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Positron scattering from magnesium

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Abstract

The elastic cross section for positron scattering from Mg has been determined by the polarized-orbital method while the excitation and ionization cross sections have been determined within a distorted-wave framework. We analyze the relative contributions of these individual cross sections to the total cross section and compare our results to recent experimental measurements. Although our results are in satisfactory agreement with the experimental measurements for energies greater than 30 eV, at lower energies there are a number of unresolved questions which need further investigation.

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1. Introduction

Recently experimental measurements of the total cross section and the positronium formation cross section for positron scattering from magnesium were presented in Ref. [1] at energies between 1 and 50 eV. These quantities have also been calculated recently by several groups. Many-body theory methods were employed in Ref. [2] in order to describe the positron-atom interaction by means of a non-local energy-dependent correlation potential, thereby including the effects of both polarization and positronium (Ps) formation. A close-coupling method was used in Ref. [3] to examine the effect of positronium formation on the elastic and excitation cross sections, and to calculate the cross section for Ps formation. As well, in Ref. [4] the elastic cross section was calculated using a relativistic polarized-orbital approximation. These results have prompted us to examine the magnitudes of the various contributions to the total cross section. It is of interest to compare the different contributions, elastic, excitation and ionization, and to show at what energies different processes are important.

Earlier work on positron Mg scattering includes that given in Ref. [5] where the elastic cross section was calculated at energies between 10 and 500 eV using a real optical potential and that presented in Ref. [6] where the Harris variational method was used for energies between 2 and 5 eV.

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For magnesium the threshold for positronium formation is 0.84 eV, while those for excitation and ionization are 4.35 and 7.65 eV, respectively. The work of Ref. [3] predicts that the effect of positronium formation on the total cross section is small above 25 eV.

We have calculated the cross sections for various contributions to the total cross section, namely, the elastic cross section from 0.5 to 200 eV, and the excitation cross section to the bound np ^{1}P states as well as the ionization cross section at energies between 10 and 200 eV. We used the polarized-orbital method for elastic scattering and the distorted-wave approximation for both excitation and ionization. However, in all our calculations the effect of positronium formation was not considered.

In Section 2 we briefly describe our theoretical methods, and in Section 3 we compare our results with the experimental data and other theoretical calculations. Finally, in Section 4 we present our conclusions.

2. Theory

Numerical atomic Hartree–Fock wave functions were used for all the calculations presented here. The ground stage Mg (3s^2 ^{1}S) wave function was obtained by a fully varied Hartree–Fock procedure. The excited Mg (3snp ^{1}P°) states were obtained in a semi frozen-core manner, in which the 1s, 2s and 2p orbitals were held fixed at their ground state values while the 3s and np orbitals were varied. The wave function for Mg$^+$ (3s ^{2}S) was determined in a similar frozen-core manner where only the 3s orbital was varied.

2.1. Elastic scattering

The elastic phase shifts for magnesium were obtained using the polarized-orbital method. The basic procedure used is identical to that which we employed previously for positron scattering from the noble gases (Ref. [7] and references cited therein). We shall therefore present only a brief outline of the theory (for details see Ref. [8]).

In the polarized-orbital method the scattering phases shifts are obtained from the solution of the differential equation

$$\left\{\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{l(l+1)}{r^2}+2[V_0(r)+V_1(r)]+k^2\right\}u_{lk}(r)=0 \tag{1}$$

subject to the boundary conditions

$$u_{lk}(0)=0 \quad \text{and}$$

$$u_{lk}(r)_{r\to\infty}\to A_l\sin\left(kr+\frac{l\pi}{2}+\delta_l(k)\right). \tag{2}$$

Here the $\delta_l(k)$ are the partial-wave phase shifts and k is the magnitude of the momentum of the incident positron. Furthermore, $V_0(r)$ is the usual static potential while $V_1(r)$ is the polarization potential as determined by the polarized-orbital method (see Ref. [8]). This polarization potential can be expressed as

$$V_1(r)=\sum_\nu V_1^\nu(r), \tag{3}$$

where asymptotically

$$V_1^\nu(r)_{r\to\infty}\to\frac{\alpha_\nu}{2r^{2\nu+2}} \tag{4}$$

with the α_ν being the multipole polarizabilities of the atom. For magnesium, all the atomic orbitals were polarized in the determination of the various contributions to $V_1^\nu(r)$ and the ν values from 1 to 9 were included in the above expansion. As with the noble gases, we estimated the higher multipole contributions $V_1^\nu(r)$, to the polarization potential, by the approximate form

$$V_1^\nu(r)=\frac{v_1(r)}{\nu^p} \qquad \nu\geqslant 10, \tag{5}$$

where the function $v_1(r)$ and the value of the parameter p were found from the calculated values of $V_1^\nu(r)$ for $\nu=8$ and 9. For magnesium p was found to have a value of 3.765. As for the noble gases, the monopole contribution ($\nu=0$) to the polarization potential was not included.

2.2. Excitation

The optically allowed transitions from the 3s^2 ^{1}S ground state of Mg to the 3snp ^{1}P° states give the most important contributions to the inelastic excitation cross section. The cross sections for the excitation of Mg to the first six excited np ^{1}P° states were calculated using a distorted-wave approximation, while those for the higher np ^{1}P° states were estimated by assuming a $1/n^3$ scaling factor. The cross sections for excitation of optically forbidden states were not calculated since their magnitude would be substantially less than that for the ^{1}P° states.

The angle integrated cross section for excitation from the ground state of Mg to an excited 3snl (^1L) state is the sum over the magnetic quantum number M of the cross section σ_M for excitation to the different M levels, where

$$\sigma_M = 4\pi^2(k_b/k_a)\int \mathrm{d}\Omega_{k_b}\,|t_{ba}^M|^2 \qquad (6)$$

with k_a and k_b being the momenta of the positron in the ground and excited state channels, respectively (Ref. [9]). The T matrix element is expressed as

$$t_{ba}^M = \int \mathrm{d}\boldsymbol{r}_0\, \chi_b^{-*}(\boldsymbol{r}_0)\chi_a^{+}(\boldsymbol{r}_0)\left\langle \Psi_b \middle| \sum_i -(1/r_{i0}) \middle| \Psi_a \right\rangle, \qquad (7)$$

where $\chi_b^{-*}(\boldsymbol{r}_0)$ and $\chi_a^{+}(\boldsymbol{r}_0)$ are the distorted waves for the two channels normalized to unit flux, Ψ_a and Ψ_b are the ground and excited state wave functions for the atom and r_{i0} is the distance from the positron to the ith electron.

The partial-wave contributions to the distorted waves were calculated in the field of the static and polarization potentials in each channel by solving Eq. (1). The static potentials were derived from the corresponding Hartree–Fock atomic wave functions. For the ground state the polarization potential given by Eq. (3) was used, so that the partial-wave functions were the same as used for elastic scattering. For the excited states the polarization potentials were calculated using an extension to Stone's method (Ref. [10]). Converged values of the T-matrix were obtained by summing typically 30–50 partial waves and using a Born subtraction technique to estimate the remainder.

2.3. Ionization

The ionization cross sections were obtained following the CPE method described in Ref. [11]. Here the total cross section for positron impact ionization of an atom (in units of πa_0^2) is expressed in terms of the following partial wave expansion

$$Q(E_\mathrm{i}) = \frac{16}{\pi E_\mathrm{i}}\int_0^E \mathrm{d}E_\mathrm{e}\sum_{l_\mathrm{i}l_\mathrm{e}l_\mathrm{f}}(2L+1) \times \left|\sum_\lambda f_\lambda(l_\mathrm{b}l_\mathrm{i}l_\mathrm{e}l_\mathrm{f};L)\langle (P_\mathrm{b}P_\mathrm{i}|2/r_1 - 2/r_{12}|P_\mathrm{e}P_\mathrm{f}\rangle\right|^2, \qquad (8)$$

where l_i and l_f are the orbital angular momentum quantum numbers of the positron in the initial and final channels respectively, l_e is the corresponding quantum number of the ejected electron and l_b is that of the electron when bound in the atom; L is the total angular momentum. The kinetic energies obey the energy conservation equation i.e.,

$$E = E_\mathrm{i} - I = E_\mathrm{e} + E_\mathrm{f}, \qquad (9)$$

where I is the ionization potential of the atom, in this case magnesium. The angular dependent factor f_λ is given in Ref. [11]. In Eq. (8), r_1 is the positron coordinate and r_2 the electron coordinate while the $P(r)$ represent radial wavefunctions. In particular, P_b is the bound-electron orbital, P_i and P_f are the initial and final positron wave functions and P_e is the wave function of the ejected electron.

In our present calculations were included contributions for the ionization of both the 3s and 2p electrons. We note that the threshold for 2p ionization is around 62 eV. The ionization of the 1s and 2s electrons makes a negligible contribution to the ionization cross section, although the 2s threshold opens around 102 eV. Our ionization calculations were carried out in the energy range from 12 to 200 eV.

The bound-state functions P_b were taken as the numerical Hartree–Fock orbitals for the 3s and 2p electrons. The incident positron partial waves P_i were obtained as solutions of Eq. (1) without the polarization potential V_1. In the CPE approximation the scattered positron and ejected electron partial waves were calculated in the field of simple Coulomb potentials as follows

$$\begin{cases} V_e = -1/r \quad V_f = 0 \quad \text{for } E_e < E_f, \\ V_e = -2/r \quad V_f = 1/r \quad \text{for } E_e > E_f. \end{cases}$$

In order to obtain converged results for these cross sections, we included up to 20 partial waves for the incident positron and up to 15 partial waves for the ejected electron. The integration over the energy of the ejected electron in Eq. (8) was carried out using 6 gaussian nodes. The number of partial waves for the scattered positron was obtained from the triangular condition among l_i, l_e and l_f, respectively.

3. Results

As a check on the quality of our bound state wave functions, we have calculated the oscillator strength for the resonance $3s^2 \rightarrow 3s3p$ transition and obtained a value of 1.99 in the length formulation. This compares well with the recent experimental determination of 1.87 ± 0.10 given in Ref. [12]. The more elaborate MCHF calculation given in Ref. [13] yielded 1.757 in the length formulation and 1.736 in the velocity formulation.

We first compare our results for various transitions contributing to the total cross section with previous theoretical calculations. We then compare these theoretical results with the experimental values of the Wayne State group who are continuing to refine their measurements and have sent us their latest though still preliminary data (Ref. [14]) and draw conclusions about the relative importance of the various cross sections for different energy ranges.

Fig. 1 shows our results for excitation to the $3snp\ ^1P^\circ$ states for $n = 3, 4, 5$. Also shown are the results of Ref. [3] for excitation to the 3s3p $^1P^\circ$ state, both with the inclusion of Ps formation and without it. Our results are of a similar shape to those of Ref. [3] and lie between their two curves. The other excitation cross sections are less by an order of magnitude. Our ionization results are also shown, as are our elastic cross sections for comparison. We have estimated the sum of the cross sections for excitation, $\sum_{n=9}^{\infty} \sigma_n$ as $3.506\sigma_8$, where σ_n is the cross section for excitation to $3snp\ ^1P^\circ$. This was done by using a $1/n^3$ scaling procedure, assuming that the $3snp\ ^1P^\circ$ states act like states in a hydrogen-like Rydberg series for $n \geqslant 8$. We checked the sensitivity to the $1/n^3$ scaling law by carrying out a similar calculation for $n > 7$ and found it affected σ_{tot} by at most 10^{-2}. In Table 1 we present our various cross sections as a function of the energy of the incident positron.

In Fig. 2 we have plotted the total cross section results of Ref. [14] as well as the 'no positronium' cross section obtained by subtracting their measured positronium formation cross section from the total. Also included are some results from other theoretical calculations. The solid line is the sum of our elastic, excitation and ionization cross sections. We note that the experimental measurements cannot discriminate against positrons elastically scattered in the forward direction. This problem is more severe at lower scattering energies and, if taken into account, would have the effect of raising the total cross sections particularly at these energies. (See Ref. [15] for a discussion of the mag-

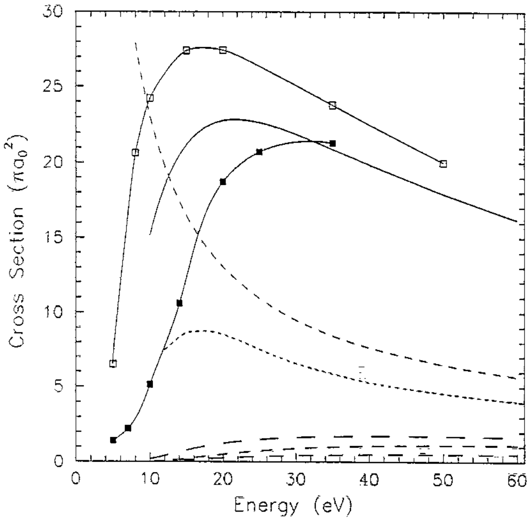

Fig. 1. Contributions to total cross section: ——, present cross section for 3p $^1P^\circ$ excitation; —— ——, for 4p $^1P^\circ$; —— —, for 5p $^1P^\circ$; — — —, for $np\ ^1P^\circ$, $n > 5$; - - -, for elastic scattering; - - -, for ionization; ■, Ref. [3], 3p $^1P^\circ$ excitation (5 state CCA); □, Ref. [3], 3p $^1P^\circ$ excitation (2 state CCA).

Table 1
Scattering cross sections (in πa_0^2) for Mg at different values of the incident energy

(eV)	σ_{el}	$\sigma_{ex}(3p)$	$\sigma_{ex}(4p)$	$\sum_{n=5}^{8}\sigma_{ex}(np)$	$\sigma_{ex}(n > 8p)$	σ_{ion}	σ_{tot}
0.5	312.315						
1.0	178.534						
2.0	94.252						
4.0	51.312						
6.0	35.851						
8.0	27.909						
10.0	23.055	15.183	0.168	0.011	0.001		
12.0	19.773	18.415	0.399	0.056	0.006	7.480	46.129
13.0	18.496	19.570	0.524	0.090	0.012	7.923	46.615
15.0	16.438	21.197	0.764	0.173	0.029	8.639	47.240
16.0	15.596	21.745	0.872	0.219	0.040	8.719	47.191
18.0	14.179	22.455	1.064	0.312	0.062	8.741	46.813
20.0	13.034	22.788	1.221	0.402	0.084	8.525	46.054
21.0	12.538	22.852	1.289	0.444	0.095	8.355	45.573
26.0	10.608	22.545	1.531	0.619	0.143	7.309	42.755
30.0	9.503	21.895	1.641	0.717	0.171	6.570	40.497
40.0	7.648	19.857	1.739	0.847	0.212	5.297	35.600
50.0	6.484	17.896	1.718	0.881	0.226	4.581	31.786
60.0	5.675	16.208	1.652	0.872	0.228	4.035	28.670
70.0	5.076	14.787	1.573	0.845	0.223	3.422	25.926
80.0	4.611	13.592	1.492	0.811	0.216	3.149	23.871
100.0	3.932	11.710	1.344	0.741	0.200	2.592	20.519
120.0	3.456	10.293	1.217	0.676	0.184	2.171	17.997
130.0	3.267	9.715	1.161	0.647	0.177	2.001	16.968
140.0	3.101	9.203	1.111	0.621	0.170	1.830	16.036
150.0	2.955	8.746	1.064	0.596	0.163	1.682	15.206
200.0	2.420	7.038	0.878	0.495	0.137	1.216	12.184

nitude of this effect for positron scattering from Rb.)

Above 30 eV where positronium formation is almost negligible, the sum of our cross sections agrees well with the experimental results. At lower energies, our results have a similar shape to that of the experimental 'no positronium' data but are considerably larger. Part of this discrepancy can be accounted for however, as noted above, by the experimental measurements of the total cross section not being able to detect positrons elastically scattered in the forward direction. The total cross section of Ref. [2], which includes positronium formation into only the 1s state, lies above the measured cross section below 7 eV. We also show the positronium formation cross section of Ref. [3] which included contributions from the 1s, 2s and 2p states of positronium.

4. Conclusions

We have investigated the contributions to the total cross section for scattering of positrons from Mg up to 200 eV. At energies up to 7 eV the elastic cross section dominate, but Ps formation into the 1s state gives an important contribution. Between 7 eV and 25 eV excitation to ^{1}P states and ionization become important, but Ps formation, to the 2s and 2p states as well as the 1s state, makes a significant contribution. Above 25 eV excitation of the 3s3p ^{1}P° excited state gives the largest contribution to the total cross section while elastic scattering and ionization are less important and comparable in magnitude. Agreement between the present calculations and the experimental measurements seems to be satisfactory above 30 eV. At lower energies there is considerable disagreement between

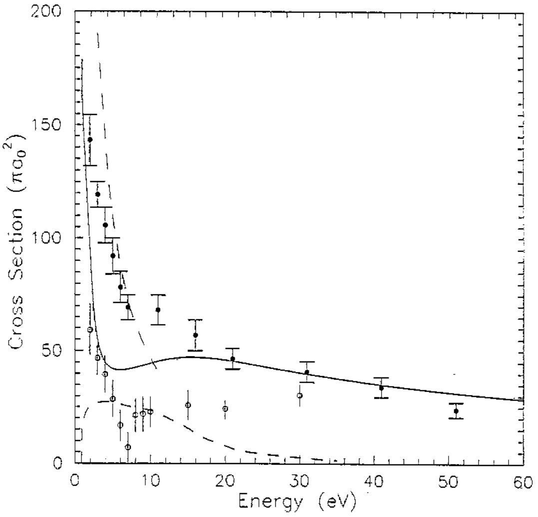

Fig. 2. Total cross section: —, present results, — —, Ref. [2]; — — —, Ps formation, Ref. [3]; Preliminary experimental data (Ref. [14]): •, total cross section, ○, total cross section minus positronium formation.

the measured positronium formation cross section and the calculations of Ref. [3]. Further theoretical and experimental investigations in this energy range would be highly desirable.

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