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Positron scattering from alkaline-earth elements

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Abstract. The total (elastic + inelastic) cross sections for e^+ impact on alkaline-earth elements from Be to Ra are calculated by employing a complex spherical optical potential. This potential has static, polarization and absorption components. The positron energy range is from a few eV to several thousand eV. We have compared our elastic cross sections for Mg and Ca with the other available results and the agreement is good for energies above 100 eV. We have also compared our absorption cross sections with e^- ionization cross sections at high energies where our absorption cross sections are in good accord. We have made Bethe plots for e^+ scattering on these elements.

Keywords. Positron; alkaline-earth elements; static potential; optical potential; polarization potential; absorption potential; inelastic and total cross sections; Bethe plot.

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1. Introduction

Since the advent of positron beams of well defined energies, the study of positron scattering from atoms and molecules has become an important branch of research in atomic physics. One of the principal objectives for obtaining cross section data for the scattering of positrons from atoms has been to compare this data with that of electrons. There are interesting differences in the cross sections for the two cases. The Coulomb static field for the electron case is attractive in contrast to the repulsive field experienced by the positrons. The dipole polarization term which arises from the second order perturbation theory is attractive in both cases. Because of the cancellation effects in static and polarization components of the interaction of positron with atoms, the elastic cross sections for positrons are smaller than the corresponding e^- case for energies up to 100 eV. Since the total cross sections for both the cases merge with each other at high energies, the inelastic cross sections for positrons would be higher than the corresponding electron case. At low energies the virtual positronium formation term must be taken into account whereas for electrons it is the exchange effect which is important. There are several interesting articles on positron impact on various targets [1–9].

Most of the experimental and theoretical work has been concentrated on positron impact on H, noble gases, alkali atoms and some diatomic and polyatomic molecules [10–21]. However, there are some calculations of elastic scattering of e^+ by Mg [22] and Ca [23] using a real optical potential. In the present work, we have calculated elastic, inelastic and total cross sections for e^+ impact on alkaline-earth atoms Be, Mg,

Ca, Ba, Sr and Ra. These atoms are characterized by two s electrons in their outermost shell. We have employed an optical potential approach in which the positron-atom interaction term is replaced by a complex potential. The real part of this complex potential consists of static and polarization terms and imaginary part accounts for the absorption of flux from the incident positrons. We report elastic, absorption and total cross sections for e^+ impact on all alkaline earth elements from Be to Ra in the energy range 10 eV to few thousand eV.

2. Theory

The basic idea of the optical model potential approach is to reduce many body problems to an equivalent one body problem. Above the first ionization threshold, the interaction between the e^+ and target is represented by a complex optical potential $V_{\text{opt}}(\mathbf{r})$. The scattering function $F(\mathbf{r})$ of the positron satisfies the differential equation

$$(\nabla^2 + k^2 - V_{\text{opt}}(\mathbf{r}))F(\mathbf{r}) = 0, \tag{1}$$

where k^2 is the energy of the incident positron. The optical potential is a complex, non local, non spherically symmetric and energy dependent potential whose evaluation is a formidable task. In the present work we have replaced $V_{\text{opt}}(\mathbf{r})$ by spherically symmetric potential $V_{\text{opt}}(r)$. We represent $V_{\text{opt}}(r)$ by various local potentials of the form [14]

$$V_{\text{opt}}(r) = V_{\text{st}}(r) + V_{\text{pol}}(r) + iV_{\text{abs}}(r). \tag{2}$$

The static potential $V_{\text{st}}(r)$ is calculated from the unperturbed target wavefunctions at the Dirac–Hartree–Fock level [24]. This relativistic potential has been parametrized as a sum of three Yukawa potentials. Its form is

$$V_{\text{st}}(r) = \frac{Z}{r}\sum_{i=1}^{3} A_i e^{-\alpha_i r}, \tag{3}$$

where A_i and α_i are parameters. In principle, these parameters can be determined so that one-electron binding energies agree with Dirac–Hartree–Fock–Slater energy eigenvalues by employing a conventional least-square fitting procedure. However, such a procedure makes the values of A_i and α_i sensitive to the initial estimate. An alternative procedure is to reproduce the expectation values of $\langle r^n \rangle$ where $n = -1, 0, 1, 2, 3$ and 4. The atomic density takes the analytic form

$$\rho(r) = \frac{Z}{r}\sum_i A_i \alpha_i^2 \exp(-\alpha_i r). \tag{4}$$

The form $V_{\text{st}}(r)$ of (3) is not a unique one. Other forms like a sum of exponential terms or a sum of exponential and Yukawa terms can be employed.

$V_{\text{pol}}(r)$ represents the polarization potential which arises due to the distortion of the electronic charge cloud by the incident positron. The effect of polarization is very important for alkaline-earth elements because of the large value of dipole polarizabilities of these atoms. The long range part of the polarization assumes its asymptotic form

$$V_{\text{pol}}(r) = \frac{-\alpha_d}{2r^4}, \quad r > r_c. \tag{5}$$

In the short range part $r < r_c$, the polarization potential is evaluated by calculating the correlation energy $\varepsilon_{corr}(r_s)$ of a single e^+ in a homogeneous electron gas [25]. The correlation energy is calculated from the ground state expectation value of the Hamiltonian which describes the fixed positron interacting with the target electrons. This polarization is different from that of the corresponding short range part of the e^- case [26] because the e^+ distorts the electronic charge cloud differently than the corresponding e^- case. The polarization potential $V_{corr}(r)$ is related to $\varepsilon_{corr}(r_s)$ by

$$V_{corr}(r) = \left[1 - \frac{1}{3} r_s \frac{d}{dr_s}\right] \varepsilon_{corr}(r_s). \tag{6}$$

Its explicit form is given as [14]

(i) for $r_s < 0{\cdot}302$,

$$2V_{corr}(r) = -\frac{1{\cdot}82}{(r_s)^{1/2}} + [0{\cdot}051 \ln(r_s) - 0{\cdot}115] \ln(r_s) + 1{\cdot}167, \tag{7a}$$

(ii) for $0{\cdot}302 \leqslant r_s \leqslant 0{\cdot}56$,

$$2V_{corr}(r) = -0{\cdot}92305 - \frac{0{\cdot}09098}{(r_s)^2} \tag{7b}$$

and

(iii) for $0{\cdot}56 \leqslant r_s \leqslant 8{\cdot}0$,

$$2V_{corr}(r) = -\frac{8{\cdot}764 r_s}{(r_s + 2{\cdot}5)^3} + \frac{0{\cdot}9552 r_s - 13{\cdot}151}{(r_s + 2{\cdot}5)^2} + \frac{2{\cdot}8655}{(r_s + 2{\cdot}5)} - 0{\cdot}6298. \tag{7c}$$

r_c in (5) is the first crossing point of the short and long range parts and r_s is defined by

$$(4/3)\Pi r_s^3 \rho(r) = 1. \tag{8}$$

It may be pointed out that in the limit $r_s \to 0$, $V_{corr}(r)$ diverges. This is due to the strong short-range correlation between the positron and the homogeneous electron gas. When $r_s \to \infty$ (or $\rho(r) \to 0$), $V_{corr}(r)$ is designed such that it approximately reproduces the binding energy of the positronium. Since we know that asymptotically, the polarization potential behaves like $-\alpha/2r^4$, we assume this form beyond the radius r_c. The formulas 7(a–c) have been derived so that the correlation-energy functionals and its derivatives are continuous over the entire range of r_s values. In other words, $V_{corr}(r)$ is a continuous function of r.

Semi-empirical models have been developed to determine the imaginary part $V_{abs}(r)$ of the optical potential for the case of e^- scattering. The imaginary part $V_{abs}(r)$ represents the total loss of flux into all accessible channels. We, in the present work, have employed the semi-empirical form [27–30] $V^-_{abs}(r)$ of e^- case modified as $V^+_{abs}(r)$ for e^+ case as prescribed earlier [14]. These are related as

$$V^+_{abs}(r) = f(k, r)\, V^-_{abs}(r). \tag{9}$$

It is a formidable task to determine the form of $f(k, r)$ from an *ab-initio* point of view. This relation is further dictated by certain conditions which hold in the electron as well

as in the positron case. The imposed conditions for the electron case are that (1) the initially unbound electron is not allowed to fall into the occupied Fermi sea, and (2) the lowest-energy state available to the initially bound electron exceeds the Fermi level by the energy gap (Δ). These conditions are also valid when the incident projectile is a positron. It has been shown [14] that by choosing $f(k,r) = 2/(kr)^{1/2}$, there is a good agreement between calculated total cross sections and the experimental results for Ar, Kr, Xe and Rn. The factor 2 accounts for the fact that exchange is absent in positron scattering. It may be pointed out that a factor of 1/2 approximately accounts for exchange effects in the evaluation of $V^{-}_{abs}(r)$. So to remove this factor, a factor of 2 appears in $V^{+}_{abs}(r)$. The factor $1/(kr)^{1/2}$ approximately accounts for Ps formation at lower energies. It is well known that the positron-atom total cross sections exhibit a sharp rise near the Ps threshold and there is a bell-shaped structure around 20–80 eV depending upon the chosen target. We have introduced the empirical factor $1/(kr)^{1/2}$ to account for this behaviour. The factor $(kr)^{1/2}$ is dimensionless since $f(k,r)$ is dimensionless. The square root factor is only an empirical one. In the present work, we have kept Δ equal to the first ionization potential of the atom.

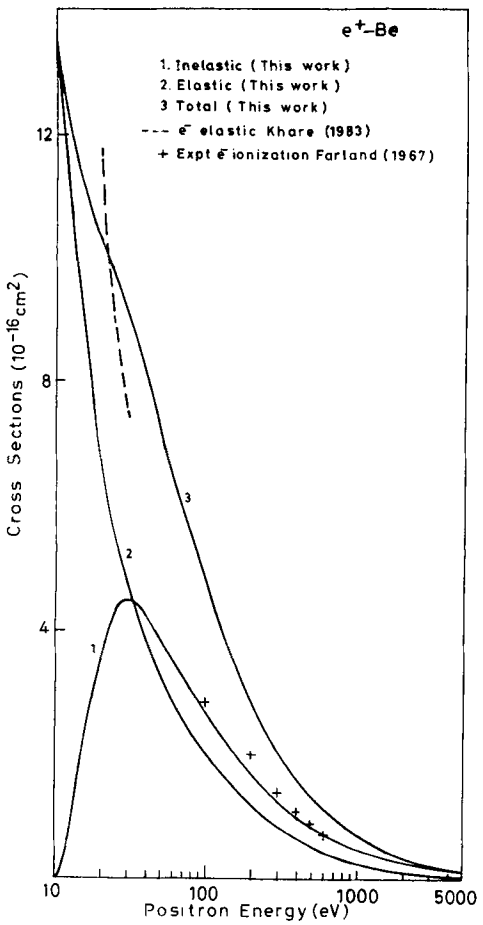

Figure 1. Cross sections for positron impact on Be.

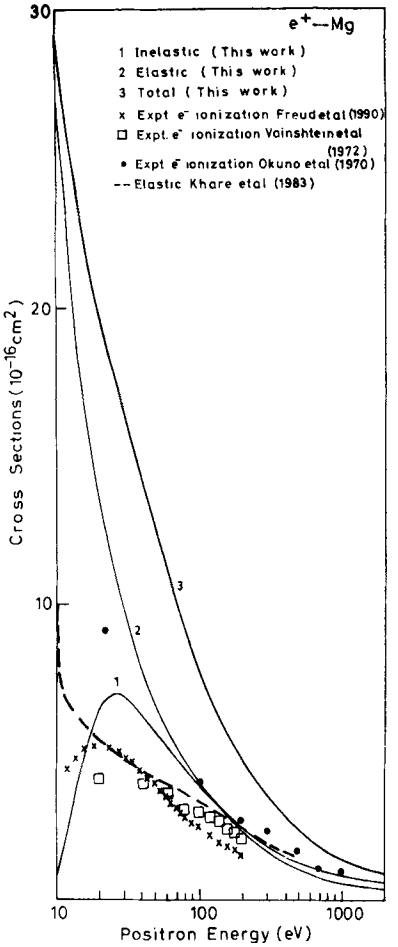

Figure 2. Cross sections for positron impact on Mg.

Since our optical potential is spherically symmetric, we now make a partial wave analysis and get the real and complex phase shifts by using a variable phase approach [14]. The S-matrix and the various cross sections are calculated. We also calculate the polarized Born phase shifts and checked their values against the numerical phase shifts. When the agreement was better than 0·1% at a particular value of the partial wave l_{max}, we switched over entirely to the polarized Born phase shifts for partial waves having value of $l > l_{max}$. Enough partial waves are included to obtain converged results.

3. Results and discussion

In figure 1 we have displayed the elastic, absorption and the total cross sections for e^+-Be scattering systems using our complex optical model potential. We notice a maximum in the absorption cross section around 30 eV. There are no other results available for comparison. However, we show elastic scattering result of e^--Be

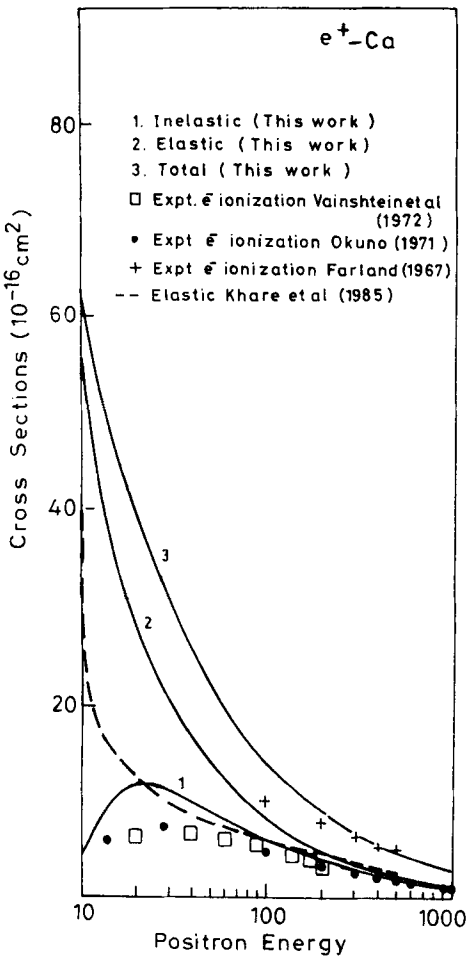

Figure 3. Cross sections for positron impact on Ca.

scattering system which also employed an optical model potential [31]. This calculation was done in the static field approximation (SF), static field polarization approximation (SFP) and static field polarization exchange approximation (SFPE). For polarization potential this calculation employed an empirical energy dependent and spherically symmetric potential [32]. These results were calculated up to 30 eV. We have shown SFP results only in figure 1 because there is no exchange in the positron case. The elastic scattering cross sections for e^- case are higher than the corresponding elastic e^+ cross sections by almost 50% up to 30 eV. The lower cross sections for e^+ case are due to the cancellation effect of repulsive static field and attractive polarization field. The absorption cross section represents the loss of incident e^+-flux into ionization channel and all other accessible excitation channels. Therefore the absorption cross section represents an upper bound to the ionization cross section. There are no results available for e^+ impact ionization of Be. However, it is well-known that at energies

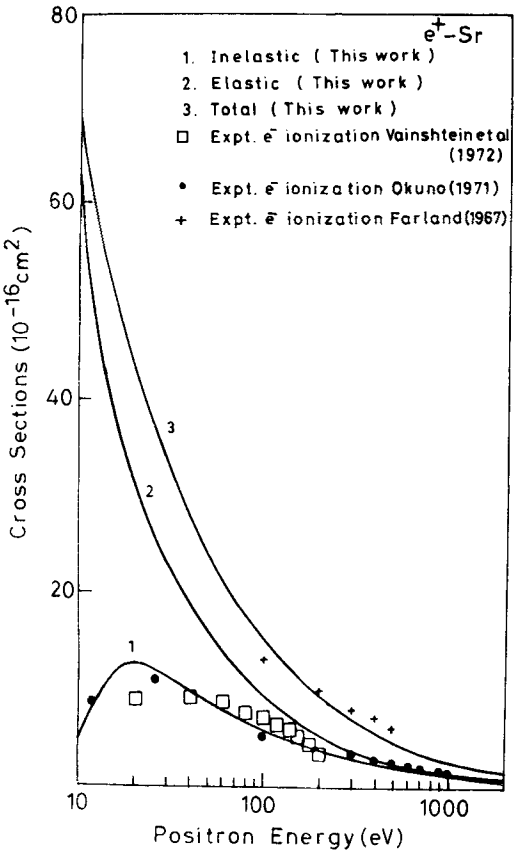

Figure 4. Cross sections for positron impact on Sr.

greater than a few hundred eV, the ionization cross section for e^- and e^+ case merge with each other. Also at such high energies the ionization cross section is the most important channel in the absorption cross section. The ionization cross section makes the bulk contribution to the absorption cross section. In figure 1 we have displayed the ionization cross section from 100–600 eV for e^- impact on Be using Gryzinski equation [33]. It is indeed satisfactory to note a good agreement between our absorption cross sections and the experimental e^- ionization cross sections [33].

Figure 2 shows various cross sections for positron-Mg scattering system. We have also shown the elastic scattering cross sections obtained via a real optical model potential [22]. This calculation employed Buckingham type polarization potential. The difference in the elastic cross section computed in our model and that of real optical model potential is due to the different polarization potentials used. However above 100 eV the two calculations agree with each other. We have no knowledge of various components of absorption cross sections for e^+-Mg scattering. However at high energies (greater than 400 eV), the ionization channel is the dominant channel among all the inelastic processes, and therefore we expect our absorption curve to approach from above the ionization curve for e^- or e^+. According to Born approximation e^-

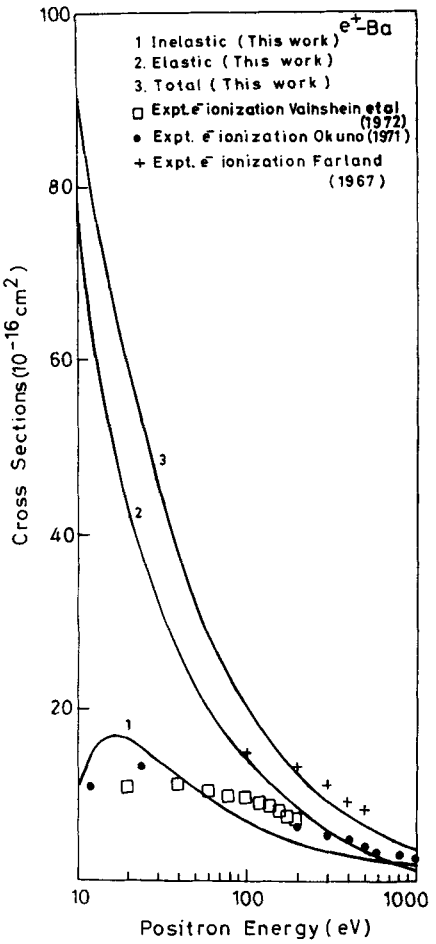

Figure 5. Cross sections for positron impact on Ba.

ionization curve coincide with e^+ ionization curve at high energies. To bring this qualitative features into focus we have shown various ionization cross sections for e^- impact on Mg [34–36]. It is interesting to note that our absorption curve peaks at 26 eV whereas the ionization curve of Freund *et al* peaks at 20 eV. The ionization cross sections of Vainshtein *et al* indicate maximum around 26 eV. It is also interesting to note that our absorption cross section lie above all the ionization cross sections shown. At energies above 200 eV our absorption curve seems to be merging with the ionization curve of Vainshtein *et al*. It is indeed satisfying to note that our simple model is capable of yielding elastic and inelastic cross sections which reveal expected qualitative features. More light on their quantitative aspects can be shed only by doing more calculations by other theoretical means and performing experiments using the positron beam. The measurements of Okudaira *et al* [37] almost agree with Okuno *et al* [36], hence are not shown in the figure.

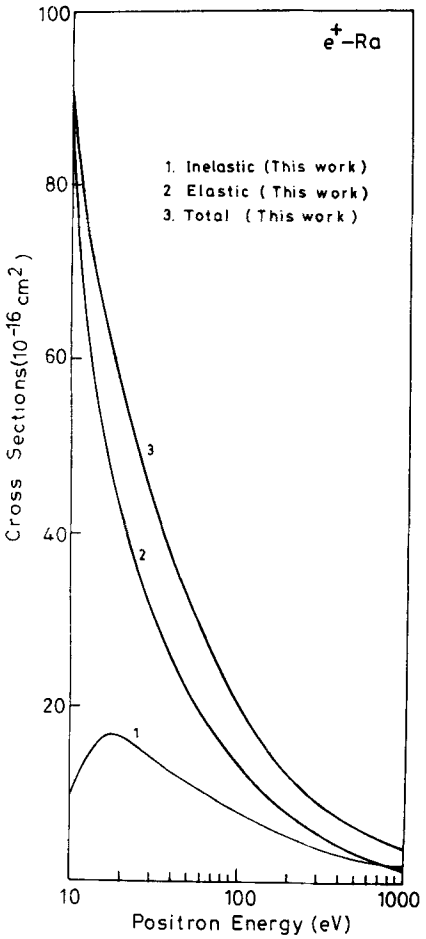

Figure 6. Cross sections for positron impact on Ra.

Our results for e^+ scattering on Ca are displayed in figure 3. Just as in Mg, our elastic cross sections agree with the real optical model potential [23] above 100 eV. Once again our absorption cross sections are close to the e^- ionization cross sections [35, 38] above 100 eV. We have also shown the experimental result of McFarland [33] which lie above our absorption curve. These higher cross sections are probably due to normalization procedure used. This experiment used Gryznski equations for normalization which may not be appropriate.

The cross sections for e^+ scattering on Sr and Ba are depicted in figures 4 and 5 respectively where the elastic, absorption and total cross sections are shown. The absorption cross sections are compared with the ionization cross sections for e^- case. Our absorption cross sections are in good accord with the e^- ionization cross sections [35, 38] above 100 eV for Sr. Once again the cross sections measured in chopped crossed beam experiment [33] are above our absorption cross section curve due to normalization process. For Ba, our absorption cross section lie slightly lower than the

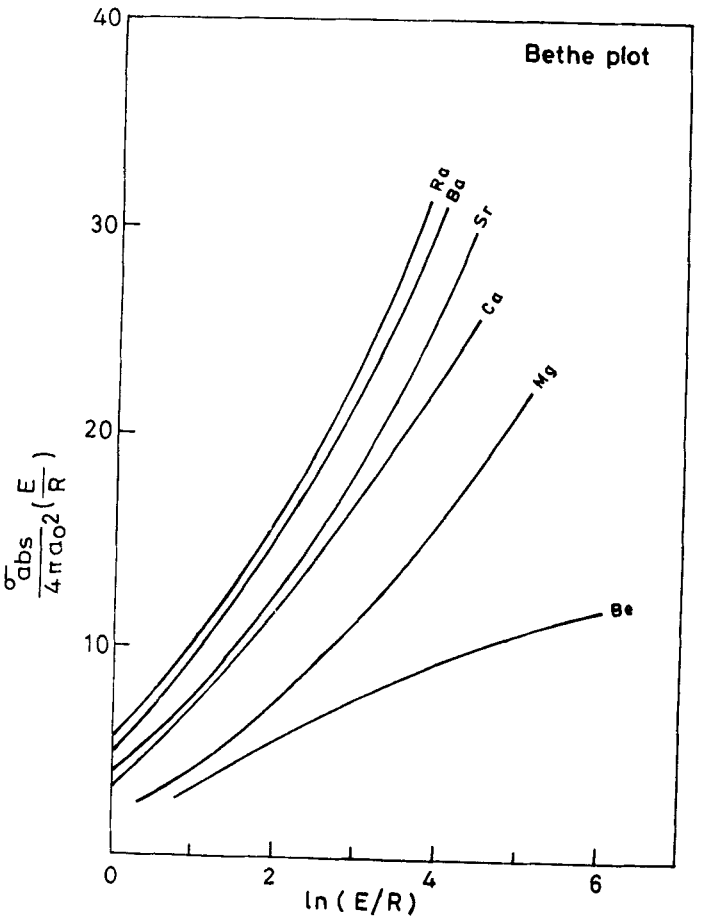

Figure 7. Bethe plot for positron impact on alkaline-earth elements.

ionization cross sections [35, 38] which indicates that the absorption potential may not be accurate for such heavier systems.

Lastly our results for e^+ scattering on Ra are given in figure 6. However there are no other results available for comparison. An interesting aspect of the ionization curve for these alkaline-earth elements reveal a maximum around 30 eV.

To probe further into the study of absorption cross section we have made Bethe plots [39] for e^+ scattering on alkaline earth elements in figure 7. The inelastic cross sections can be conveniently parametrized by Bethe asymptotic formula [39]

$$\frac{\sigma_{\text{abs}}E}{4\pi a_0^2 R} = M_{\text{tot}}^2 \ln(4C_{\text{tot}}E/R), \tag{10}$$

where M_{tot}^2 is the total dipole matrix element [39]. R is the Rydberg energy. We notice that for all the elements, there is a region of linearity at energies above 300 eV. The slope of these curves directly yields the value of M_{tot}^2. The values extracted are $M_{\text{tot}}^2 = 1{\cdot}86$,

5·17, 6·08, 7·8 and 8·6 for Be, Mg, Ca, Sr, Ba and Ra respectively. We note that the values of M_{tot}^2 increases from Be to Ra. This implies that the effect of absorption increases from Be to Ra. For energies above 1 keV, we expect our cross sections to merge with the corresponding electron case.

In conclusion, we have shown that a complex spherical model optical potential is capable of producing elastic, absorption and total cross sections for rare earth elements showing their expected qualitative features. There is internal consistency in our calculations which is embedded in Bethe plots.

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