

Analytical Expression of Photoionization Cross Sections for Rare Gases

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The theoretical photoionization cross sections for subshells in rare gases have been fitted to an appropriate polynomial on a log-log scale. The obtained results are compared with the theoretical values and also with the similar results of McMaster *et al.*

KEY WORDS: Photoionization cross sections/ Rare gases/ Analytical expression

1. INTRODUCTION

The photoelectric effect is one of the most important processes in interaction of photons with atoms and plays a dominant role in attenuation of low-energy photons in matter. There have been reported extensive experimental and theoretical studies for wide range of photon energy and for variety of target elements.^{1,2)}

Old theoretical calculations were made with hydrogenic or screened hydrogenic wave functions. However, in recent years theoretical photoionization cross sections based on realistic atomic models, such as the Hartree-Fock (HF) method, are available as numerical tables. McGuire³⁾ used the Hartree-Fock-Slater (HFS) method and calculated nonrelativistic photoionization cross sections. Storm and Israel⁴⁾ performed the similar calculations from 1 keV to 100 MeV for elements with $Z=1$ to 100. On the other hand, Veigle⁵⁾ published the table of photoionization cross sections for element from H to Pu from 0.1 keV to 1 MeV. In the energy region between 1 keV and 1 MeV, he obtained the values of photoionization cross sections from experimental photon attenuation data by subtracting the theoretical scattering cross sections. For lower photon energies, the HFS method was used to calculate nonrelativistic photoionization cross sections.

Scofield⁶⁾ calculated the relativistic cross sections for photoionization from various atomic subshells for elements up to $Z=101$ and for photon energy from 1 to 1,500 keV by the use of the relativistic HFS (RHFS) model. The similar calculations were made by Band *et al.*⁷⁾ for elements from $Z=1$ to 100 in the energy range between 0.132 and 4.509 MeV. These numerical tables have been frequently applied to analyze the experimental data and good agreement with

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experimental data has been observed.

However, in these tables the photoionization cross sections are available only at given energy points and the value for an intermediate energy should be evaluated by interpolation. With recent advent of synchrotron radiation facilities, it becomes quite easy to obtain strong monochromatic photon beams with arbitrary energy and the photoionization cross sections for various energies are often necessary.

In such a case, it is very useful to express the photoionization cross sections for atoms in the form of analytical functions with respect to incident photon energy. McMaster *et al.*⁸⁾ obtained the analytical expressions of the experimental photoionization cross sections for various elements in the energy range of 1 keV to 1 MeV by fitting them to a polynomial in the log-log scale. In order to derive the experimental photoionization cross sections, they computed the incoherent scattering cross sections from form factors of Cromer and Mann⁹⁾ and the coherent scattering cross sections from form factors of Cromer and Waber.¹⁰⁾

The photoionization cross sections were estimated by subtracting the sum of theoretical incoherent and coherent cross sections from the experimental total attenuation cross sections. For high energy photons, the theoretical photoionization cross sections by Schmickley and Pratt¹¹⁾ were used.

The results of McMaster *et al.*¹¹⁾ are very convenient and have been widely used in x-ray spectroscopy. However, they tabulated the coefficients of polynomial only for the total photoionization cross sections of atomic shells. It is worthwhile to derive the similar analytical expression for the subshell photoionization cross sections. In the present work, we use the relativistic photoionization cross sections for subshells computed by Scofield⁶⁾ and fit the logarithm of them to the power series of the logarithm of the photon energy. The calculations have been performed for all subshells of Ne, Ar, and Kr in the energy range from 1 to 1,500 keV.

2. METHOD

For photoionization cross sections, we use the theoretical values of Scofield.⁶⁾ He performed the fully relativistic calculations for the photoelectric process with the RHFS method,¹²⁾ including the contributions from all multipoles and retardation effects. The obtained results are tabulated for elements from $Z=1$ to 101 and for photon energies from 1 to 1,500 keV.

Following the method of McMaster *et al.*,⁸⁾ we use the equation

$$\ln \sigma = \sum_{i=0}^n A_i (\ln E)^i, \quad (1)$$

where σ is the subshell photoionization cross section in barns/atom at the incident photon energy E in keV, n is the degree of polynomial, and A_i is the fit coefficient. The same equation was also used by Veigele.⁵⁾

We choose $n=3$ in the whole calculations in the present work. For each subshell in each element, a set of data points, (E_j, σ_j) , where σ_j is the photoionization cross sections at photon energy E_j , are taken from the table of Scofield⁶⁾ and the fit coefficients in Eq. (1) are determined with the least-squares method. All the data points given in the table are used, i.e. all the cross sections available at energy points between 1 and 1,500 keV are used in fitting.

3. RESULTS AND DISCUSSION

The calculated results of the coefficients in Eq. (1), A_i , are listed Tables I for Ne, Ar and Kr, respectively. The fitting is generally good. The deviation of the σ values obtained from Eq. (1) using A_i in the tables is less than 10%, except for the lowest and highest energies, 1 and 1,500 keV. The maximum deviation is found to be 17% at 1,500 keV for M_1 shell of Ar and Kr. It is interesting to note that each fit coefficient has similar values and same sign for all elements and for all subshells, except for K shell in Kr where A_1 is positive. Especially, for the subshells with the same relativistic quantum number κ , i.e. K, L_1 , M_1 , N_1 shells ($\kappa=-1$), L_2 , M_2 , N_2 shells ($\kappa=1$), and L_3 , M_3 , N_3 shells ($\kappa=-2$), the A_i values are almost same.

Table I. Fit coefficients for Ne.

Shell	A_0	A_1	A_2	A_3
K	1.2260E+01 ¹⁾	-2.2097E+00	-2.9998E-01	2.7968E-02
L_1	9.1635E+00	-2.0846E+00	-3.2023E-01	2.9055E-02
L_2	7.4243E+00	-3.0720E+00	-3.3302E-01	3.5866E-02
L_3	8.0585E+00	-2.9576E+00	-3.8951E-01	4.1886E-02

¹⁾ 1.2260E+01 means 1.2260×10^1 .

Table II. Fit coefficients for Ar.

Shell	A_0	A_1	A_2	A_3
K	1.3218E+01 ¹⁾	-1.2428E+00	-4.8107E-01	3.9625E-02
L_1	1.0865E+01	-1.6078E+00	-3.6585E-01	3.0076E-02
L_2	1.0619E+01	-2.5864E+00	-3.7840E-01	3.7003E-02
L_3	1.1246E+01	-2.4929E+00	-4.2684E-01	4.1910E-02
M_1	8.7187E+00	-1.6518E+00	-3.5307E-01	2.9053E-02
M_2	8.0443E+00	-2.4773E+00	-3.9878E-01	3.8208E-02
M_3	8.6679E+00	-2.3785E+00	-4.5043E-01	4.3543E-02

¹⁾ 1.3218E+01 means 1.3218×10^1 .

Table III. Fit coefficients for Kr.

Shell	A_0	A_1	A_2	A_3
K	1.2550E+01 ¹⁾	5.9167E-01	-7.8575E-01	5.7107E-02
L_1	1.1704E+01	-7.0400E-01	-4.7571E-01	3.4944E-02
L_2	1.3208E+01	-1.8509E+00	-4.4264E-01	3.8609E-02
L_3	1.3825E+01	-1.7783E+00	-4.9087E-01	4.3209E-02
M_1	1.0530E+01	-1.2432E+00	-3.4351E-01	2.5149E-02
M_2	1.0840E+01	-1.5912E+00	-4.7950E-01	4.0276E-02
M_3	1.1482E+01	-1.5539E+00	-5.1719E-01	4.4001E-02
M_4	1.0997E+01	-2.7032E+00	-4.8882E-01	4.6599E-02
M_5	1.1331E+01	-2.6010E+00	-5.4614E-01	5.3072E-02
N_1	8.5110E+00	-1.3055E+00	-3.2822E-01	2.4020E-02
N_2	8.4013E+00	-1.6046E+00	-4.7183E-01	3.9534E-02
N_3	9.0201E+00	-1.5429E+00	-5.1811E-01	4.4036E-02

¹⁾ 1.2550E+01 means 1.2550×10^1 .

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 Table IV. Comparison of fit coefficients in the present work with those by McMaster *et al.* for K shell.

Element		A_0	A_1	A_2	A_3
Ne	MCM ¹⁾	1.24485E+01 ³⁾	-2.45819E+00	-2.12591E-01	1.96489E-02
	MITE ²⁾	1.2260E+01	-2.2097 E+00	-2.9998 E-01	2.7968 E-02
Ar	MCM	1.39491E+01	-1.82276E+00	-3.28827E-01	2.74382E-02
	MITE	1.3218E+01	-1.2428 E+00	-4.8107 E-01	3.9625 E-02
Kr	MCM	1.35927E+01	-3.05214E-02	-6.51340E-01	4.77616E-02
	MITE	1.2550E+01	5.9167 E-01	-7.8575 E-01	5.7107 E-02

¹⁾ McMaster *et al.* (Ref. 8).

²⁾ Present work.

³⁾ 1.24485E+01 means 1.24485×10^1 .

Table IV represents the comparison of the present fit coefficients with the values of McMaster *et al.*⁸⁾ for K shell. The results for other shells cannot be compared with their values because in their table only the values for the total shells are listed and the coefficients for subshells are not given separately. It can be seen from the table that there are small difference in A_2 and A_3 values, but the present results for K shell are generally in agreement with the values of McMaster *et al.*⁸⁾

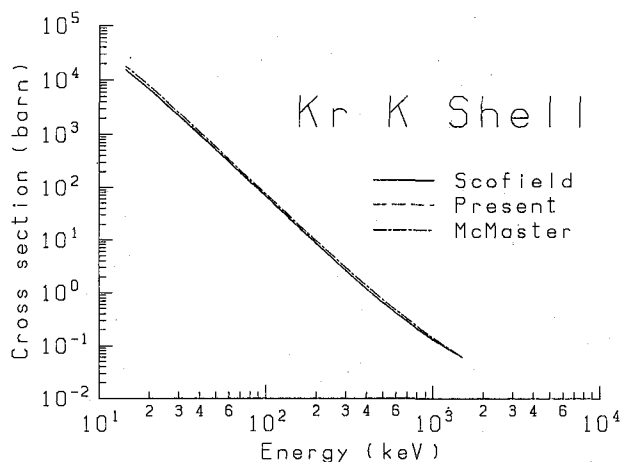


Fig. 1. Comparison of the K shell photoionization cross sections for Kr. The solid line represents the calculated values of Scofield (Ref. 6). The dashed line indicates the present results, and the dot dashed line shows the results of McMaster *et al.* (Ref. 8).

Figure 1 shows the comparison of the K shell photoionization cross sections for Kr obtained in the present work with the tabulated values of Scofield⁶⁾ and the results of McMaster *et al.*⁸⁾ The present results are in good agreement with the Scofield's values. On the other hand, the analytical expression of McMaster *et al.* yields higher values than the calculated ones by Scofield.

In Fig. 2, the relative ratios of the photoionization cross sections of the present work and of McMaster *et al.*⁸⁾ for K shell in Kr to the tabulated values of Scofield.⁶⁾ In this case, the deviation of the present results are less than 4%. The analytical expression of McMaster *et al.*

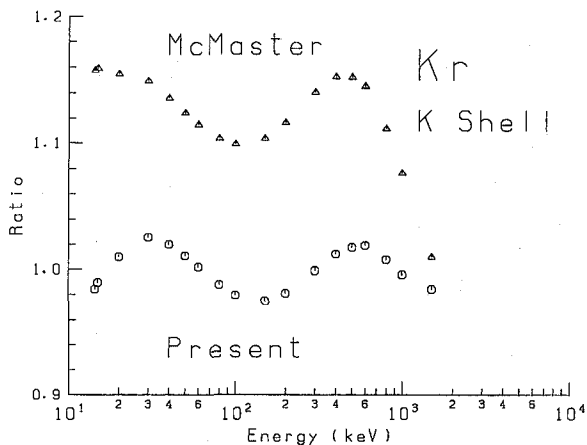


Fig. 2. Ratios of the K shell photoionization cross sections for Kr calculated by the analytical expressions to those of the numerical values of Scofield (Ref. 6). The circles represent the present results and the triangles indicate the results of McMaster *et al.* (Ref. 8).

gives about 10% larger values and deviation is also larger. It is natural because the present results are obtained by fitting to the theoretical photoionization cross sections of Scofield, while McMaster *et al.* used the experimental cross sections estimated from the total attenuation cross sections.

In conclusion, we have derived analytical expressions for subshell photoionization cross sections in rare gases. The theoretical photoionization cross sections of Scofield as a function of photon energy in the range from 1 to 1,500 keV were fitted to polynomials in log-log scale with the least-squares method. The obtained results are in agreement with the tabulated values within 10% except for 1 keV and 1,500 keV. The present results are very useful to analyze the experimental data.

REFERENCE

- (1) R.H. Pratt, A. Ron and K.H. Tseng, *Rev. Mod. Phys.*, **45**, 273 (1973).
- (2) S.T. Manson, *Adv. Electron. Electron Phys.*, **41**, 73 (1976).
- (3) E.J. McGuire, *Phys. Rev.*, **175**, 20 (1968).
- (4) E. Storm and H.I. Israel, *Nucl. Data Tables*, **A7**, 565 (1970).
- (5) W.J. Veigele, *Atomic Data*, **5**, 51 (1973).
- (6) J.H. Scofield, Lawrence Livermore Laboratory Report No. UCRL-51326 (1973), unpublished.
- (7) I.M. Band, Yu. I. Kharitonov and M.B. Trzhaskovskaya, *Atomic Data Nucl. Data Tables*, **23**, 443 (1979).
- (8) W.H. McMaster, N.K. Del Grande, J.H. Mallett and J.H. Hubbel, Lawrence Livermore Laboratory Report No. UCRL-50174 (1969), unpublished.
- (9) D.T. Cromer and J.B. Mann, Los Alamos Scientific Laboratory Report No. LA-DC-8819 (1967), unpublished.
- (10) D.T. Cromer and J.T. Waber, *Acta Crystall.*, **18**, 104 (1965).
- (11) R.D. Schickley and R.H. Pratt, *Phys. Rev.*, **164**, 104 (1967).
- (12) D.A. Liebermann, J.T. Waber and D.J. Cromer, *Phys. Rev.*, **137**, A27 (1965).