar in positron impact were measured by Knudsen *et al* [13], Jacobsen *et al* [14] and Moxom *et al* [15]. Parcell *et al* [16] have determined all cross-sections of Ar and Kr using the method of polarized orbital and distorted waves up to 200 eV. Campeanu *et al* [17] have calculated ionization cross-sections of all noble gases using distorted wave model. Kara *et al* [18] have measured single and double ionization cross-sections of Kr. Fornari *et al* [19] measured the positronium formation cross-section of He, Ar and H_2. Marler *et al* [20] have measured positronium formation as well as ionization cross-sections of all noble gases. Recently, McEachran and Stauffer [21] have calculated elastic differential cross-sections of Ar using optical potential approach.

Krishnakumar and Srivastava [22] have measured the electron impact ionization of Ar and Kr. Vinodkumar *et al* [23] have calculated elastic, ionization and total cross-sections for all noble gases by electron impact except for radon, using spherical complex optical potential (SCOP) method along with CSP-ic approach in the energy region from ionization threshold to 2000 eV. We have recently examined the relative contribution of excitations and ionization in e^+-He, Ne, N_2 and CO scattering [24–26].

Now the present paper investigates positron scattering from Ar and Kr atoms.

2. Theory

For positrons, our theoretical method CSP-ic has been discussed in detail in [26] and is well explained for electrons in [27–30]. Therefore, only essential details of the calculations are given here. The method basically starts with positron scattering in complex potential as follows:

$$V(r, E_i) = V_{st}(r) + V_{pol}(r) + iV_{abs}(r, E_i). \tag{1}$$

In eq. (1), the real part consists of static potential $V_{st}(r)$ and polarization potential $V_{pol}(r)$ and imaginary part consists of absorption potential $V_{abs}(r)$ as described in [10]. The polarization potential we have used is described in [9]. The imaginary absorption term V_{abs} in the complex potential is an energy-dependent potential that accounts for all possible inelastic scattering channels cumulatively, and has the generic form, developed by [10,26,27]. Presently, for Ar and Kr we have fixed the energy gap Δ at E_{Ps} [25,26], as shown in table 1.

After generating the full complex potential of eq. (1) for a given positron–atom system, we treat it exactly in a partial wave analysis by solving the first-order differential equations for the real (δ_R) and imaginary (δ_I) parts of the complex phase shifts function. This is done using the variable phase approach of [31].

The total (complete) cross-sections Q_T obtained from the complex spherical potential are such that

$$Q_T(E_i) = Q_{el}(E_i) + Q_{inel}(E_i), \tag{2}$$

Table 1. Properties of the present targets used in the calculations.

Target	Ionization potential (I_p) [32] (eV)	Polarizability a_0^3	Energy gap Δ (eV)
Ar	15.76	11.08	8.96
Kr	13.99	16.76	7.19

where Q_{el} is the total elastic cross-section and Q_{inel} is the total (cumulative) inelastic cross-section at a given incident energy E_i. The total inelastic cross-section results from contributions of positronium formation, excitations and ionizations of the target atom, so that [26]

$$Q_{inel}(E_i) = Q_{Ps} + \sum Q_{exc} + \sum Q_{ion}. \tag{3}$$

The first term on the right-hand side of eq. (3) is positronium formation cross-section, second term is the sum over total discrete-excitation cross-sections for all accessible transitions in the atom, while the third term indicates the sum of the total cross-sections of all allowed (single, double etc.) ionization processes. Presently the last term will be simply denoted by Q_{ion}.

Now, we introduce the quantity

$$Q_{in}(E_i) = Q_{inel} - Q_{Ps}. \tag{4}$$

This is such that $V_{abs} = 0$, for $E_i \leq \Delta$. The cross-section Q_{inel} as calculated from our complex potential contains Q_{Ps}, $\sum Q_{exc}$ and Q_{ion} as in eq. (3).

To ascertain the contribution of Q_{ion}, first we have to subtract Q_{Ps} from the calculated Q_{inel} in order to obtain Q_{in}, i.e. ($Q_{ion} + \sum Q_{exc}$). It is possible to extend the usual complex potential formulation by a method called complex scattering potential-ionization contribution (CSP-ic) to deduce Q_{ion} from the Q_{in}. To employ the method presently for positrons, let us introduce a break-up ratio function,

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{in}(E_i)}. \tag{5}$$

Obviously $R = 0$ when $E_i \leq I$.

Let $E_{p'}$ denote the incident energy at which Q_{in} achieves its maximum value (table 2). R_p is the value of the above ratio at incident energy equal to $E_{p'}$ and it is found to be around 0.7 to 0.8 at the peak of Q_{inel} in the case of electrons, and we had $R_p = 0.7$ in e^--Ar, Kr scattering [23]. We adopt the same value here for the ionization of Ar, Kr by positron scattering.

Now, for the actual calculation of Q_{ion} from our Q_{in} we need $R(E_i)$ as a continuous function of energy E_i. Therefore, [23,27,28]

$$R(E_i) = 1 - f(U) = 1 - C_1\left[\frac{C_2}{(U+a)} + \frac{\ln U}{U}\right] \tag{6}$$

Table 2. Parameters of the present targets used in the calculations.

Target	Energy at the peak $E_{p'}$ (eV)	a	C_1	C_2
Ar	90	5.634	−0.965	−6.875
Kr	85	7.454	−1.093	−7.728

with

$$U = \frac{E_i}{I}. \tag{7}$$

Details of evaluation of parameters a, C_1 and C_2 are explained in [26].

The target properties, viz., ionization potential, polarizability, energy at the peak E_p and energy gap Δ, together with the three parameters of the present targets are listed in tables 1 and 2.

3. Results and discussion

Our interest in this paper is to calculate ionization cross-sections in the background of total (complete) scattering of positrons, inclusive of all the allowed channels. It is meaningful to calculate the important cross-section Q_{ion} from Q_{in} which is complicated by the presence of positronium formation. We have organized the discussion of our present results along with comparisons separately for Ar and Kr in two parts as follows.

3.1 *e^+-Argon scattering*

Let us start the discussion with the total (complete) cross-sections Q_T for positrons upon Ar atoms, for which the measurements over a wide energy range were done by Kauppila *et al* [2], as against the high-energy measurements of Brenton *et al* [4] and Griffith *et al* [5]. As can be seen from figure 1, the present results on Q_T of e^+-Ar scattering are satisfactorily matching with all the above experimental results [2–5]. Theoretical calculations for these targets were done by Baluja and Jain [9] and also by Reid and Wadehra [10]. Notably, at low energies, the shape of positron Q_T curve differs significantly from the electron Q_T curve of a given target due to difference in the interaction potentials, apart from the Ps formation. In this context, the present calculations on e^+-Ar system correctly reproduce the shape of the Q_T curve and the peak around 30 eV. We have compared the present Q_{el} cross-sections with calculated differential elastic cross-sections of McEachran and Stauffer [21] (by integrating their results) in table 3. For clarity, we have not compared our elastic cross-sections and also not shown our total inelastic cross-sections Q_{inel} in figure 1. We have tabulated these results in table 3.

Next we discuss our calculated ionization cross-sections. A good comparison is possible with the available data of Q_{ion} [13,14,16,17,20]. Below 100 eV, the present Q_{ion} seems to be a good match with other results. The measurements of Knudsen *et al* [13] are much higher at peak energy of Q_{ion}. Our present Q_{ion} are slightly higher at high energies. The results of Parcell *et al* [16] are also higher than other results at peak energy. The

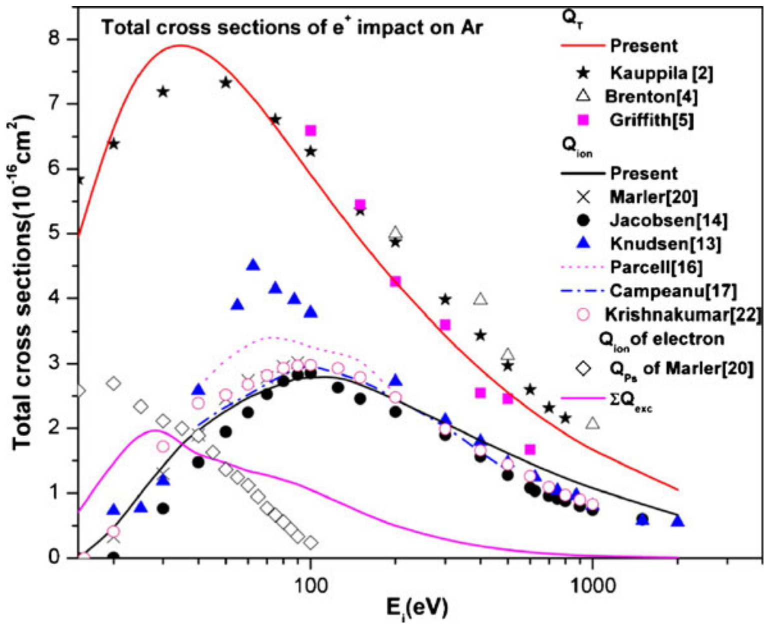

Figure 1. Various total cross-sections for e^+-Ar scattering. Red solid line: present Q_T; black star: Kauppila *et al* [2] Q_T; magenta square: Griffith *et al* [5] Q_T; white triangle: Brenton *et al* [4] Q_T; black solid line: present Q_ion; black filled circle: Jacobsen *et al* [14]Q_ion; blue filled triangle: Knudsen *et al* [13] Q_ion; cross: Marler *et al* [20] Q_ion; magenta dot: Parcell *et al* [16] Q_ion; blue dash–dot: Campeanu *et al* [17] Q_ion; pink open circle: Krishnakumar and Srivastava [22] Q_ion of the electron; white tetragonal: Marler *et al* [20] Q_Ps; magenta solid line: present $\sum Q_\mathrm{exc}$.

results of Campaneu *et al* [17] are in good accord with our results in 40–200 eV energy range. At high energies, our results of Q_ion are higher than other measurements. The electron impact ionization of Krishnakumar and Srivastava [22] is found to be higher than positron impact ionizations at low energies. At peak position, electron impact Q_ion are nearly equal to positron impact Q_ion.

The Ps formation cross-sections required to calculate the present Q_ion are adopted from Marler *et al* [20], and the same are also shown in figure 1. The lowest curve in this figure is $\sum Q_\mathrm{exc}$. Above 50 eV, the excitation sum exceeds the Ps formation cross-sections. Our present total excitation cross-sections are higher than Q_Ps above 50 eV. The peak of Q_in (not shown in figure for clarity) is found to be at 90 eV for present results on Ar.

3.2 e^+-*Krypton scattering*

Consider first the total (complete) cross-sections Q_T for Kr atoms. The experimental total cross-sections of e^+-Kr scattering were measured by Dababneh *et al* [6,7] and these are found to be close to our results at low and high energy. There is some disagreement at

Table 3. Present elastic, total inelastic and ionization cross-sections of Ar and Kr.

	Ar				Kr			
E (eV)	Present Q_{el}	Q_{el} of [21]	Present Q_{inel}	Q_{ion}	Present Q_{el}	Q_{el} of [21]	Present Q_{inel}	Q_{ion}
15	2.03	2.53	2.92	0	3.40		6.26	0.16
20	2.10	2.37	4.62	0.42	3.52	3.46	7.42	1.22
30	2.35	2.31	5.51	1.41	3.60		7.45	2.31
40	2.40		5.44	1.97	3.47		6.98	2.84
50	2.35	2.19	5.19	2.27	3.28		6.52	3.19
60	2.25		4.92	2.47	3.09	2.61	6.13	3.44
70	2.14		4.67	2.60	2.92		5.80	3.61
80	2.03		4.45	2.69	2.77		5.51	3.72
90	1.93		4.25	2.78	2.64		5.27	3.73
100	1.84		4.07	2.78	2.52		5.05	3.69
200	1.30	1.5	2.93	2.44	1.80		3.75	3.05
300	1.06	1.35	2.35	2.07	1.45		3.10	2.68
400	0.91		1.99	1.81	1.24		2.69	2.41
500	0.81		1.74	1.61	1.10		2.40	2.19
600	0.73		1.55	1.45	1.00		2.18	2.02
700	0.67		1.40	1.33	0.93		2.01	1.88
800	0.62		1.28	1.23	0.86		1.86	1.76
900	0.59		1.18	1.14	0.81		1.74	1.66
1000	0.55		1.10	1.06	0.77		1.64	1.57
2000	0.37		0.67	0.66	0.54		1.07	1.05

intermediate energy. The shape of our Q_T curve is similar to that of the theoretical results of [9] and [10]. For elastic scattering we have differential elastic cross-sections, only at 20 and 60 eV, which we got from McEachran and Stauffer [21]. In table 3, we have compared the integrated elastic cross-sections of [21] with our present elastic cross-sections Q_{el}.

In the case of Kr, in order to calculate Q_{in}, we subtracted Q_{Ps} of Marler *et al* [20] from our present calculated values of Q_{inel}. We have calculated the ionization cross-sections Q_{ion} using the CSP-ic method given in eqs (7)–(9), as in Ar. The peak position of Q_{in} (not shown in figure 2) of our present results is at 85 eV.

At peak position, our positron impact Q_{ion} are lower than the results of [18,20], but matches with calculated results of Campaneu *et al* [17]. Results of Marler *et al* [20] are higher than other results at peak position. At high energies, our positron impact Q_{ion} are higher than that of Kara *et al* [18]. We have shown that electron impact ionization of Krishnakumar and Srivastava [22] are close to our results at high energies. At low energies, the electron impact Q_{ion} are higher than positron impact Q_{ion}. The Ps formation cross-sections of Marler *et al* [20] are also shown in figure 2. The lowest curve of the present $\sum Q_{exc}$ exceeds Q_{Ps} after 40 eV.

The peak of Q_{in} (not shown in figure for clarity) is found to be at 85 eV for the present results on Kr. In table 3 we have shown present elastic (Q_{el}), inelastic (Q_{inel}) cross-sections and Q_{ion} of both targets.

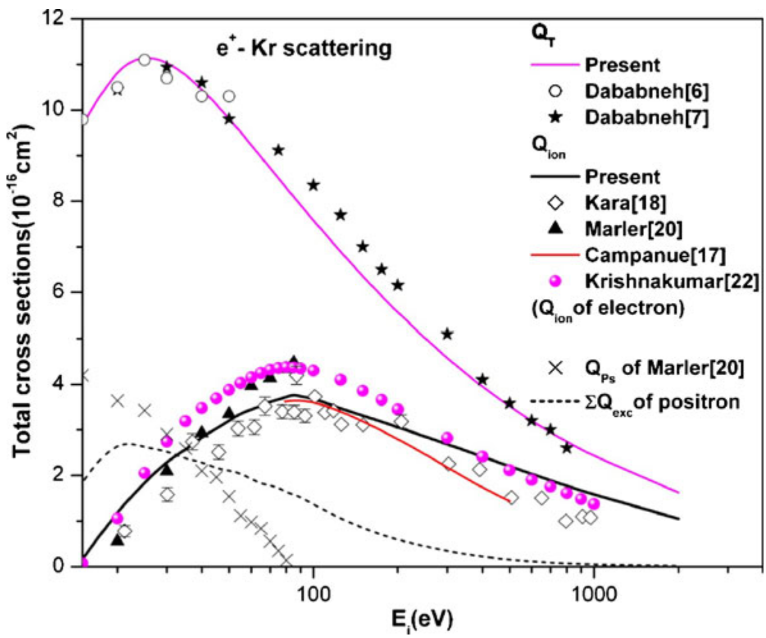

Figure 2. Various total cross-sections for e^+-Kr scattering. Magenta solid line: present Q_T; white circle: Dababneh *et al* [6] Q_T; black filled circle: Dababneh *et al* [7] Q_T; black solid line: present Q_{ion}; black filled triangle: Marler *et al* [20]; white tetragonal: Kara *et al* [18]; red solid line: Campeanu *et al* [17] Q_{ion}; magenta sphere: Krishnakumar and Srivastava [22] Q_{ion} of the electron; cross: Q_{Ps} of Marler [20]; short dash: present $\sum Q_{exc}$.

4. Conclusions

In conclusion, the application of complex potential formulation along with the present CSP-ic approximation enables us to calculate the major total cross-sections of positron impact with target atoms Ar and Kr. In this paper, the basic approach of complex positron scattering potential is employed to derive the important total cross-sections for Ar and Kr atoms which gives reasonably good agreement with other measurements [2,4–7], as discussed already. From the well-established CSP-ic method, we can calculate Q_{ion} successfully with $\sum Q_{exc}$ as an important by-product. We also find that in the case of Ar and Kr atoms, electrons are more ionizing compared to positrons at lower energies. Our present e^+ impact Q_{ion} of Kr is lower than e^- impact Q_{ion} at peak energy, whereas in the case of e^+ impact Q_{ion} of Ar, at peak and after the peak both are nearly equal. Our present results of Q_{ion} are well-matched with theoretical results of Campaneu *et al* [17] at peak region. But, some discrepancies are still there with experimental measurements.

Our present elastic cross-sections are slightly different from the results of McEachran and Stauffer [21]. The nature of our present elastic cross-sections of Ar and Kr is quite similar to Ne as in [25]. In view of the present results and comparisons made in this paper, it seems possible to prepare recommended data sets for various total cross-sections of positron scattering with Ar and Kr atoms.

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