

Elastic Scattering of Electron and Positron by Radium and Radon Atoms

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ABSTRACT

The Differential Cross Sections (DCS's), Total Cross Sections (TCS's) and Momentum Transfer Cross Sections (MTCS's) of electron and positron scattering by radium and radon atoms were calculated in the range of energy (5–500) eV using a total potential consisting of combining the static, exchange and polarization potentials at long distances. In addition, the correlation potential of Perdew–Zunger at short distances for electrons was used, as well as the correlation potential of Jain for positrons. The exchange potential for positrons was neglected. In this study, a good agreement with other experimental values and theoretical values of many investigators was found.

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الاستطارة المرنة للإلكترونات والبوزترونات بواسطة ذرات الراديوم والرادون

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الكلمات المفتاحية:

معادلة ديراك النسبية

استطارة الإلكترونات

استطارة البوزترونات

ذرات الراديوم

ذرات الرادون

الخلاصة

تم حساب المقاطع العرضية التفاضلية، والمقاطع العرضية الكلية وزخم الانتقال للمقاطع العرضية لاستطارة الإلكترونات والبوزترونات بواسطة ذرات الراديوم والرادون عند مدى الطاقة (5-500) إلكترون فولت باستخدام الجهد الكلي الذي يتكون من ربط الجهد المستقر وجهد التبادل وجهد الاستقطاب عند المسافات الطويلة وجهد الارتباط للباحثين برادون – زنكر عند المسافات القصيرة للإلكترونات بالإضافة إلى ذلك جهد الارتباط للباحث (جين) في حالة البوزترونات، مع حذف جهد التبادل؛ وجدنا في هذه الدراسة توافق جيد مع القيم العملية والنظرية لعدة باحثين.

1. INTRODUCTION

The study of electrons and positrons scattering from neutral atoms provides a fundamental knowledge for the theoretical understanding of this process. This can lead to understanding the technological potential of light-temperature plasmas, especially after the development of X-ray lasers. The analysis of such plasmas requires knowledge of the processes of elastic scattering, excitation and ionization of atomic and ionic targets [1]. From the literature review [2–5], the Differential Cross Sections (DCS's), Total Cross Sections (TCS's) and Momentum Transfer Cross Sections (MTCSs) for electrons and positrons scattering from atoms were studied by using a total potential $V(r)$. The similarities and differences between electrons and positrons means that the positron scattering is useful to test the mechanism which is used to study the scattering processes.

Experimental measurements for the scattering of positrons by atoms are not only interesting, since they might, also, involve the interactions of antimatter with matter. In addition, it helps to provide a better understanding of the scattering of electrons by atoms, which is considered a very important method in many different fields of science and technology, such as plasma physics, including fusion research, laser development, gaseous electronics, astrophysics, aeronomy [2].

The similarities among electrons and positrons in term of their masses, spin and magnitude of charge, suggest a consistent way to describe the model potential should consist of these quantities. The differences between electrons and positrons are presented in the sign of the charge, the possibility of positronium formation and the fact that positron projectiles are distinguishable from the electrons of the atom target, whereas electrons are not. Elastic scattering is very important in many fields, including the physics of stars and plasmas [6] and collaboration between experimental and theoretical research areas that deal with determining DCS's, TCS's and MTCS's. In this paper, the theoretical study of elastic electrons and positrons scattering by radium and radon

atoms was achieved using the relativistic wave functions obtained from the Multi configuration Dirac–Fock (MCDF) method to perform the calculations. The relativistic Dirac equation is solved for both elastic and inelastic scattering of electrons and positrons of different energies. The total potential $V(r)$ for electrons is represented as:

$$V(r) = V_{st}(r) + V_{ex}(r) + V_{cor}(r) + V_{pol}(r) \quad (1)$$

It consists of a static potential $V_{st}(r)$ which is obtained from the Dirac–Hartree–Fock–Slater (DHFS) function [7]. $V_{ex}(r)$ is the exchange potential obtained from the Free Electron Gas (FEG) model [8], $V_{pol}(r)$ is the polarization potential at large distances and the correlation potential $V_{cor}(r)$ at short distances. For positrons, the total potential $V(r)$ is represented as:

$$V(r) = V_{st}(r) + V_{cor}(r) + V_{pol}(r) \quad ---(2)$$

The term $V_{ex}(r)$ for positrons was omitted.

2. Theory

The Dirac equation for the motion of the projectile electron with the velocity v in a central field is given by [1]:

$$H_0 \psi(r) = E \psi(r) \quad ----(3)$$

Here ,

$$H_0 = c \alpha \cdot P + \beta mc^2 + V(r) \quad ---(4)$$

Where, $E = m_0 \gamma c^2 = E_i + m_0 c^2$ is the total energy, m_0 is the rest mass of the matrices .The relativistic wave function $\psi(r)$ includes the four components spinor with quantum numbers k , m which describes the motion of the projectile, and $\gamma = 1/\sqrt{(1 - v^2/c^2)}$, where c is the velocity of light in vacuum , E_i is the kinetic energy of the incident particle, α and β are the usual 4x4 Dirac scattered electron that is given by [1].

$$\psi_{Ekm}(r) = \frac{1}{r} \begin{pmatrix} P_{Ek}(r) & \Omega_{km}(\hat{r}) \\ iQ_{Ek}(r) & \Omega_{-km}(\hat{r}) \end{pmatrix} \quad ---(5)$$

Here, $P_{Ek}(r)$ and $Q_{Ek}(r)$ represent the radial parts of the large and small components of the scattered wave function and $\Omega_{km}(r)$ is the spherical spinors .The relativistic quantum number , $k = (\ell - j) (2j + 1)$, where j

and ℓ are the total and orbital angular momentum quantum numbers that are both determined by the value of k as : ($j = [k] - \frac{1}{2}$, $\ell = j + \frac{1}{2}$) . Here the elastic interactions of an electron or positron are considered having kinetic energy E_i , with a target atom of atomic number Z_0 It has been assumed that the charge distribution of the target is spherically symmetric and the effective interaction between a projectile at r and the target is described by means of an optical model potential as given by [1]

$$V(\bar{r}) = V_{st}(\bar{r}) + V_{ex}(\bar{r}) + V_{cp}(\bar{r}) + V_{abs}(\bar{r}) \quad \text{---(6)}$$

$V_{st}(\bar{r})$ is the electrostatic interaction potential , $V_{ex}(\bar{r})$ is the exchange potential, $V_{cp}(\bar{r})$ is the correlation polarization and W_{abs} is the absorption potential. The calculation of this project deals with elastic scattering, so, the absorption part of eq. (6) will vanishes, therefor eq. (6) becomes [1]:

$$V(\bar{r}) = V_{st}(\bar{r}) + V_{ex}(\bar{r}) + V_{cp}(\bar{r}) \quad \text{---(7)}$$

with this approximation, the structure of the target is fully characterized by the charge distributions . The electronic densities $\rho(r)$ of free atoms used in the present calculations were generated by means of the multi-configuration Dirac – Fock code of Desclaux [2] . The potential energy of the projectile at a distance r from nucleus of the target is given by [1] :

$$V_{st}(\bar{r}) = Z_0 e^2 \left(\frac{1}{r} \int_0^r \rho(r') \cdot 4\pi r'^2 dr' + \int_r^\infty \rho(r') \cdot 4\pi r' dr' \right) \quad \text{---(8)}$$

where, e is the absolute value of the electron charge and Z_0 is the charge of the projectile. When the projectile is an electron , it is necessary to account for the accuracy of rearrangement collision is required in which the projectile exchanges place with an atomic electron. In the present calculation, the exchange potential of Furness and McCarthy [3] were used which is derived directly from the expression of non-local exchange interaction by using a WKB-like approximation for the wave function [1]:

$$V_{ex}(\bar{r}) = \frac{1}{2} [E - V_{st}(\bar{r})] - \frac{1}{2} \{ [E - V_{st}(\bar{r})]^2 + 4\pi a_0 e^4 \rho(\bar{r}) \}^{\frac{1}{2}} \quad \text{---(9)}$$

where a_0 is the Bohr radius for positron and the exchange potential vanishes. In the present work, the correlation-polarization potential as a combination of the parameter for free long range polarization potential and Local Density Approximation (LDA) correlation potential was used accordingly to the following :

$$V_{cp}(r) = \begin{cases} V_{cor}(r) & \text{if } r < r_c \\ V_{pol}(r) & \text{if } r \geq r_c \end{cases} \quad \text{---(10)}$$

where r_c is the outer radius at a short range $V_{cor}(r)$ and long range $V_{pol}(r)$ first intersect for a slow projectile causes the polarization of the charge cloud of the target atom and the induced dipole moment acts on the projectile to turn it back . When the projectile is far from the atom , the polarization potential energy can be approximated by following Buckingham potential [4]

$$V_{POL}(\bar{r}) = - \left[\frac{\alpha_D e^2}{2(r^2 + d^2)^2} \right] \quad \text{---(11)}$$

where α_D is the dipole polarizability of the target atom [4], and d is a cut off parameter, which was utilized to prevent the polarization potential from diverging at $r = 0$, where it is given by the expression of Mittleman and Watson [5] as:

$$d^4 = \frac{1}{2} \alpha_D a_0 Z^{-1/3} b_{pol}^2 \quad \text{---(12)}$$

Where a_0 is an atomic unit that assumed equal to one and b_{pol} is an adjustable energy-dependent parameter, which can be determined by fitting the DCS's at small angles [6] .

The correlation potential was calculated as a function of the density parameter r_s which be given by [6] :

$$r_s = 1/a_0 \left[\frac{3}{4\pi\rho(r)} \right]^{\frac{1}{3}} \quad \text{---(13)}$$

For electrons, the parameterization of the correlation potential given by Perdew and Zunger [7] is adopted, for $r_s < 1$:

$$V_{cor}(r) = -\frac{e^2}{a_0} [0.0311 \ln(r_s) - 0.058 + 0.0013r_s \ln(r_s) - 0.0084r_s] \quad \text{---(14)}$$

And for $r_s \geq 1$:

$$V_{cor}(r) = -\frac{e^2}{a_0} \beta_0 \frac{1 + (\frac{7}{6})\beta_1 r_s^{1/2} + (\frac{4}{3})\beta_2 r_s}{(1 + \beta_1 r_s^{1/2} + \beta_2 r_s)^2} \quad \text{---(15)}$$

where:

$$\beta_0 = 0.1423 ; \beta_1 = 1.0529 ; \beta_2 = 0.3334$$

For positrons in this study, we use the parameterization of the correlation potential that was proposed by Jain [8], where for $r_s < 0.302$:

$$V_{cor}(r) = \frac{+e^2}{a_0} \{ 0.5835 + 0.91 r_s - \frac{1}{2} + [0.00255 \ln r_s - 0.0575] \ln r_s \} \quad \text{---(16)}$$

For $0.302 \leq r_s < 0.56$:

$$V_{cor}(r) = \frac{e^2}{a_0} [0.461525 - 0.04549 r_s^{-2}] \quad \text{---(17)}$$

For $0.56 \leq r_s < 8.0$:

$$V_{cor}(r) = \frac{e^2}{a_0} \left[-\frac{4.3637}{(r_s + 2.5)^3} + \frac{-6.5755 + 0.4776 r_s}{(r_s + 2.5)^2} + \frac{1.43275}{r_s + 2.5} - 0.3149 \right] \quad \text{---(18)}$$

And for $r_s \geq 8.0$:

$$V_{cor}(r) = \frac{e^2}{a_0} [-15375.8679 r_s^{-6} + 44.5047 r_s^{-3} - 0.262] \quad \text{---(19)}$$

So, the Dirac equation can be reduced to a set of two equations [1] :

$$\frac{dP_{Ek}}{dr} = -\frac{k}{r} P_{Ek} + \frac{E - V(r) + 2m_0 c^2}{\hbar} Q_{Ek}(r) \quad \text{---(20)}$$

And

$$\frac{dQ_{Ek}}{dr} = -\frac{E - V(r)}{\hbar} P_{Ek} + \frac{k}{r} Q_{Ek}(r) \quad \text{---(21)}$$

The relativistic quantum number k is defined as $k = (l - j)(2j + 1)$, where j and l are the total and orbital angular momentum quantum numbers that are both determined by the value of k ; $j = |k| - 1/2$. Therefore, the spherical waves should be normalized so that the upper-component radial function $P_{Ek}(r)$ oscillates asymptotically with unit amplitude. For finite-range fields and $r \rightarrow \infty$, the result is [9]:

$$P_{Ek}(r) = \sin(kr - l\frac{\pi}{2} + \delta_k) \quad \text{---(22)}$$

It was noticed that, the scattering information is determined from the asymptotic form of the large component P_{Ek} of the scattering wave function expressed in terms of the phase shift δ_k . Equations (20) and (21) are satisfying the asymptotic condition of eq.(22) which were solved numerically using the subroutine package RADIAL [10] by the relativistic partial wave analysis, after that the relativistic phase shift

δ_k are obtained then we can calculate the other scattering observables to complete the information of scattering processes, where the direct and spin – flip scattering amplitudes [1], are respectively given by :

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \{ (l+1) [\exp(2i\delta_{k=-l-1}) - 1] + l [\exp(2i\delta_{k=l}) - 1] \} P_l(\cos\theta) \quad \text{---(23)}$$

And

$$g(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} [\exp(2i\delta_{k=l}) - \exp(2i\delta_{k=-l-1})] P_l^1(\cos\theta) \quad \text{---(24)}$$

Here, $P_l(\cos\theta)$ and $P_l^1(\cos\theta)$ denote the Legendre polynomial and associated Legendre functions respectively, k is the relativistic wave number of the projectile. So, The differential cross-section is given by [1] :

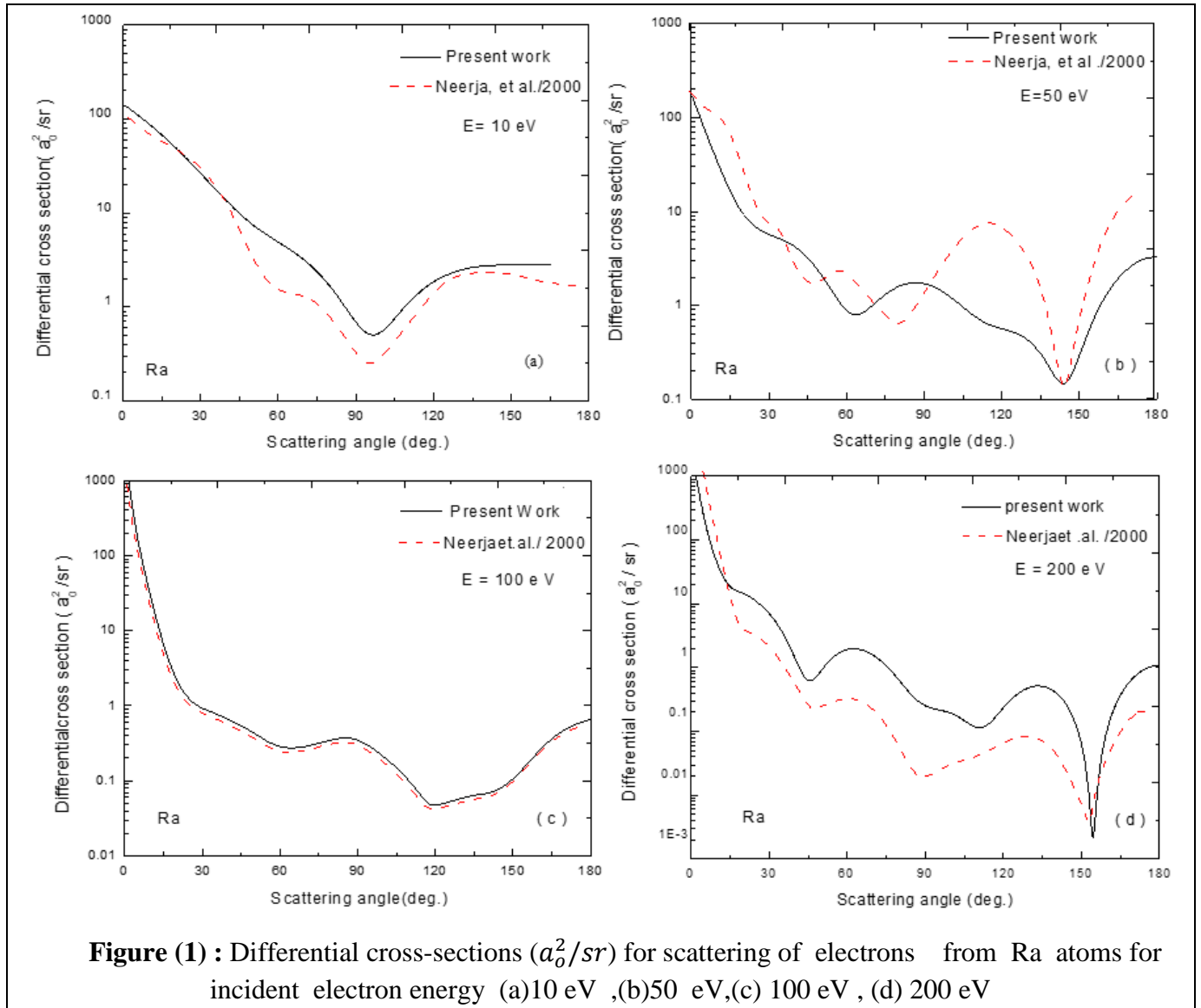
$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2 \quad \text{--- (25)}$$

3. Results and Discussion :

a- Scattering of electrons by Radium and Radon

Radium is considered a heavy element in the alkaline earth atoms. To explain the scattering of electrons and calculates the DCS's, Figure (1) for different energies (10, 50, 100, 200) eV was plotted. The results are compatible with the Neerja et.al. results [19] at different

energies (50, 100) eV. At energy of 10 eV, there was relative consensus, thus, we can conclude from these calculations that the average energies had a compatibility. In contrast, at high energies, the reason for that the potential did not contain the imaginary part. Also, the central potential becomes less effective on the falling electron beam, i.e., the probability of the reaction of the incident beams of electrons with the system potential is weak.



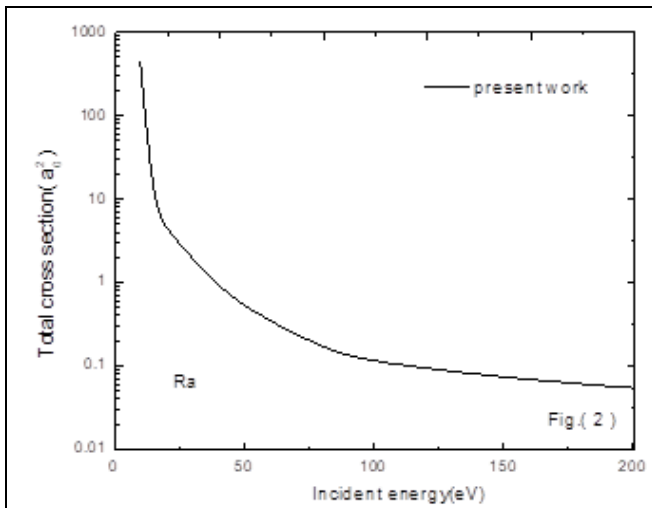


Figure (2) : Total cross sections (a_0^2) for electrons scattering from Ra atoms.

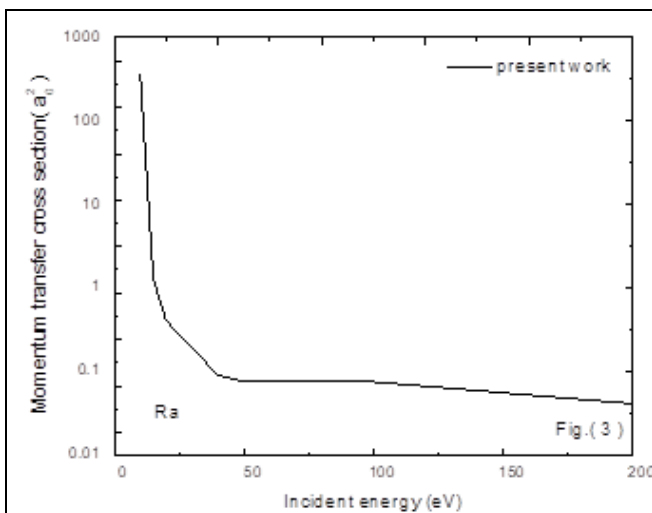
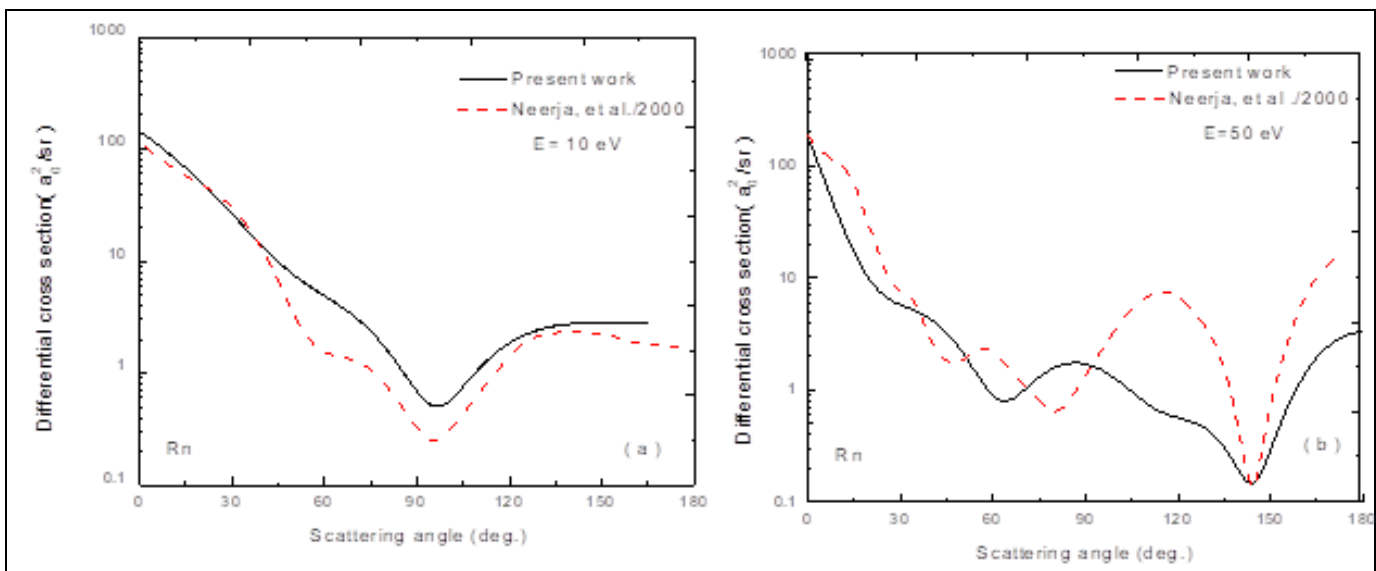
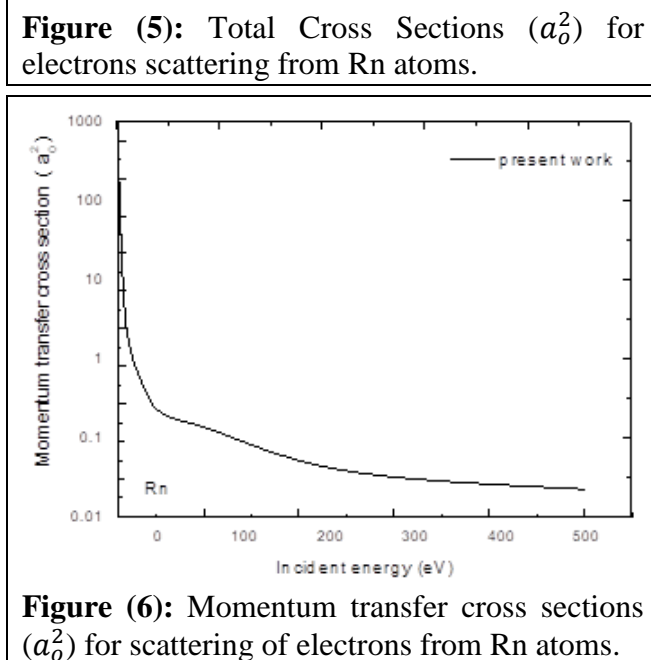
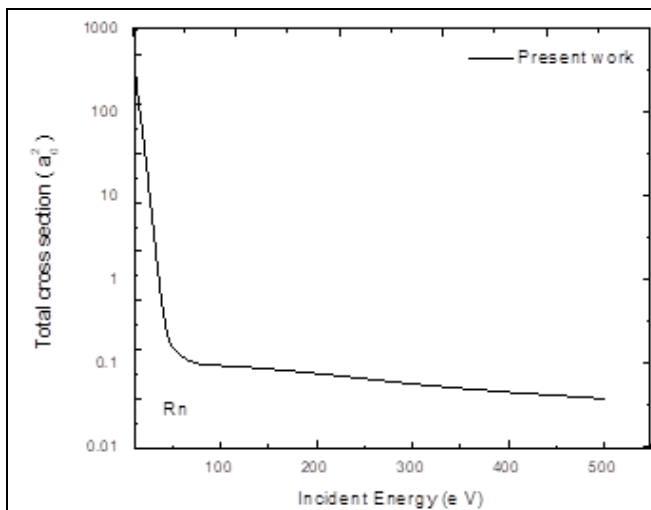
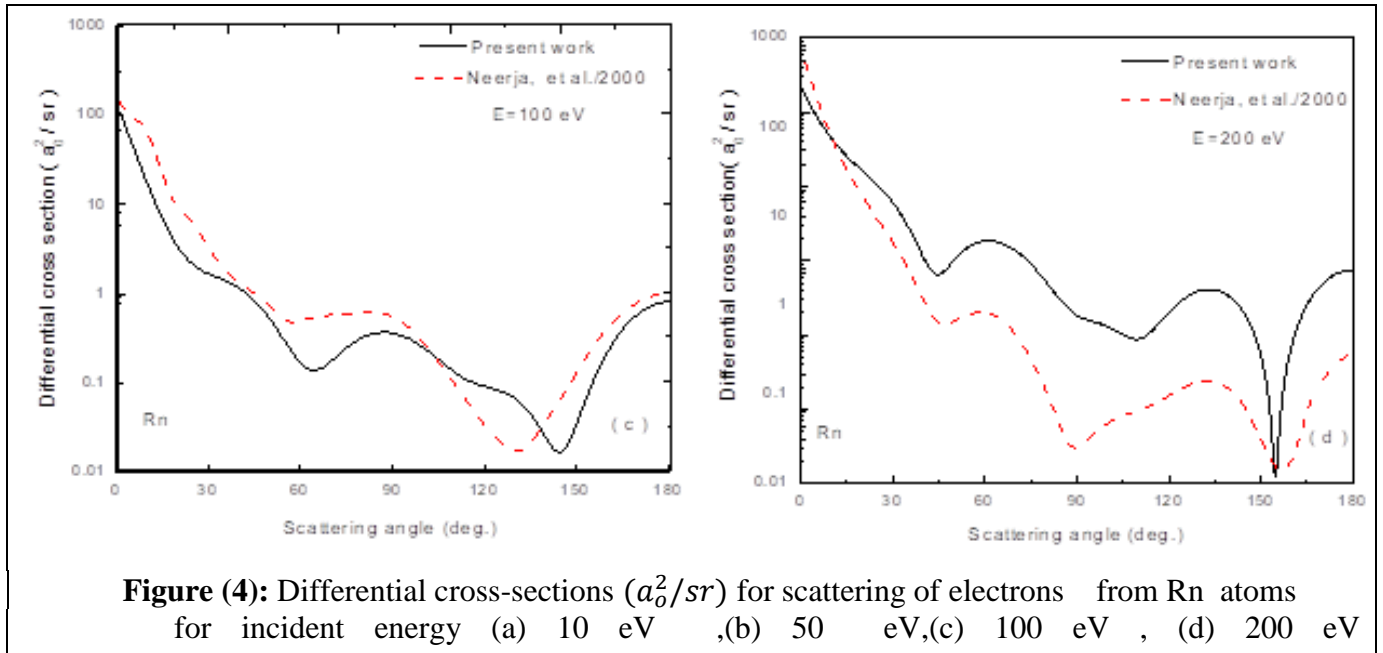


Figure (3): Momentum transfer cross-sections (a_0^2) for electrons scattering from Ra atoms.

From the above figures (2) and (3) , it can be observed that the TCS's and MTCS's had

the highest values at low energies, because the beam of electrons is affected by the central potential. The energy in this section was increased exponentially, because phase shifts gradually decreases. The noble gas was selected (radon atoms) with high atomic number (closed shell), these atoms are characterized by being highly bounded and fully occupied shells. Therefore, the ionization potentials are high, and the elastic scattering sections of these atoms are larger than the inelastic scattering sections. The DCS's of radon atoms are showing in Figure (4) for different energies (10, 50, 100, 200) eV. The theoretical results at energies more than 10 eV are not compatible with the results found by Neerja et al. [19]. This is, also due to the construction of the potential as well as the high electronic structure of the atom. The differential cross section had largest probability especially at small angles because phase shifts are the largest possible, then start decreasing gradually because the incident electron beam is close to the center of the control, which is represented by the central potential of the target. At intermediate angles ($70 \leq \theta \leq 160$) the values of DCS's provide there projections that as are salt for effects of the weak potential and causes decreases in phase shifts, so the incident electrons passes away from the center of the scattering.





on phase shifts in these calculations, because the potential of the atom has a large impact which is greater than the incident energies, while the effect of the potential is weak on the incident electron beams at high energies, which leads to lower values of TCS's and MTCS's, as a result of decreases in phase shifts, as shown in Figures (5) and (6), respectively.

b- Scattering of positrons by Radium and Radon atoms

The differential cross sections for scattering of positrons by radium and radon atoms were calculated for different energies. It is known that alkaline earth atoms have a closed subshell. Figure (7) shows DCSs for scattering of positrons from Ra atoms ($Z = 88$) for different incident energies (5, 10, 50, 500) eV. When compared with Sharma et. al. [20], the results show a good compatibility.

An additionally, the TCS's reach high values at low energies, which depend entirely

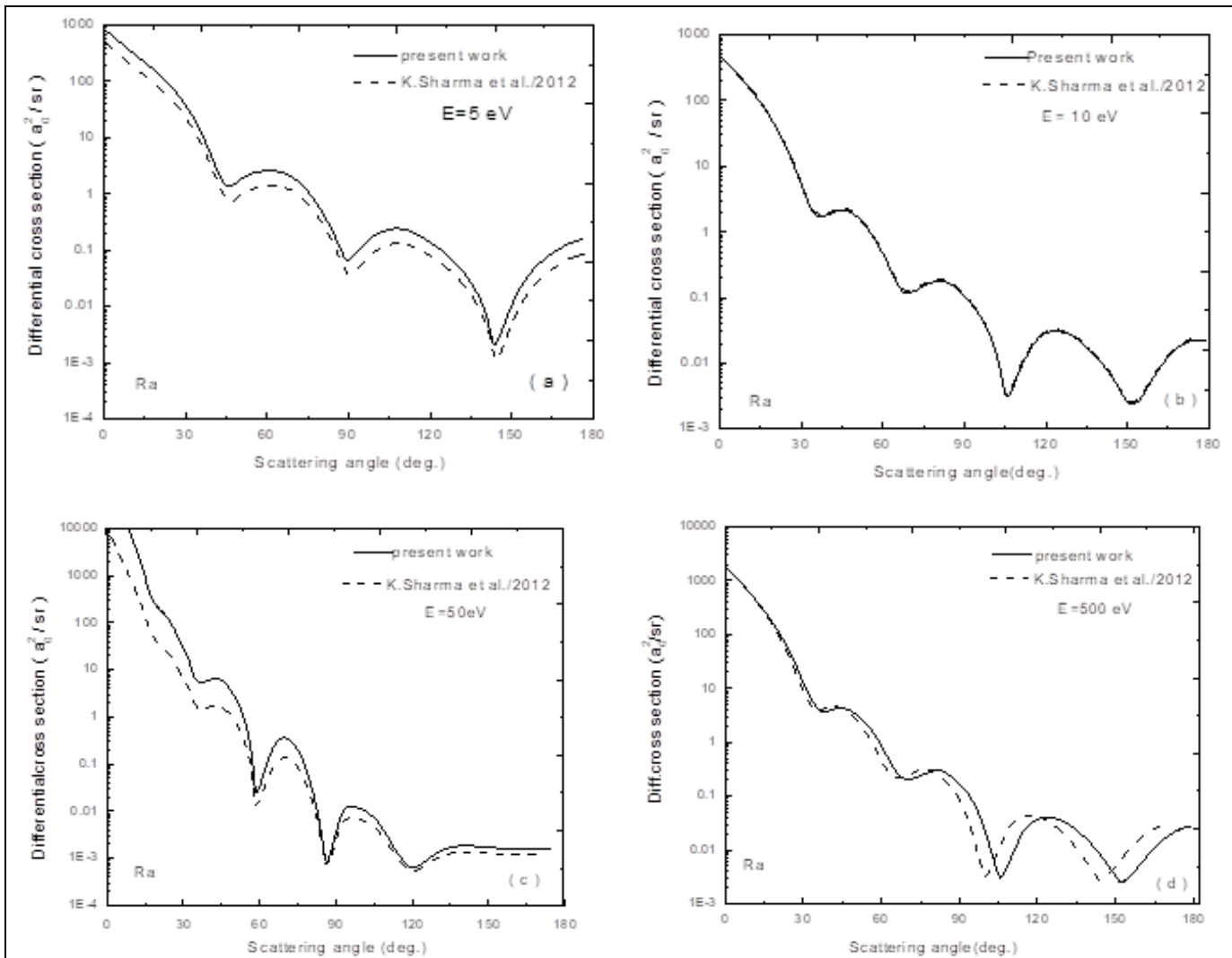


Figure (7): Differential cross sections (a_0^2/sr) for scattering of positrons from Ra atoms for positron energy (a) 5 eV, (b) 10 eV, (c) 50 eV, (d) 100 eV.

The TCS's and MTCS's are shown in Figures (8) and (9), respectively. There are no previous data to compare with, so these results can serve as new addition in this field.

Figure (8): Total cross sections (a_0^2) for positron scattering from Ra atom.

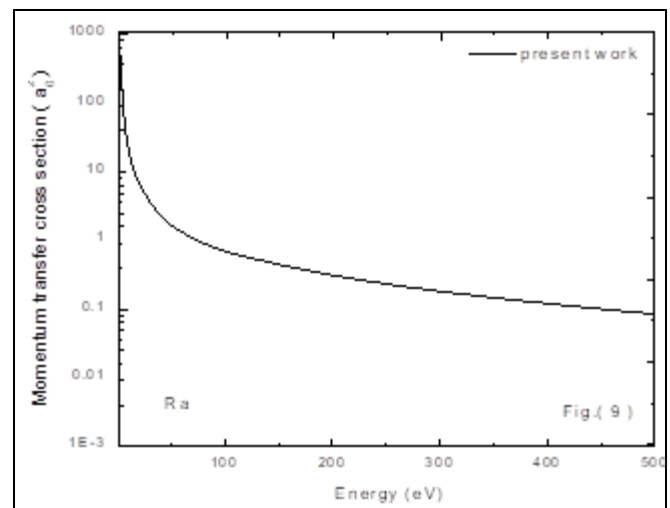
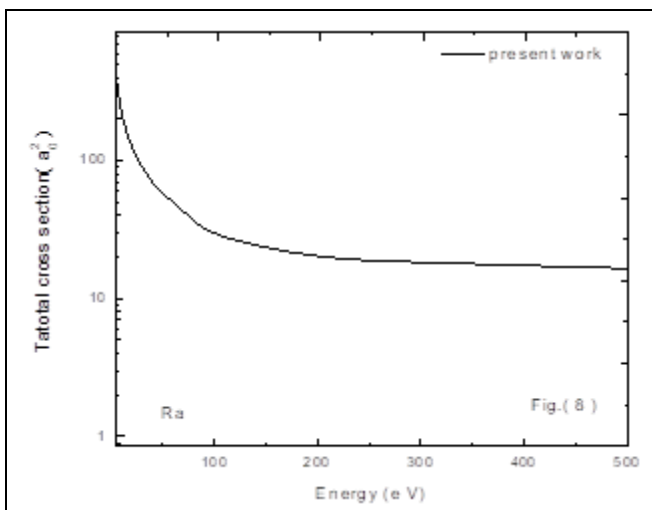


Figure (9): Momentum transfer cross sections (a_0^2) for the scattering of positrons from Ra.

Also, Figure (10) shows the differential cross sections for the scattering of positrons from Rn atoms ($Z = 86$) with incident energies (5, 10, 50, 100, 500) eV, which was compatible with Sharma et al.

[20]. The TCSs and MTCs were calculated as shown in Figures (11) and (12), respectively. Also, Figure (10) shows the differential cross sections for the scattering of positrons from Rn atoms ($Z = 86$) with incident energies (5, 10, 50, 100, 500) eV, which was compatible with Sharma et al. [20].

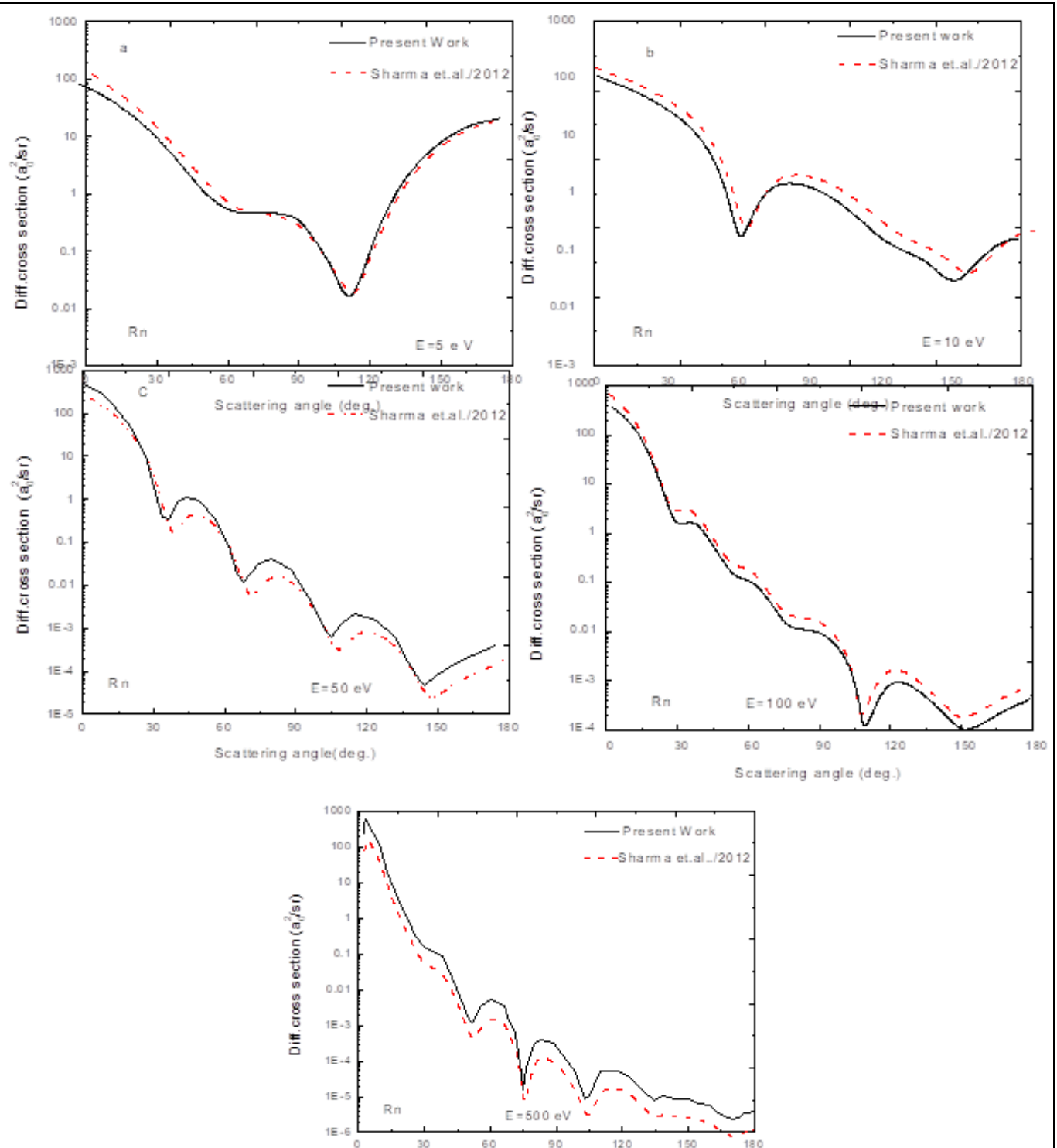


Figure (10): Differential cross-sections (a_0^2/sr) for scattering of positrons from Rn –atoms at incident positron energies: (a) 5 eV, (b) 10 eV, (c) 50 eV, (d) 100 eV, (e) 500 eV

The TCSs and MTCSs were calculated as shown in Figures (11) and (12), respectively. There is no results for comparison, so our results can serve as results for comparison.

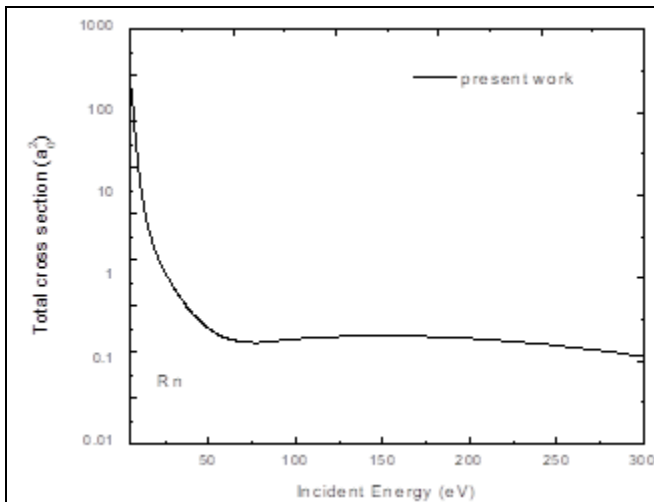


Figure (11) : Total cross sections (a_0^2) for positrons scattering from Rn atoms.

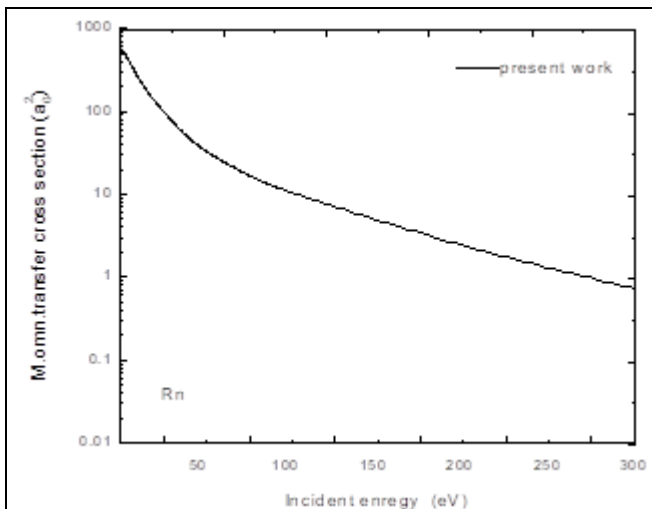


Figure (12) : Momentum transfer cross sections (a_0^2) for scattering of positron from Rn atoms.

4. Conclusion :

The elastic scattering of electrons and positrons from radium and radon atom has been treated relativistically by solving the Dirac equation numerically for the model potential representing the projectile-target interaction which consists of static, exchange and correlation-polarization terms for electrons and omitted exchange term for positrons. These

terms are important for radium and radon atoms as well as the other atomic systems especially when the atomic number increases. The relativistic correction terms according to the spin-orbit interaction becomes more sensitive at low impact energies, where the dependence of the electron exchange, correlation and polarization potentials on the radial distance, according to the relativistic effects in the Dirac equation, becomes more important at low energies especially for electron scattering than positron scattering. Generally, the scattering functions obtained in this work show good agreement with the results of other investigators, but there is a slightly some differences between our calculations with results of others especially at low energies, because of the optical potential which differ from the potential used by others.

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