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Elastic scattering of electrons and positrons by magnesium atoms at intermediate energies

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Abstract. Differential and total cross sections for the elastic scattering of electrons and positrons by magnesium atoms in the intermediate energy region from 10 to 500 eV are calculated using a real optical potential and are compared with the available theoretical and experimental results. The agreement with the experimental data is only moderate but that with the theoretical values of Gregory and Fink is fairly good.

1. Introduction

Optical model calculations of electron–atom elastic scattering have attracted considerable interest in the past few years. A large number of calculations of elastic scattering of electrons by H, He, C, N, O and inert gases (Furness and McCarthy 1973, Jhanwar and Khare 1976, McCarthy *et al* 1977, Joachain *et al* 1977, Byron and Jochain 1977, Jhanwar *et al* 1978, Khare and Kumar 1978, Khare and Raj 1979, Kaushik *et al* 1982, Khare *et al* 1982) have been carried out using the optical potential model. However, there have been only two theoretical investigations of the elastic scattering of electrons by magnesium. Gregory and Fink (1974) solved the Dirac equation for energies varying from 100 eV to 2 keV and Fabrikant (1980) investigated the scattering in the close-coupling approximation at energies of 10 and 20 eV.

In the present investigation we have employed the partial-wave method to obtain differential (DCS) and total cross sections (TCS) for the elastic scattering of electrons and positrons by magnesium atoms in the energy range from 10 to 500 eV. The static and exchange potentials are constructed by using Hartree–Fock wavefunctions and they are taken as local, spherically symmetric and energy-dependent potentials. The second-order polarisation effects are taken into account through the Buckingham-type potential of Jhanwar *et al* (1978). DCS and TCS results are compared with the results of Fabrikant (1980), Gregory and Fink (1974) and the experimental results of Williams and Trajmar (1978). As far as e^+–Mg scattering is concerned no other investigations, theoretical or experimental, are available for comparison.

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2. Theory

In the optical potential method, the many-body problem is reduced to a one-body problem. In this model, the equation describing the scattering of the incident particle is given by

$$(\nabla^2 + k^2 - V_{op}(\boldsymbol{r}))F(\boldsymbol{r}) = 0 \tag{1}$$

where k^2 is the energy of the incident particle (we employ atomic units unless stated otherwise), $V_{op}(\boldsymbol{r})$ is the optical potential of the system which, in general, is a complex, non-local, non-spherically symmetric and energy-dependent potential. An exact evaluation of V_{op} has not yet been achieved. Its evaluation is as difficult as the evaluation of the original many-body problem. Therefore, in the present investigation, we represent it by a spherically symmetric, localised and real potential so that we can solve equation (1) using the partial-wave method. The optical potential consists of static, exchange and polarisation potentials:

$$V_{op}(r) = V_{00}(r) + V_{ex}(r) + V_{pol}(r) \tag{2}$$

where $V_{00}(r)$ is the static potential given as $\langle 0|V(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N; \boldsymbol{r})|0\rangle$ with $|0\rangle$ representing the ground state of Mg having $N = 12$ and $V(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N; \boldsymbol{r})$ the interaction potential given by

$$V(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N; \boldsymbol{r}) = \frac{NQ}{r} - Q\sum_{j=1}^{N} \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_j|} \tag{3}$$

where $Q = -1$ for electrons and $+1$ for positrons. V_{ex} is the exchange potential. In general, it is non-local but it is converted into an equivalent local exchange potential following Vanderpoorten (1975). The local energy-dependent exchange potential is given by

$$V_{ex}(r) = \tfrac{1}{2}\{(k^2 - V^D) - [(k^2 - V^D)^2 - 32\pi\rho(r)]^{1/2}\} \tag{4}$$

with $V^D = V_{00} + V_{pol}$ and $\rho(r)$ is the spherical charge density of the atom. For positron scattering, exchange is absent hence V_{ex} is taken to be zero. For the evaluation of the static and the exchange potentials, we have used the Hartree–Fock wavefunctions for the ground state of Mg given by Clementi and Roetti (1974).

For the polarisation potential, we have employed the same energy-dependent and spherically symmetric Buckingham-type expression as used by Jhanwar and Khare (1976). The expression is given as

$$V_{pol}(r) = -\frac{\alpha_d r^2}{(r^2 + d^2)^3} - \frac{\alpha_q r^4}{(r^2 + d^2)^5} \tag{5}$$

with $d = 0.75k/\Delta$. α_d and α_q are the dipole and quadrupole polarisabilities and Δ, the mean excitation energy, is given as

$$\Delta = \exp[L(-1)/S(-1)] \tag{6}$$

where $L(-1)$ and $S(-1)$ are the properties of the atom and require the oscillator strength distribution for their determination (Inokuti *et al* 1967). To calculate Δ, we have used the values of $L(-1)$ and $S(-1)$ given by Dehmer *et al* (1975) which are -8.825 and 8.619, respectively, and obtain $\Delta = 0.3592$. Jhanwar *et al* (1978) have

shown that the above polarisation potential is not adequate for energies less than 3.56Δ and does not even give qualitative agreement with experiment in this energy range. To remove this inadequacy we have replaced, following Kaushik *et al* (1982), d by a constant value d_c equal to $0.75(3.56/\Delta)^{1/2}$ for $E < 3.56\Delta$.

Recently Eades *et al* (1982) have given adiabatic polarisation potentials for the elastic scattering of electrons by Be and Mg atoms. They have compared the polarisation potential given by (5) with their adiabatic polarisation potential at 50 and 100 eV. They have mentioned in their results that V_{pol} results obtained from (5) at 50 eV are close to their results for $r \geq 1.5$. However, their conclusion seems to be misleading for the following reasons. In the computation of V_{pol} from the expression (5), they have taken Δ equal to the ionisation potential (say Δ_i) of the atom instead of the mean excitation energy given by (6) and V_{pol} is very sensitive to the value of Δ. For example if we take Δ equal to the mean excitation energy (say Δ_e) the results obtained are very much less than those obtained by using Δ_i. It is evident from table 1 that the values of V_{pol} obtained from (5) with Δ_e at 50 eV are of much smaller magnitude than the values of the adiabatic polarisation potential of Eades *et al* (1982). Furthermore V_{pol} is energy independent only for $E < 3.56\Delta$. Therefore it is better to compare the present polarisation potential with the adiabatic polarisation potential of Eades *et al* (1982) at 10 eV instead of 50 eV. The examination of the results at 10 eV shows that the results with Δ_i are much higher in magnitude than the values obtained by Eades *et al* whereas the results with Δ_e are close to the results of Eades *et al.* Hence the replacement of the mean excitation energy by the ionisation potential is not justifiable. In the present investigation, we take $\alpha_d = 75.0$ and $\alpha_q = 919.54$ as given by Stwallay (1971) and Sen and Schmidt (1981), respectively.

After thus obtaining $V_{op}(r)$, which is spherically symmetric, we substitute equation (2) in equation (1) and expand the scattering function $F(r)$ in partial waves. We get

$$\left(\nabla^2 + k^2 - V_{op}(r) - \frac{l(l+1)}{r^2}\right) f_l(r) = 0 \tag{7}$$

Table 1. Comparison of polarisation potentials with different values of Δ.

		Present polarisation potential			
r (a_0)	Adiabatic polarisation potential[a]	$E = 50$ eV $\Delta = \Delta_i$	$E = 50$ eV $\Delta = \Delta_e$	$E = 10$ eV $\Delta = \Delta_i$	$E = 10$ eV $\Delta = \Delta_e$
0.5	−1.2196	−0.0680	−0.0047	−0.4322	−0.1104
1.0	−0.5014	−0.2237	−0.0170	−1.2951	−0.3561
1.5	−0.3724	−0.3515	−0.0320	−1.5972	−0.5317
2.0	−0.3214	−0.3833	−0.0446	−1.3169	−0.5436
2.5	−0.2782	−0.3412	−0.0520	−0.9128	−0.4545
3.0	−0.2314	−0.2720	−0.0537	−0.5949	−0.3436
3.5	−0.1856	−0.2054	−0.0511	−0.3841	−0.2484
4.0	−0.1452	−0.1515	−0.0461	−0.2514	−0.1771
5.0	−0.0850	−0.0820	−0.0340	−0.1157	−0.0913
6.0	−0.0492	−0.0459	−0.0237	−0.0588	−0.0497
8.0	−0.0180	−0.0168	−0.0112	−0.0193	−0.0176
10.0	−0.0078	−0.0073	−0.0056	−0.0080	−0.0075

[a] Eades *et al* (1982).

where $f_l(r)$ represents the radially scattered wavefunction which varies asymptotically as

$$f_l(r) \underset{r\to\infty}{\sim} \frac{1}{k}\sin(kr-\tfrac{1}{2}l\pi+\delta_l). \tag{8}$$

δ_l is the phaseshift corresponding to lth partial wave. The scattering amplitude is obtained from the following expression

$$f(\theta)=\frac{1}{k}\sum_{l=0}^{M}(2l+1)\exp(\mathrm{i}\delta_l)\sin\delta_l P_l(\cos\theta)+f_{\mathrm{dp}}^{\mathrm{B}}(\theta)-\frac{1}{k}\sum_{l=0}^{M}(2l+1)\delta_l^{\mathrm{B}}P_l(\cos\theta)$$

where $f_{\mathrm{dp}}^{\mathrm{B}}$ is the scattering amplitude in the Born approximation due to the long-range polarisation potential and δ_l^{B} are the corresponding Born phaseshifts. The calculation of δ_l^{S} from the relation

$$\delta_l^{\mathrm{B}}=-k\int_0^{\infty} r^2 V_{\mathrm{pol}}(r)(j_l(kr))^2\,\mathrm{d}r$$

for higher partial waves becomes time consuming as it involves Bessel functions, therefore following Khare and Raj (1979) we have replaced it by the semiclassical phaseshift δ_l^{S} given by LaBahn and Callaway (1969) as

$$\delta_l^{\mathrm{S}}=-\frac{1}{k}\int_0^{\infty}\frac{rV_{\mathrm{pol}}(r)\,\mathrm{d}r}{(r^2-r_0^2)^{1/2}}$$

with $r_0=(l+0.5)/k$ (for details see Raj 1981). The differential cross sections are obtained by taking the modulus squared of the scattering amplitude $f(\theta)$ and the total elastic cross sections are obtained by using the optical theorem.

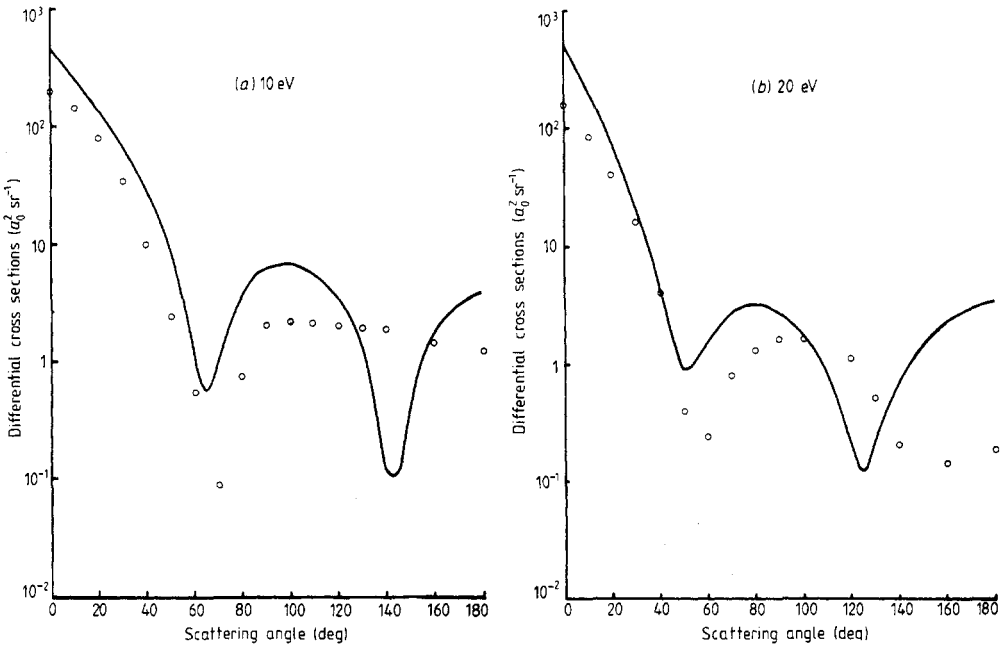

Figure 1.

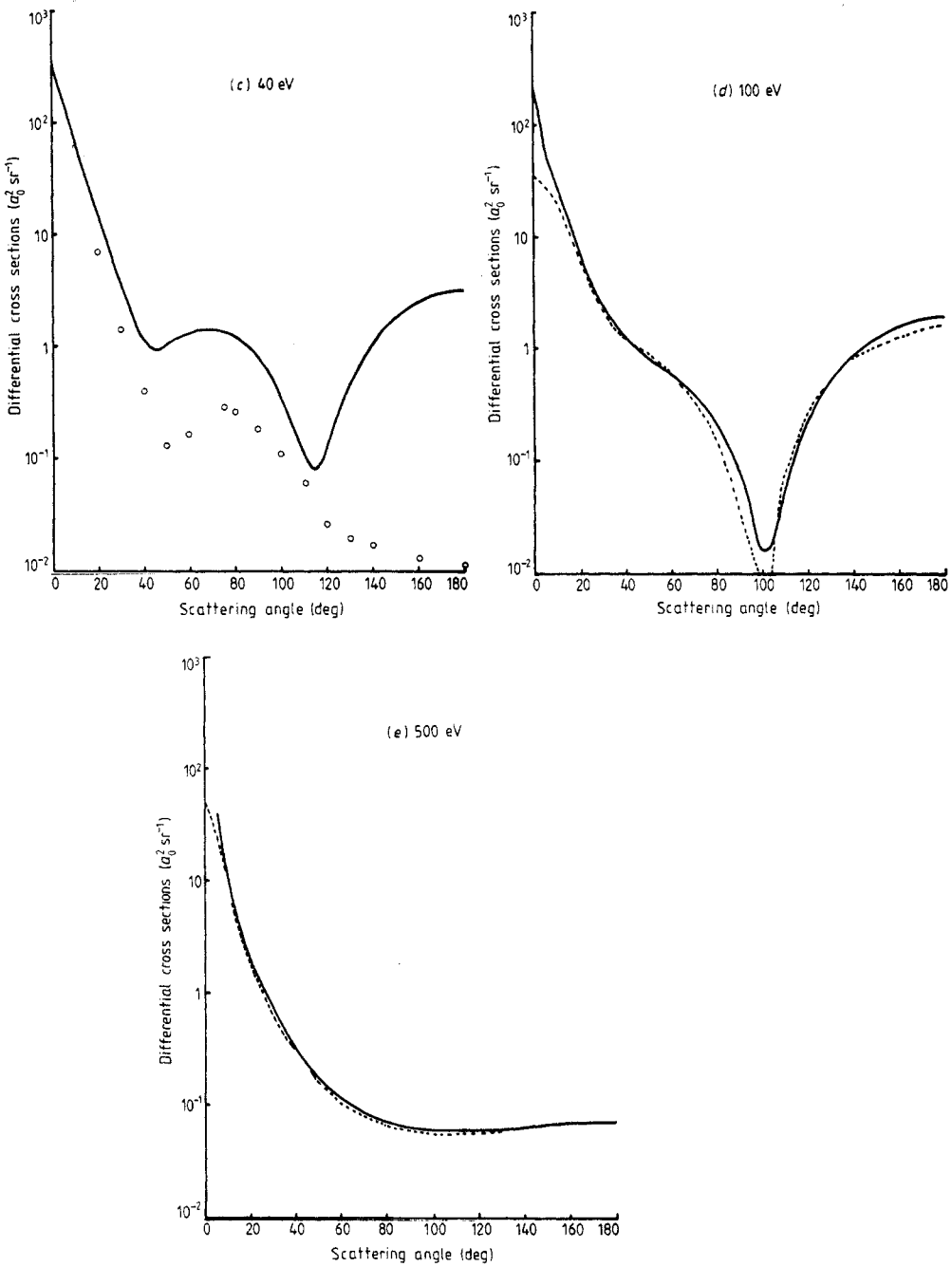

Figure 1. The differential cross sections (in a_0^2 sr^{-1}) for the elastic scattering of the electrons by the magnesium atoms at (*a*) 10 eV, (*b*) 20 eV, (*c*) 40 eV, (*d*) 100 eV and (*e*) 500 eV. ——; the present results; – – –, Gregory and Fink (1974) results; O, experimental results of Williams and Trajmar (1978).

3. Results and discussion

In figure 1 we have presented our differential cross section results for the elastic scattering of electrons by Mg atoms in the energy range from 10 to 500 eV and

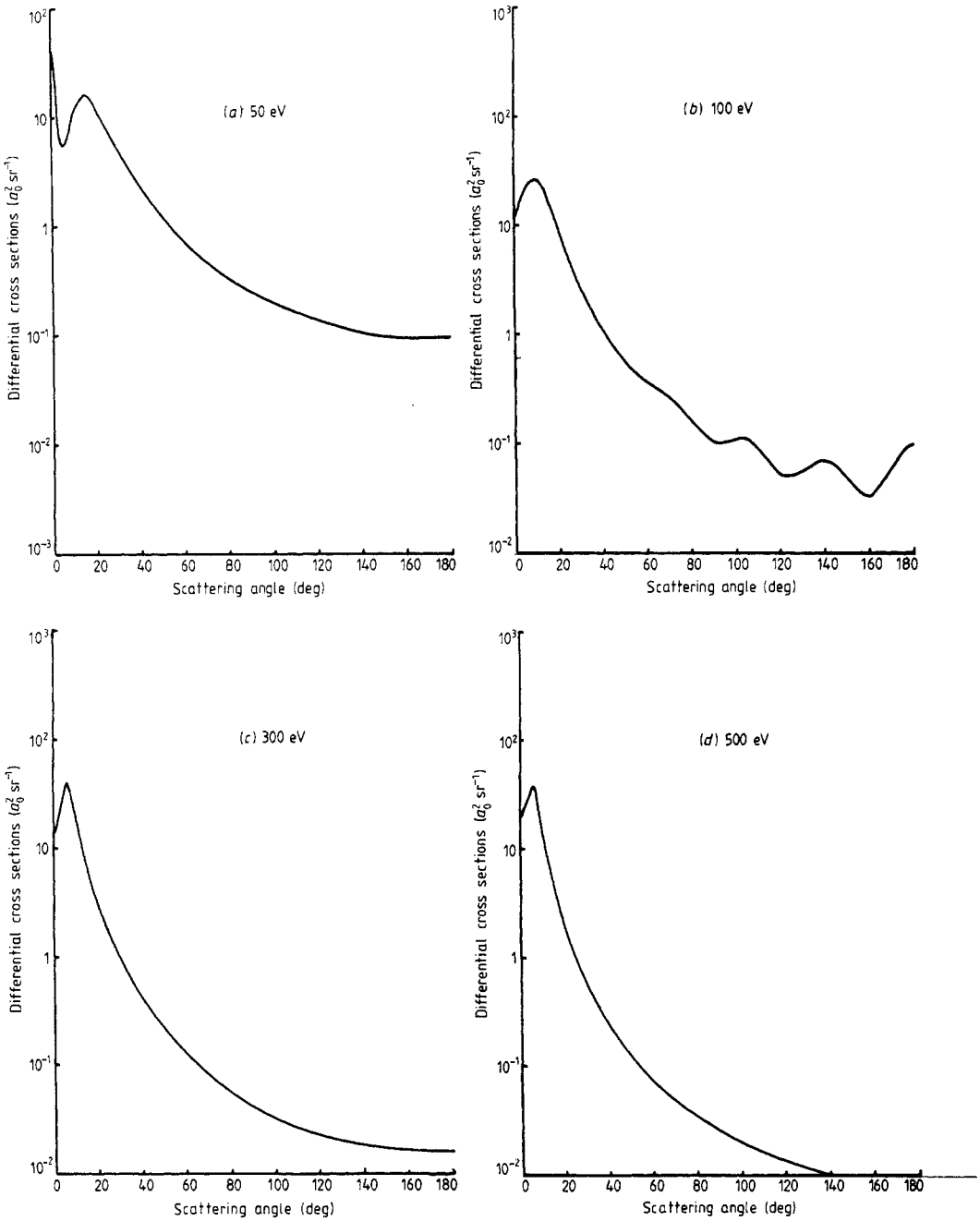

Figure 2. The differential cross sections (in a_0^2 sr^{-1}) for the elastic scattering of the positrons by magnesium atoms at (*a*) 50 eV, (*b*) 100 eV, (*c*) 300 eV and (*d*) 500 eV.

compared them with the experimental results of Williams and Trajmar (1978) at 10, 20 and 40 eV. They have measured differential cross sections between 10 to 130°. These results are normalised and have an uncertainty of ±50%. The normalisation is done by using the 3^1P excitation function measurements of Leep and Gallagher (1976). The extrapolation at higher angles is probably not corrrect. At 10 eV our results show two minima, one at 65° and the other at 140°, whereas the experimental results show only one minimum at 70°. Comparison of our results at different impact energies shows that the agreement is good at small angles. At higher angles the results disagree. The same thing was observed by Fabrikant (1980) for his results at 10 and 20 eV. Perhaps the normalised and extrapolated results of Williams and Trajmar require reinvestigation. At 100 and 500 eV, we have compared our results with the results of Gregory and Fink (1974) and found that the two calculations give nearly the same results, except in the forward direction, because they have not included polarisation effects. Such an agreement indicates that the spin–orbit effect is not appreciable for energies varying from 100 to 500 eV.

In figure 2, we show our differential cross section results for the elastic scattering of positrons by Mg atoms. Because of the absence of any other theoretical or experimental results, no comparison is possible. In the present calculations, we have not included absorption effects. The inclusion of absorption effects is expected to increase the differential cross sections in the forward direction (as noted by Khare *et al* (1982) for e^+–Ar scattering).

Table 2. Total elastic cross sections (in a_0^2) for electron–Mg and positron–Mg scattering.

	Theoretical results		Experimental data	
	e^-–Mg		e^+–Mg	e^-–Mg
Energy (eV)	Present values	Fabrikant (1980)	Present values	Williams and Trajmar (1978)
10	198.7	91.11	35.05	103.6
20	104.8	43.98	18.57	57.17
40	35.55	—	15.85	23.58
50	28.23	—	15.47	
100	17.17	—	12.43	
200	11.12	—	8.75	
300	8.51	—	6.91	
400	7.00	—	5.79	
500	6.00	—	5.02	

In table 2, we have presented our total elastic cross sections for the scattering of electrons and positrons by Mg atoms along with the results of Fabrikant (1980) and the experimental data of Williams and Trajmar (1978). For electron scattering our results overestimate the cross sections whereas Fabrikant's results underestimate them. As the main contribution to the total cross sections comes from the low-angle region, where extrapolation has been employed the total cross sections of Williams and Trajmar (1978) are suspect. The reason for such a big difference between the present values and those obtained by Fabrikant remains obscure. For positron–Mg total elastic cross sections no comparison is possible due to the absence of any other theoretical or

experimental results. Finally, we conclude that more experimental measurements are needed for the elastic scattering of electrons as well as positrons by Mg atoms covering a wide energy region.

Acknowledgments

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