

IONIZATION AND EXCITATION  
OF HELIUM BY PROTON IMPACT

By

Barney B. Roberts

Thesis Submitted in Partial Fulfillment of  
the Requirements for a Master of Science

Degree in Physics

Commencement August, 1972

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## ABSTRACT

Cross sections for the simultaneous ionization and excitation of helium by proton impact were calculated using a first Born approximation. The main purpose of this theoretical investigation was to further investigate a thesis by Byron and Joachain<sup>1</sup> that only atomic wave functions containing electron-electron correlation terms are sufficiently accurate to describe double-processes in helium, that is, processes which cause a transition of both electrons. For the final state wave function a symmetric product of a hydrogen-like wave function and a positive energy Coulomb wave function were used. For the initial state three different wave functions were used, a 12-term correlated wave function, an uncorrelated product of hydrogen-like wave functions, and a Green's expansion of the Hartree-Fock wave function which is also uncorrelated. Comparisons were made with the analytical results of Bell and Kingston<sup>7</sup> who investigated the single ionization of helium by proton impact using a correlated wave function; however, in their work they considered the case only for the residual ion in the ground state. The analysis of Mapleton<sup>2</sup> for simultaneous ionization and excitation of helium using uncorrelated wave functions was also used for comparison. Although for single processes (i.e. transition of one electron) correlation effects are not important, the results for multiple processes show significant differences between cross sections using correlated wave functions and cross sections using uncorrelated wave functions.

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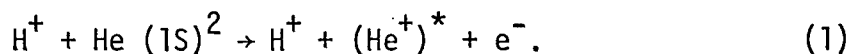
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## I. Introduction

When a fast heavy particle passes through matter, its energy is dissipated in excitation and ionization of the target particles. Knowledge of the relevant cross sections are of considerable practical and theoretical interest. For example, in the field of controlled thermonuclear research, high energy injection is used to initiate the thermonuclear process. Excitation and ionization cross sections also enter into consideration of upper atmospheric phenomena. Ions and electrons in the upper atmosphere are produced to some extent by collisions with particles from space. Some of the electrons produced contribute to the excitation of the auroras and to the population of the electronic component of the Van Allen Radiation Belt. Any detailed interpretation of auroral spectra must be based on a knowledge of excitation cross sections. Spectral observations show that high energy protons penetrate to auroral heights in the atmosphere during auroral displays, and Doppler-shifted lines of the Balmer series appear in the majority of auroral forms. Thus, from the viewpoint of thermonuclear processes and upper atmospheric phenomena, the knowledge of the interaction of protons with various gases is of considerable interest.

The subject of this particular theoretical investigation is simultaneous ionization and excitation of helium by proton impact as represented by:



(2)

The process (1) was first examined by Mapleton in 1957. Mapleton derived the following expressions for the Born scattering amplitude and total cross sections:

$$f_o = -\frac{2\mu_2 e^2}{A^2 \hbar^2} \int d\vec{r}_1 d\vec{r}_2 \psi_{k,n}^* (\vec{r}_1 \vec{r}_2) \left( e^{i\vec{A} \cdot \vec{r}_1} + e^{i\vec{A} \cdot \vec{r}_2} \right) \psi_o (\vec{r}_1 \vec{r}_2) \quad (2)$$

$$Q_o^{nk} = \int dk dA k^2 |f_o^{nk}|^2 \quad (3)$$

where:

$r_1$  C.M. Coordinate of Electron 1

$r_2$  C.M. Coordinate of Electron 2

$\psi_{k,n}^*$  Final state wave function of the helium atom

$\psi_o$  Initial state wave function of the helium atom

$A$  Momentum change vector of incident proton

Since exact wave functions are not known for helium, some type of approximate wave function must be devised. The most accurate are those of Hylleraas<sup>4</sup> and Pekeris.<sup>5</sup> The initial state wave function used by Mapleton is a product of normalized hydrogen-like ground state wave functions which do not account for electron-electron correlation. This point is emphasized here, because according to Byron and Joachain, ground state wave functions without correlation terms cannot give accurate results for collision processes in helium which cause a transition of both electrons (i.e. multiple processes). Byron and Joachain demonstrated this thesis by considering



double ionization of helium by photon absorption. They obtained excellent agreement with experimental results and showed that use of the wave function for the Hartree-Fock initial state yields poor results.

Peach<sup>6</sup>, Bell and Kingston also investigated the single ionization of helium by proton impact; however, they did not consider excited final states of the residual ion. For the initial state Peach used analytical fits to a Hartree-Fock wave function. Bell and Kingston used the correlated wave function of Stewart and Webb, which is a reevaluation of the Hylleraas six parameter wave function. However, the literature yields no analytical work on the total cross section for the multiple process of ionization and excitation of helium by proton impact using correlated wave functions.

This Thesis considers the process (1) with the residual ion in the excited states: 2s, 2p, 3s, 3p, and 3d, and also the case with the residual ion remaining in the ground state.

Of obvious importance in these calculations is the question of orthogonality between the initial and final states, that is, to guarantee anything but absurd results it must be true that

$$\langle \psi_0 | \psi_{kn} \rangle = 0.$$

It is well known (shown in detail later) that orthogonality naturally exists between the initial and final state when they are not of the same parity. For example, in Mapleton's work, and in any similar analysis using uncorrelated ground state wave functions in conjunction with the same final state

(4)

approximation,  $\Psi_{k,n}(\bar{r}_1, \bar{r}_2)$ , used herein, orthogonality is assured for all final states except those having an angular momentum quantum number of zero (s states), and likewise for initial states containing both s waves and p waves orthogonality naturally occurs for final states other than s states or p states. Therefore, for the 12-term wave function (see Section II.A) and for the final states of the residual ion considered herein, orthogonality exists only for the 3d final state. For all other final states a correction to the final state wave function must be made.

One way to overcome this problem, is to subtract from the final state wave function the projection of the initial state onto the final state. Then, giving the new final state the symbol  $\Psi_f(\bar{r}_1, \bar{r}_2)$ , it is written as

$$\Psi_f(\bar{r}_1, \bar{r}_2) = \Psi_{k,n}(\bar{r}_1, \bar{r}_2) - \langle \Psi_{k,n}(\bar{r}_1, \bar{r}_2) | \Psi_o(\bar{r}_1, \bar{r}_2) \rangle \Psi_o(\bar{r}_1, \bar{r}_2)$$

Now  $\Psi_f(\bar{r}_1, \bar{r}_2)$  is obviously orthogonal to the initial state. This is the technique used by Oldham and Miller<sup>8</sup> in calculating the differential cross sections for simultaneous ionization and excitation of helium by proton impact using the 12-term correlated ground state wave function. They calculated the overlap integral,  $\langle \Psi_{k,n}(\bar{r}_1, \bar{r}_2) | \Psi_o(\bar{r}_1, \bar{r}_2) \rangle$ , and computed the matrix elements to the final states of interest here. The computer program of Oldham and Miller was utilized for this analysis by adding the required integration routines to calculate the total cross sections to the final states other than 3d.

(5)

For the uncorrelated ground state wave functions, the hydrogen-like and the Hartree-Fock, several cases could be considered without this additional complication, thus final states 2p, 3p, and 3d are computed using the uncorrected final state wave function,

## II. Analysis

### II.A Scattering Cross Section, Wave Functions

The first Born approximation to the cross section for simultaneous ionization and excitation of helium by proton impact where the residual  $\text{He}^+$  ion is in the quantum state represented by  $n$  is given by Mapleton as follows:

$$\begin{aligned} Q_0^{n,k} &= \int |f_0^{n,k}|^2 d\bar{k} d\bar{r} \\ f_0^{n,k} &= \frac{4\mu}{A} \int \Psi_{k,n}^* (\bar{r}_1 \bar{r}_2) e^{i\mathbf{A} \cdot \mathbf{r}_1} \Psi_0 (\bar{r}_1 \bar{r}_2) d\bar{r}_1 d\bar{r}_2 \\ d\bar{k} &= k^2 dk \sin \theta d\theta d\phi \\ d\bar{r} &= \sin \omega d\omega d\xi \simeq \frac{AdA}{K_0} d\xi \end{aligned} \tag{4}$$

where

$k$  momentum vector of ejected electron

$\mu$  reduced mass

$A$  momentum change vector

$\Psi_0$  initial state wave function of the helium atom

$r_i$  radius vector to electron  $i$

(6)

- $\theta$  polar angle, ejected electron
- $\phi$  azimuth angle, ejected electron
- $\omega$  polar angle, final momentum vector of incident proton
- $\xi$  azimuth angle, final momentum vector of incident proton
- $K_0$  initial momentum of incident proton

$Q_0^{n,k}$  is the total cross section for single ionization and excitation of the bound electron to the state represented by  $n$ .  $\psi_{k,n}(\vec{r}_1, \vec{r}_2)$  is the final state wave function for the helium atom with one electron free and the residual  $H_e^+$  ion in the state represented by  $n$  where  $n$  collectively specifies the three usual quantum numbers  $n, \ell$ , and  $m$ .  $f_0^{k,n}$  is the Born matrix element.

Since the main purpose of this Thesis is to compare the cross sections using correlated initial state wave functions with those resulting from the use of uncorrelated wave functions, a general representation for the initial state was devised that embodied the details of several possible wave functions. By doing this, only one set of integrals needed to be evaluated that would be applicable to all of the assumed initial state wave functions. This was accomplished by formulating the initial state as:

$$\psi_0(\vec{r}_1, \vec{r}_2) = \sum_{\lambda, \rho, \omega} r_1^\lambda r_2^\rho P_\omega(\cos \theta_{12}) e^{-\alpha_1 r_1 - \alpha_2 r_2}$$

$$\cos \theta_{12} = \frac{\vec{r}_1 \cdot \vec{r}_2}{r_1 r_2} \quad (5)$$

Table I gives the values of the parameters required to generate 1) a hydrogen-like initial state, 2) a Green's expansion of the Hartree-Fock,

(7)

and 3) a 12-term correlated initial state. 1) and 2) above are chosen because of their simplicity and lack of correlation terms. The first, 1), was also attractive because it is the same wave function used by Mapleton<sup>2</sup> and provides a very useful check on this analysis.

For the correlated initial state wave function many choices were available. The Hylleraas wave functions (or the Stewart and Webb six parameter wave function used by Bryon and Joachain) are the most accurate; however, they contain terms of  $1/r_{12}$  which hopelessly complicates the evaluation of the integrals herein. The 45-term correlated wave function<sup>7</sup> contains s, p, and d relative partial waves and consequently is quite complex and (shown later) will not be othogonal to any of the final states to be considered here. The 12-term wave function contains angular terms through the relative p wave and appears to be the simplest correlated wave function available. The 12-term wave function is not as accurate as the other functions mentioned but combines the advantages of simplicity, fewer terms, and correlation terms. One measure of accuracy is the ability of the ground state wave function to predict the ground state energy.

<u>wave function</u>	<u>ground state energy</u>
Hartree-Fock	-2.862 (a.u.)
12-term	-2.89852 (a.u.)
45-term	-2.9020 (a.u.)
Hylleraas (6-term)	-2.9032 (a.u.)
experimental	-2.90372 (a.u.)

(8)

Therefore, the 12-term wave function is an excellent compromise and should show any dramatic effects due to correlation. The final state,  $\psi_{k,n}(\bar{r}_1, \bar{r}_2)$ , is approximated by a symmetrized product of a hydrogen-like wave function for the bound electron,  $\phi_n(Z_2|r)$ , and a positive energy Coulomb wave function for the ejected electron,  $\psi_k(Z_3|r)^2$ .

Although Bryon and Joachain showed that correlation effects are important in the final state as well as the initial state, of primary importance here was the need to keep this problem soluable yet still consider correlation effects in the initial state, hence the choice of this final state:

$$\psi_{k,n}(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}} \left\{ \phi_n(Z_2|\bar{r}_1) \psi_k(Z_3|\bar{r}_2) + \phi_n(Z_2|\bar{r}_2) \psi_k(Z_3|\bar{r}_1) \right\}$$

Substitution of the above into equation (1) yields the following expression for the scattering amplitude:

$$f_o^{n,k} = \frac{4\mu}{A^2 \sqrt{2}} \sum_{\lambda, \rho, \omega} N_{\lambda, \rho, \omega} \left[ \frac{4\pi}{2\omega+1} \right]^{1/2} [I_1 + I_2]$$

where:

$$I_1 = \int \phi_n^*(Z_2|\bar{r}_1) \psi_k^*(Z_3|\bar{r}_2) r_1^\lambda r_2^\rho Y_{\omega,0}(\theta_{12}, \phi_2) \\ \times e^{i\bar{A} \cdot \bar{r}_1} e^{-\alpha_1 r_1 - \alpha_2 r_2} dr_1 dr_2$$

$$I_2 = \int \phi_n^*(Z_2|\bar{r}_2) \psi_k^*(Z_3|\bar{r}_1) r_1^\lambda r_2^\rho Y_{\omega,0}(\theta_{12}, \phi_2) \\ \times e^{i\bar{A} \cdot \bar{r}_1} e^{-\alpha_1 r_1 - \alpha_2 r_2} d\bar{r}_1 d\bar{r}_2 \quad (6)$$

(9)

And in the above,  $\phi_n^*(Z_2|r)$  is a hydrogen-like wave function for a one electron atom with a nuclear charge of  $Z_2e$ . The subscript  $n$  represents collectively the usual quantum numbers,  $n$ ,  $\ell$ , and  $m$ .  $\psi_k(Z_3|r)$  is the Coulomb wave function with wave propagation vector  $k$ , and with a field of  $Z_3e$ . Now, the problem consists of evaluation of  $I_1$  and  $I_2$  and subsequent summation over the parameters  $\alpha_1$ ,  $\alpha_2$ ,  $\lambda$ ,  $\rho$ , and  $\omega$ .

As noted earlier the initial state and final state are not orthogonal for the 12-term wave function except for final states with angular momentum quantum numbers which are greater than  $\omega$ , i.e. final states must not contain the same partial waves as contained in the initial state. Since the 12-term wave function contains s and p waves ( $\omega = 0$  and  $\omega = 1$ ), the final state is restricted to the 3d state. This is shown by considering the angular parts of the overlap integral, which are

$$\sum_{m=-\omega}^{\omega} \left\{ \int \psi_k(Z_3|\bar{r}_2) Y_{\omega,m}(\theta_{2A}, \phi_A) d\Omega_2 \phi_n(Z_2|\bar{r}_1) Y_{\omega,m}^*(\theta_{1A}, \phi_A) d\Omega_1 \right. \\ \left. + \int \psi_k(Z_3|\bar{r}_1) Y_{\omega,m}(\theta_{1A}, \phi_A) d\Omega_1 \phi_n(Z_2|\bar{r}_2) Y_{\omega,m}^*(\theta_{2A}, \phi_A) d\Omega_2 \right\}.$$

Then if  $\omega = 0$ , the above integrals are zero for all final states,  $\phi_n(Z_2|\bar{r}_1)$ , which do not contain s waves. For the 12-term initial state wave function,  $\omega$  has values 0, and 1, therefore, the integrals are orthogonal only if the angular parts of  $\phi_n(Z_2|\bar{r}_2)$  do not contain s or p waves. Therefore, for the uncorrelated initial state wave functions, orthogonality corrections are not required if transitions to the 2p, 3p, and 3d final states are considered, and for the 12-term correlated wave function corrections are not required if the  $\text{He}^+$  ion is in the 3d state.

(10)

Now  $I_2$  of equation (6) can be expressed as:

$$I_2 = \sum_{m=-\omega}^{\omega} \left[ \frac{4\pi}{2\omega+1} \right] \int e^{i\vec{A} \cdot \vec{r}} e^{-\alpha_1 r_1} \psi_k^* (Z_3 | \vec{r}_1) r_1^\lambda Y_{\omega, m}^* (\theta_{1A}, \phi_{1A}) d\vec{r}_1 \\ \times \int e^{-\alpha_2 r_2} \phi_n^* (Z_2 | \vec{r}_2) Y_{\omega, m} (\theta_{2A}, \phi_{2A}) r_2^\rho d\vec{r}_2$$

and by the same reasoning above,  $I_2 = 0$  for the final states considered here. Thus, this problem has been reduced to evaluation of  $I_1$  in general for the parameters  $\lambda$ ,  $\rho$ ,  $\omega$ ,  $\alpha_1$  and  $\alpha_2$ .



(11)

## II.B. Separation of the Integrals of the Born Matrix Elements

The positive energy Coulomb wave function,  $\psi_k$ , is written as:

$$\psi_k(Z_3|r) = \gamma' C e^{i k r} \sum_{\ell=0}^{\infty} i^{\ell} \frac{\Gamma(\ell+1+n)}{(2\ell)!} \\ \times P_{\ell}(\cos \theta_{r_k}) F(\ell+1+n, 2\ell+2, -2i k r)$$

where:

$$\gamma' = \left[ \frac{i n}{1 - e^{-2i\pi n}} \right]^{1/2} \quad n = Z_3 / i k \\ C = \frac{1}{2\pi \Gamma(n+1)} \quad \cos \theta_{r_k} = \frac{\vec{r} \cdot \vec{k}}{r k}$$

Substitution into equation (6) for  $I_1$  yields:

$$I_1 = I_{1A} I_{1B}$$

where:

$$I_{1A} = \left[ \frac{4\pi}{2\omega+1} \right] \int Y_{\omega,0}(\theta_{1k}, \phi_k) e^{i \vec{\lambda} \cdot \vec{r}_1} r_1^{\lambda} \phi_n^*(Z_2|\vec{r}_1) e^{-\alpha_1 r_1} d\vec{r}_1$$

and:

$$I_{1B} = \gamma' C i^{\omega} \frac{\Gamma(\omega+1+n)}{(2\omega)!} (2k)^{\omega} \\ \times \int e^{i k r_2 - \alpha_2 r_2} r_2^{\omega+2+\rho} F(\omega+1+n, 2\omega+2, -2i k r_2) dr_2$$

The integrals,  $I_{1A}$  and  $I_{1B}$ , are evaluated in the appendices and only the results given here.  $I_{1B}$  can be evaluated in general for the parameters,  $\omega$ ,  $\alpha_2$ , and  $\rho$ ; however,  $I_{1A}$  cannot, thus,  $I_{1A}$  is evaluated for each final state and each value of  $\omega$  ( $\omega = 0$  except for cases involving 12-term wave function, i.e.  $3d\ 0$  and  $3d \pm 1$ ).

(11)

## II.B. Separation of the Integrals of the Born Matrix Elements

The positive energy Coulomb wave function,<sup>2</sup>  $\psi_k$ , is written as:

$$\psi_k(Z_3|r) = \gamma' C e^{ikr} \sum_{\ell=0}^{\infty} i^{\ell} \frac{\Gamma(\ell+1+n)}{(2\ell)!} \\ \times P_{\ell}(\cos \theta_{r_k}) F(\ell+1+n, 2\ell+2, -2ikr)$$

where:

$$\gamma' = \left[ \frac{in}{1-e^{-2i\pi n}} \right]^{1/2} \quad n = Z_3/ik \\ C = \frac{1}{2\pi\Gamma(n+1)} \quad \cos \theta_{r_k} = \frac{\vec{r} \cdot \vec{k}}{r_k}$$

Substitution into equation (6) for  $I_1$  yields:

$$I_1 = I_{1A} I_{1B}$$

where:

$$I_{1A} = \left[ \frac{4\pi}{2\omega+1} \right] \int Y_{\omega,0}(\theta_{1k}, \phi_k) e^{i\vec{A} \cdot \vec{r}_1} r_1^{\lambda} \phi_n^*(Z_2|\vec{r}_1) e^{-\alpha_1 r_1} d\vec{r}_1$$

and:

$$I_{1B} = \gamma' C i^{\omega} \frac{\Gamma(\omega+1+n)}{(2\omega)!} (2k)^{\omega} \\ \times \int e^{ikr_2 - \alpha_2 r_2} r_2^{\omega+2+\rho} F(\omega+1+n, 2\omega+2, -2ikr_2) dr_2$$

The integrals,  $I_{1A}$  and  $I_{1B}$ , are evaluated in the appendices and only the results given here.  $I_{1B}$  can be evaluated in general for the parameters,  $\omega$ ,  $\alpha_2$ , and  $\rho$ ; however,  $I_{1A}$  cannot, thus,  $I_{1A}$  is evaluated for each final state and each value of  $\omega$  ( $\omega = 0$  except for cases involving 12-term wave function, i.e. 3d 0 and 3d  $\pm 1$ ).

(12)

II.C. Value of the Integral,  $I_{1A}$

1. Final state = 2P

$$I_{1A} = C_1 S(\lambda, \beta_1 + \alpha_1, 1)$$

2. Final state = 3P

$$I_{1A} = C_2 S(\lambda, \beta_2 + \alpha_1, 1) + C_3 S(\lambda + 1, \beta_2 + \alpha_1, 1)$$

3. Final state = 3d<sub>0</sub>

$$\omega = 0, I_{1A} = C_4 S(\lambda, \beta_2 + \alpha_1, 2) + C_5 S(\lambda + 2, \beta_2 + \alpha_1, 0)$$

$$\omega = 1, I_{1A} = C_6 S(\lambda - 1, \beta_2 + \alpha_1, 3) + C_7 S(\lambda + 1, \beta_2 + \alpha_1, 1)$$

4. Final state = 3d<sub>±1</sub>

$$I_{1A} = C_8 S(\lambda + 1, \beta_2 + \alpha_1, 1) + S(\lambda - 1, \beta_2 + \alpha_1, 3)$$

where:

$$C_1 = -2i$$

$$C_2 = \frac{96}{81} i$$

$$C_3 = -\frac{32}{81} i$$

$$C_4 = -\frac{48}{81\sqrt{3}}$$

$$C_5 = -\frac{16}{81\sqrt{3}}$$

$$C_6 = \frac{16}{81} \cos \theta_{Ak}$$

$$C_7 = \frac{16}{(81)(3)} \cos \theta_{Ak}$$

$$C_8 = i \frac{32}{\sqrt{8} (27)^{3/2}} (1 - \cos \theta_{Ak})^{1/2} e^{\pm i\phi_{Ak}}$$

(13)

$$\beta_1 = 1 \quad \beta_2 = 2/3$$

and:

$$\frac{\partial^n}{\partial A^n} F(A) = \frac{\partial^n}{\partial A^n} \frac{1}{A} = \frac{(-1)^n}{A^{n+1}} (n!) \quad (7a)$$

and:

$$\begin{aligned} \frac{\partial^n}{\partial A^n} G(A) &= \frac{\partial^n}{\partial A^n} \left[ \frac{1}{(a+iA)^{\lambda+2}} - \frac{1}{(a-iA)^{\lambda+2}} \right] \\ &= \frac{(\lambda+n+1)!}{(\lambda+1)!} \left[ \frac{i^n (-1)^n}{(a+iA)^{\lambda+2+n}} - \frac{i^n}{(a-iA)^{\lambda+2+n}} \right] \end{aligned} \quad (7b)$$

$$s(\lambda, a, n) = 2\pi i (\lambda+1)! \sum_{L=0}^n \binom{n}{L} \frac{\partial^L}{\partial A^L} F(A) \frac{\partial^{n-L}}{\partial A^{n-L}} G(A).$$

(14)

II.D. Value of the Integral,  $I_{1B}$ 

$$I_{1B} = \gamma^r C i^r (\omega+1+n) (2k)^\omega (-1)^{\rho+1-\omega} \frac{(2\omega+1)}{(2\omega)!} \\ \times \frac{\partial^{\rho+1-\omega}}{\partial \alpha_2^{\rho+1-\omega}} \frac{(\alpha-ik)^{n-\omega-1}}{(\alpha+ik)^{n+\omega+1}}$$

let:

$$F_n = \frac{\partial^n}{\partial \alpha_2^n} \frac{(\alpha-ik)^{n-\omega-1}}{(\alpha+ik)^{n+\omega+1}} = \frac{\partial^n}{\partial \alpha^n} \frac{e^{\Gamma}}{(\alpha^2+k^2)^{\omega+1}} \quad (8)$$

$$\Gamma = -\frac{Z_3}{k} \left[ \frac{\pi}{2} - \tan^{-1} \frac{\alpha^2-k^2}{2\alpha k} \right]$$

Then:

$$F_0 = \frac{e^{\Gamma}}{(\alpha^2+k^2)^{\omega+1}}$$

$$F_1 = \frac{\partial}{\partial \alpha} F_0 = (C_1+C_2\alpha) F_0 (\alpha^2+k^2)^{-1}$$

$$F_2 = \frac{\partial}{\partial \alpha} F_1 = (C_2F_0+C_1F_1+C_2\alpha F_1) (\alpha^2+k^2)^{-1}$$

$$F_3 = \frac{\partial}{\partial \alpha} F_2 = (C_4F_1+C_1F_2+C_5\alpha F_2) (\alpha^2+k^2)^{-1}$$

$$F_4 = \frac{\partial}{\partial \alpha} F_3 = (C_6F_2+C_1F_3+C_7\alpha F_3) (\alpha^2+k^2)^{-1}$$

$$F_5 = \frac{\partial}{\partial \alpha} F_4 = (C_8F_3+C_1F_4+C_9\alpha F_4) (\alpha^2+k^2)^{-1}$$

where

$$C_1 = 2Z_3$$

$$C_6 = C_4 + C_5$$

$$C_2 = -2(\omega+1)$$

$$C_7 = C_5 - 2$$

$$C_3 = C_2 - 2$$

$$C_8 = C_6 + C_7$$

$$C_4 = C_2 + C_3$$

$$C_9 = C_7 - 2$$

$$C_5 = C_3 - 2$$

Orthogonality conditions guarantee only zero contributions from final states having magnetic quantum numbers not equal to zero except in the case considered for the 12-term correlated wave function. For this case a contribution is received from the  $3d_{\pm 1}$  state as well as the  $3d_0$  state; however, orthogonality conditions yield zero contribution from the  $3d_{\pm 2}$  state. Therefore, the total cross section to the 3d final state for the 12-term wave function is the sum of the  $3d_0$ , and the  $3d_{\pm 1}$  cross sections. These equations were incorporated into a computer program to evaluate the scattering cross sections to the final states 2p, 3p, and 3d for uncorrelated initial state wave functions, and final state, 3d, for the 12-term correlated initial state wave function.

### III. Numerical Techniques and Results

#### III.A Numerical Integration and Check Cases

The cross sections were numerically integrated over the variables  $A$ ,  $\cos \theta_{Ak}$ , and  $k$  with a Simpson's rule program for a Univac 1108 computer. The accuracy of the results is dependent on the step size. As the step size is decreased, truncation error will approach zero, unfortunately to do so requires more calculations resulting in greater computer usage time and increased round-off error. The results were checked for accuracy by halving the integration step sizes and observing the differences. If the change in step size produced less than .5% change in the total integrated result for the cross section, then it was assumed that the previous step sizes were adequate for a range of incident proton

energies about the checked point. Accuracy was further assured by adjusting step sizes such that the third differences in the differential cross sections were negligibly small, thus insuring a good fit by a parabola, which is the basis of Simpson's rule.

As shown in equations (7) and (8) the matrix element is composed of a great number of terms, which can be obtained by parametric differentiation of  $F(A)$ ,  $G(A)$ , and  $F_0$ . The analytical work required to obtain these terms is tedious and subject to many errors and, needless to say, there are numerous opportunities for coding errors in preparation of the computer program required to compute these functions. To obtain a check on both the coding and the analytical work, numerical differentiation using a forward difference formula was applied to each term and compared to hand calculation as well as compared to the computer calculation of the derivative. A further check was made by calculating the scattering cross sections using the same hydrogen-like wave function that was used by Mapleton. The agreement with Mapleton's results was excellent, and this check case also gave confidence in the integration step sizes chosen.

### III.B Results and Comparisons

The computer programs developed for this work were used to calculate cross sections for incident energies,  $E_0$ , between  $10^{-2}$  and 10 Mev. and for final states of the residual  $H_e^+$  ion of 1s, 2s, 2p, 3s, 3p, and 3d. Three different wave functions were used to describe the ground state of the helium atom, two of which were products of one

electron orbitals, a Hartree-Fock and a hydrogen-like, and the third wave function used was a 12-term correlated. The results are presented in Figures 1-7, in Table II, and in a selection of computer generated plots in Appendix B. The high energy results for the 2p and 3p final states are not intuitively appealing because of the difference in the slope from the s and d final states. However, many checks (described above) were made of the computer program and no errors could be found.

The plots presented in Appendix B were generated using coarse mesh sizes to conserve computer time, however, they are sufficiently accurate (within 5% of values in Table II) to show trends. At very high energies in the neighborhood of  $\cos \theta = 1$  there is a sharp dip in the totally differential cross section, see Figure B-1 through Figure B-5, and in this same neighborhood of  $\cos \theta$ , the doubly differential cross section exhibits a very sharp peak, see Figures B-6 through B-11. The dip cannot be explained, however, it has only negligible effect on the cross sections. The sharp peak in the doubly differential cross section is a result of the conservation of momentum. Due to a change of variable in the computer program,  $\cos \theta$  actually represents the negative of the ejection angle, thus the peak corresponds to the scattered electron moving opposite to the momentum change vector,  $A$ , which would be expected for conservation of momentum at high incident energies. This peak begins to take the form of a delta function as energy is increased, and it is possible that the numerical integration used herein could not adequately handle the calculations with sufficient accuracy in this region, thereby, offering a possible explanation for the unappealing results for the 2p



and 3p final states. An exact explanation can only come from further analytical and numerical studies which could not be done within the scope of this Thesis.

Comparisons were made with the analytical works of Peach, Mapleton, and Bell and Kingston. The results from Mapleton's work agree with the results developed herein for the hydrogen-like ground state wave function. Peach's results are very close and the results from the Hartree-Fock ground state wave function fall in line also. Bell and Kingston's results are for ionization with the residual ion remaining in the 1s state. They used a correlated six parameter Stewart and Webb ground state wave function. The results agree to within 1% with the 1s results from this work using the 12-term correlated wave function.

Experimental data is available only for total cross sections, that is for single ionization with the residual ion in all possible states. Thus, to match experimental data, the cross sections presented herein using the 12-term ground state wave function must be summed over all possible final states. However, this poses an additional problem, that is, whether or not to include the suspicious results of the 2p, and 3p final states. This problem was sidestepped by making two plots, one labeled A for a total cross section using all final states as calculated, and one labeled B where the 2p and 3p results were replaced with the less objectionable results from the hydrogen-like ground state wave function (see Table II). These plots are shown in Figure 8 together with the results from Mapleton's paper and available experimental results. The agreement, as expected, is very good at high energies and poor at low energies.

#### IV. Conclusions

The total cross section for single ionization without excitation is plotted in Figure 1 versus incident proton energy. This particular case is defined as a single process since only one electron makes a transition. As the plot shows, there is little difference in the results regardless of initial state wave function used. The uncorrelated wave function gives results which differ at worse by only 15% of the results obtained using the correlated wave function, and the 12-term wave plots on top of the results reported by Bell and Kingston, having a maximum difference of only 1%. These results are of great importance for two reasons. Firstly, the Stewart and Webb wave function used by Bell and Kingston (a reevaluation of the Hylleraas wave function) is regarded as being one of the most accurate descriptions of the helium atom, therefore, it is very satisfying to have the much simpler 12-term wave function agree so closely. Secondly, the close agreement of all the results for this case indicates that for single processes very simple uncorrelated wave functions may be used, and it is reasonable to assume that single processes involving more complicated atoms may also be analyzed using simple uncorrelated hydrogen-like ground state wave functions.

The remaining cases consider multiple processes involving both electrons, specifically, single ionization with the residual helium ion excited to the state 2s, 2p, 3s, 3p or 3d (Figures 2-7). As expected, there are large differences in the computed cross sections using an uncorrelated wave function as compared to using one that is correlated. The results for the 2s case, Figure 2, show the 12-term wave function

predicts a cross section that is almost twice that resulting from using the hydrogen-like or the Hartree-Fock wave function. For the 3s final state, Figure 4, there is again a factor of two difference in the low to moderate energy range, however, this difference decreases somewhat as the incident energy increases. The cross section for the 3d final state, Figure 6, using the 12-term ground state wave function is initially lower than the two uncorrelated wave functions, but as energy increases the 12-term wave function again yields a cross section twice as large as that due to the uncorrelated wave functions. The 2p and 3p results (Figures 3 and 5) for the 12-term wave function are an order of magnitude greater than the results from the uncorrelated functions, however, as stated in Section III, there may be numerical problems causing the unexpected behavior of these cross sections.

These results clearly show that whenever multiple processes are considered for helium, the analysis should definitely consider a correlated initial state wave function, however, for single processes the results using an uncorrelated wave function are not significantly different. This conclusion is in agreement with that presented by Bryon and Joachain in their analysis of multiple processes in helium due to electron impact. One can further conclude that these excited states must be included in the analysis, because, as shown in Table II and Figure 8, the excited states contribute a significant amount to the total cross section, specifically in the high energy range this contribution amounts to 5 - 20% of the 1s cross section at 1.25 and .229 MEV. respectively. Thus, to be very

accurate, the contributions to the total cross section due to the excited states must be included in the calculations.

Since the 12-term wave function produced results almost identical to the results from Bell and Kingston, it would seem reasonable to approach future work on this problem by concentrating on the final state approximations. As demonstrated by Bell and Kingston, the final state should also contain correlation terms, however, they also showed that by computing the velocity matrix element rather than the length element (used herein), the effects of correlation in the final state were not as significant for the case of double ionization. It is reasonable to assume that these results would also apply to this problem, ionization and excitation. Thus, for future work on this problem it is recommended that the results from the Born velocity element be compared with the results herein, and possibly results from acceleration element also. At first glance, it appears that these additional calculations would only require minor modifications to the integrals evaluated herein. To improve the final state wave function using correlation terms would be a more difficult task but should be accomplished in conjunction with an investigation of the other matrix elements to accurately assess the effects of correlation.

(22)

## APPENDIX A

EVALUATION OF INTEGRALS  $I_{1A}$  AND  $I_{1B}$ A.1 EVALUATION OF  $I_{1A}$ 

$$I_{1A} = \left[ \frac{4\pi}{2\omega+1} \right] \int Y_{\omega,0}(\theta_{1,k}, \phi_{1,k}) e^{i\vec{A} \cdot \vec{r}_1} r_1^\lambda \phi_n^*(Z_2|\vec{r}_1) e^{-\alpha_1 r_1} d\vec{r}_1$$

Consider first only cases for which  $\omega = 0$ , then  $Y_{\omega,0} = \frac{1}{\sqrt{4\pi}}$  yielding:

$$I_{1A} = \sqrt{4\pi} \int e^{i\vec{A} \cdot \vec{r}_1} r_1^\lambda \phi_n^*(Z_2|r_1) e^{-\alpha_1 r_1} d\vec{r}_1. \quad (1)$$

Now  $I_{1A}$  is evaluated for each final state representation of  $\phi_n(Z_2|r_1)$ .

$$\phi_{2p,0}(Z_2|r_1) = \frac{1}{\sqrt{\pi}} r_1 e^{-\beta_1 r_1} \cos \theta_{1A} \quad (2)$$

$$\phi_{3p,0}(Z_2|r_1) = \left\{ 3 - r_1 \right\} r_1 e^{-\beta_2 r_1} \frac{16}{81\sqrt{\pi}} \cos \theta_{1A} \quad (3)$$

$$\phi_{3d,0}(Z_2|r_1) = \left\{ 3 \cos^2 \theta_{1A} - 1 \right\} r_1^2 e^{-\beta_2 r_1} \frac{8}{81\sqrt{3\pi}} \quad (4)$$

For 2p final state substitution of (2) into (1) yields:

$$I_{1A} = 2 \int e^{i\vec{A} \cdot \vec{r}_1} r_1^{\lambda+1} e^{-\beta_1 r_1} \cos \theta_{1A} e^{-\alpha_1 r_1} d\vec{r}_1$$

$$I_{1A} = -2i \frac{\partial}{\partial A} \int e^{i\vec{A} \cdot \vec{r}_1} r_1^{\lambda+1} e^{-(\beta_1+\alpha)r_1} d\vec{r}_1$$

$$I_{1A} = C_1 s(\lambda, \beta_1+\alpha, 1)$$

(23)

where:

$$s(\lambda, a, n) = \frac{\partial^n}{\partial A^n} \int r_1^\lambda e^{-ar_1} e^{iAr_1} \cos \theta_{1A} d\vec{r}_1$$

and

$$C_1 = -2i$$

Following the same procedure gives:

3p final state

$$I_{1A} = C_2 s(\lambda, \beta_2 + \alpha_1, 1) + C_3 s(\lambda + 1, \beta_2 + \alpha_1, 1)$$

3d final state

$$I_{1A} = C_4 s(\lambda, \beta_2 + \alpha_1, 2) - C_5 s(\lambda + 2, \beta_2 + \alpha_1, 0)$$

where:

$$C_2 = \frac{96}{81} i$$

$$C_3 = -\frac{C_2}{3}$$

$$C_4 = -\frac{48}{81\sqrt{3}}$$

$$C_5 = -\frac{C_4}{3}$$

Now for  $\omega = 1$  only the 3d final state will be considered. First write  $Y_{\omega,0}$  in (1) as:

$$Y_{\omega,0}(\theta_{1k}, \phi_{1k}) = \left[ \frac{4\pi}{2\omega+1} \right]^{1/2} \sum_{m'=-\omega}^{\omega} Y_{\omega,m'}^*(\theta_{Ak}, \phi_{Ak}) Y_{\omega,m'}(\theta_{1A}, \phi_{1A})$$

(24)

and then equation (1) is:

$$I_{1A} = \left[ \frac{4\pi}{2\omega+1} \right]^{3/2} \sum_{m=-\omega}^{\omega} Y_{\omega, m}^* (\theta_{Ak}, \phi_{Ak}) \\ \times \int Y_{\omega, m} (\theta_{1A}, \phi_{1A}) e^{i\vec{A} \cdot \vec{r}_1} r_1^{\lambda} e^{-\alpha r_1} \phi_n (Z_2 | r_1) d\vec{r}_1$$

Now  $\phi_n (Z_2 | r_1)$  is written for the 3d,0 and 3d $\pm 1$  final state:

$$\phi_n (Z_2 | r_1) = \phi_{3d_0} (Z_2 | r_1) = R_{3,2} (Z_2 | r_1) Y_{2,0} (\cos \theta_{1A})$$

$$\phi_n (Z_2 | r_1) = \phi_{3d_{\pm 1}} (Z_2 | r_1) = R_{3,2} (Z_2 | r_k) Y_{2,\pm 1} (\cos \theta_{1A}),$$

with

$$R_{3,2} (Z_2 | r_1) = e^{-\beta_2 r_1} \frac{2^5}{81\sqrt{15}} r_1^2$$

For 3d<sub>0</sub> final state

$$I_{1A} = \left[ \frac{4\pi}{2} \right]^{3/2} \left[ \frac{3}{4\pi} \right] \cos \theta_{Ak} \left[ \frac{3}{4\pi} \right]^{1/2} \left[ \frac{5}{4\pi} \right]^{1/2} \left[ \frac{2^5}{\sqrt{15}} \right] \left[ \frac{1}{81} \right] \frac{1}{2} \\ \times \int \cos \theta_{1A} (3 \cos^2 \theta_{1A} - 1) e^{i\vec{A} \cdot \vec{r}_1} r^{\lambda+2} e^{-(\alpha+\beta_2)r_1} d\vec{r}_1$$

$$I_{1A} = C_6 s (\lambda-1, \beta_2+\alpha_1, 3) + C_7 s (\lambda+1, \beta_2+\alpha_1, 1)$$

where:

$$C_6 = \frac{16}{81} \cos \theta_{Ak}$$

$$C_7 = \frac{16}{(81)(3)} \cos \theta_{Ak}.$$

(25)

Similarly:

for  $3d_{\pm 1}$  final state

$$I_{1A} = C_8 \left\{ s(\lambda+1, \beta_2+\alpha_1, 1) + s(\lambda-1, \beta_2+\alpha_1, 3) \right\}$$

where:

$$C_8 = i \frac{32}{\sqrt{8} (27)^{3/2}} (1 - \cos \theta_{Ak})^{1/2} e^{\pm i\phi_{Ak}}.$$

Now only a solution of  $s(\lambda, a, n)$  is required.

$$\begin{aligned} s(\lambda, a, n) &= \frac{\partial^n}{\partial A^n} \int e^{i\bar{A} \bar{r}} r^\lambda e^{-ar} d\bar{r} \\ &= \frac{\partial^n}{\partial A^n} 2\pi \int r^{\lambda+2} e^{-ar} dr \int_0^\pi e^{i\text{Arcos}\theta} \sin \theta d\theta \\ &= \frac{\partial^n}{\partial A^n} i \frac{2}{A} \int r^{\lambda+1} e^{-ar} e^{i\text{Arcos}\theta} \Big|_\pi^0 dr \\ &= \frac{\partial^n}{\partial A^n} i \frac{2\pi}{A} \int r^{\lambda+1} \sin Ar e^{-ar} dr \\ s(\lambda, a, n) &= \frac{\partial^n}{\partial A^n} \frac{2\pi i}{A} (\lambda+1)! \left[ \frac{(a-iA)^{\lambda+2} - (a+iA)^{\lambda+2}}{(a^2+A^2)^{\lambda+2}} \right] \end{aligned}$$

or

$$\begin{aligned} s(\lambda, a, n) &= 2\pi i (\lambda+1)! \frac{\partial^n}{\partial A^n} F(A) G(A) \\ s(\lambda, a, n) &= 2\pi i (\lambda+1)! \sum_{L=0}^n \binom{n}{L} \frac{\partial^L}{\partial A^L} F(A) \frac{\partial^{n-L}}{\partial A^{n-L}} G(A) \end{aligned}$$



(26)

where:

$$F(A) = \frac{1}{A} \quad \text{and} \quad \frac{\partial^n F(A)}{\partial A^n} = \frac{(-1)^n}{A^{n+1}} \quad (n!)$$

$$G(A) = \left[ \frac{1}{(a+iA)^{\lambda+2}} - \frac{1}{(a-iA)^{\lambda+2}} \right]$$

and

$$\frac{\partial^n G(A)}{\partial A^n} = \frac{(\lambda+n+1)!}{(\lambda+1)!} \left\{ \frac{i^n (-1)^n}{(a+iA)^{\lambda+2+n}} - \frac{i^n}{(a-iA)^{\lambda+2+n}} \right\}.$$

(27)

A.2 EVALUATION OF  $I_{1B}$ 

$$I_{1B} = \gamma' C i^\omega \frac{\Gamma(\omega+1+n)}{(2\omega)!} (2k)^\omega \quad (1)$$

$$\times \int e^{ikr_2 - \alpha_2 r_2} r_2^{\omega+2+p} F(\omega+1+n, 2\omega+2, -2ikr_2) dr_2.$$

Now

$$J(r) = e^{ikr - \alpha r} r^{\omega+p+2} F(\omega+1+n, 2\omega+2, -2ikr_2)$$

$$= e^{-\alpha r} r^{p+2} r^\omega e^{ikr} F(\omega+1+n, 2\omega+2, -2ikr_2)$$

$$= e^{-\alpha r} r^{p+1} \frac{(-2ikr)^{\mu+1/2}}{(-2ik)^{\mu+1/2}} e^{ikr} F(\omega+1+n, 2\mu+1, -2ikr_2)$$

where

$$\mu = \omega + 1/2, \text{ now let } Z = -2ikr$$

$$= \frac{e^{-\alpha r} r^{p+1}}{(-2ik)^{\mu+1/2}} Z^{\mu+1/2} e^{-iZ/2} F(\mu+1/2, 2\mu+1, -i2kr) \quad (2)$$

Gradsthteyn and Rhyzik give the following definition:

$$M_{\lambda\mu}(Z) = Z^{\mu+1/2} e^{-Z/2} F(\mu-\lambda+1/2, 2\mu+1, Z).$$

Now substitution into (2) yields:

$$J(r) = \frac{e^{-r}}{(-2ik)^{\mu+1/2}} M_{-n\mu}(-i2kr),$$

(28)

and then (1) is written as:

$$I_{1A} = \gamma' C i^\omega \frac{\Gamma(\omega+1+n)}{(2\omega)!} (2k)^\omega \quad (3)$$

$$\times \int \frac{e^{-\alpha r}}{(-2ik)^{\mu+1/2}} r^{\rho+1} M_{-n\mu}(-2ikr) dr.$$

Now choose

$$q = -i2k$$

$$s = \alpha$$

$$\lambda = -n$$

Then (3) is

$$I_{1A} = (-1)^{\rho+1-\omega} \frac{\gamma' C i^\omega \Gamma(\omega+1+n) (2k)^\omega}{(2\omega)! (-2ik)^{\mu+1/2}} \frac{\partial^{\rho+1-\omega}}{\partial \alpha^{\rho+1-\omega}} \int_0^\infty r^{\mu-1/2} M_{\lambda\mu}(qr) e^{-sr} dr.$$

Page 860, equation (2), Gradshteyn and Ryzik gives:

$$\int_0^\infty e^{-st} r^{\mu-1/2} M_{\lambda\mu}(qr) dt = q^{\mu+1/2} (2\mu+1) (s-1/2q)^{\lambda-\mu-1/2} \times (s+1/2q)^{-\lambda-\mu-1/2}$$

with

$$R_e \mu > -1/2$$

$$R_e s > \frac{|R_e q|}{2}.$$

(29)

Thus:

$$I_{1A} = \frac{\gamma' C i^\omega \Gamma(\omega+1+n) (2k)^\omega}{(2\omega)! (-2ik)^{\omega+1/2}} (-2ik)^{\omega+1/2} \Gamma(2\omega+2)$$

$$\times \frac{(\alpha-ik)^{n-\omega-1}}{(\alpha+ik)^{n+\omega+1}}$$

$$I_{1A} = \gamma' C i^\omega \Gamma(\omega+1+n) (2k)^\omega (-1)^{\rho+1-\omega} \frac{(2\omega+1)}{(2\omega)!}$$

(4)

$$\times \frac{\partial^{\rho+1-\omega}}{\partial \alpha_2^{\rho+1-\omega}} \frac{\{\alpha_2-ik\}^{n-\omega-1}}{\{\alpha_2+ik\}^{n+\omega+1}}$$

Now consider the various derivatives required for equation (4);

let:

$$F_n = \frac{\partial^n}{\partial \alpha_2^n} \frac{\{\alpha_2-ik\}^{n-\omega-1}}{\{\alpha_2+ik\}^{n+\omega+1}} = \frac{\partial^n}{\partial \alpha^n} \frac{e^\Gamma}{\{\alpha_2^2+k^2\}^{\omega+1}}$$

where:

$$\Gamma = -\frac{Z_3}{k} \left[ \frac{\pi}{2} - \tan^{-1} \left( \frac{\alpha^2 - k^2}{2\alpha k} \right) \right].$$

For  $n = 0$ 

$$F_0 = \frac{e^\Gamma}{\{\alpha_2^2+k^2\}^{\omega+1}}$$

For  $n = 1$ 

$$F_1 = \frac{\partial}{\partial \alpha_2} \frac{e^\Gamma}{\{\alpha_2^2+k^2\}^{\omega+1}}$$

$$F_1 = (C_1 + C_2 \alpha_2) F_0 \frac{1}{\{\alpha_2^2+k^2\}},$$

(30)

where:

$$C_1 = 2Z_3$$

$$C_2 = -2 (\omega+1)$$

For  $n = 2$

$$F_2 = \frac{\partial^2}{\partial \alpha_2^2} F_0 = \frac{\partial}{\partial \alpha} F_1 = \frac{\partial}{\partial \alpha_2} (C_1 + C_2 \alpha_2) F_0 \frac{1}{\{\alpha_2^2 + k^2\}}$$

$$F_2 = \frac{C_1 F_1}{\{\alpha_2^2 + k^2\}} + \frac{C_2 F_0}{\{\alpha_2^2 + k^2\}} + \frac{C_2 \alpha_2 (-2\alpha_2)}{\{\alpha_2^2 + k^2\}^2} F_0 + \frac{C_2 2 F_1}{\{\alpha_2^2 + k^2\}} - \frac{C_1 2 \alpha_2 F_0}{\{\alpha_2^2 + k^2\}}$$

$$F_2 = [C_1 F_1 + C_2 F_0 + C_3 \alpha_2 F_1] \frac{1}{\{\alpha_2^2 + k^2\}}$$

where:

$$C_3 = C_2 - 2$$

Continuing in a similar manner:

$$F_3 = [C_4 F_1 + C_1 F_2 + C_5 \alpha_2 F_2] \frac{1}{\{\alpha_2^2 + k^2\}}$$

$$F_4 = [C_6 F_2 + C_1 F_3 + C_7 \alpha_2 F_3] \frac{1}{\{\alpha_2^2 + k^2\}}$$

$$F_5 = [C_8 F_3 + C_1 F_4 + C_9 \alpha_2 F_4] \frac{1}{\{\alpha_2^2 + k^2\}}$$

(31)

where :

$$c_4 = c_2 + c_3$$

$$c_5 = c_3 - 2$$

$$c_6 = c_4 + c_5$$

$$c_7 = c_5 - 2$$

$$c_8 = c_6 + c_7$$

$$c_9 = c_7 - 2 \quad .$$

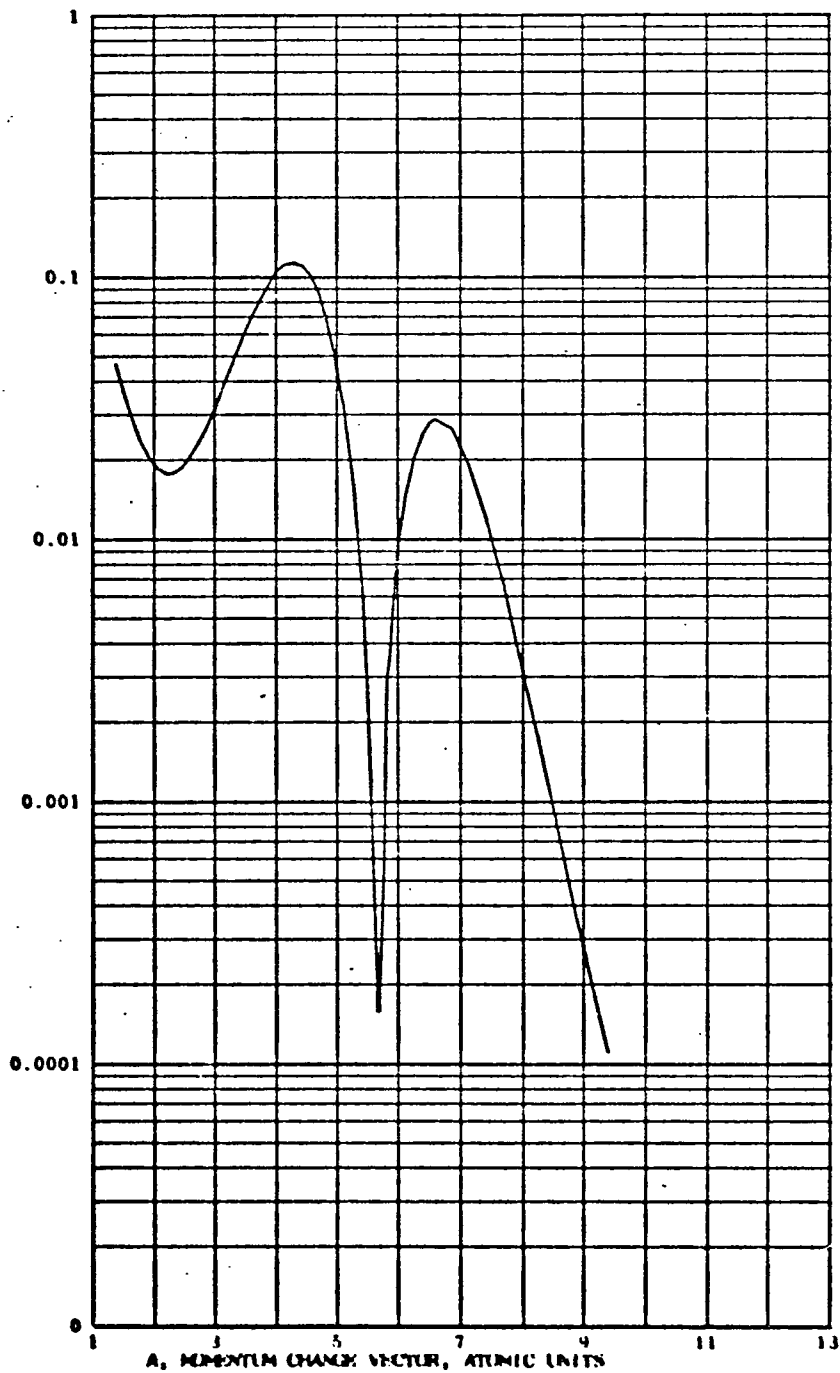
## APPENDIX B - PLOTS OF DIFFERENTIAL CROSS SECTIONS

Figure B-1. - (Final State = 2p)

INCIDENT ENERGY= .39020+04  
 EJECTED ELECTRON ENERGY .55000+01  
 COS(THETA)= .10000+01

SCALE FACTOR=10\*\* 4

T  
O  
T  
A  
L  
L  
Y  
  
D  
I  
F  
F  
E  
R  
E  
N  
T  
I  
A  
L  
  
C  
R  
O  
S  
S  
  
S  
E  
C  
T  
I  
O  
N  
,  
  
U  
N  
I  
T  
S  
  
O  
F  
  
P  
I  
\*  
A  
0  
\*  
\*  
2





(34)

Figure B-2. - (Final State = 2p)

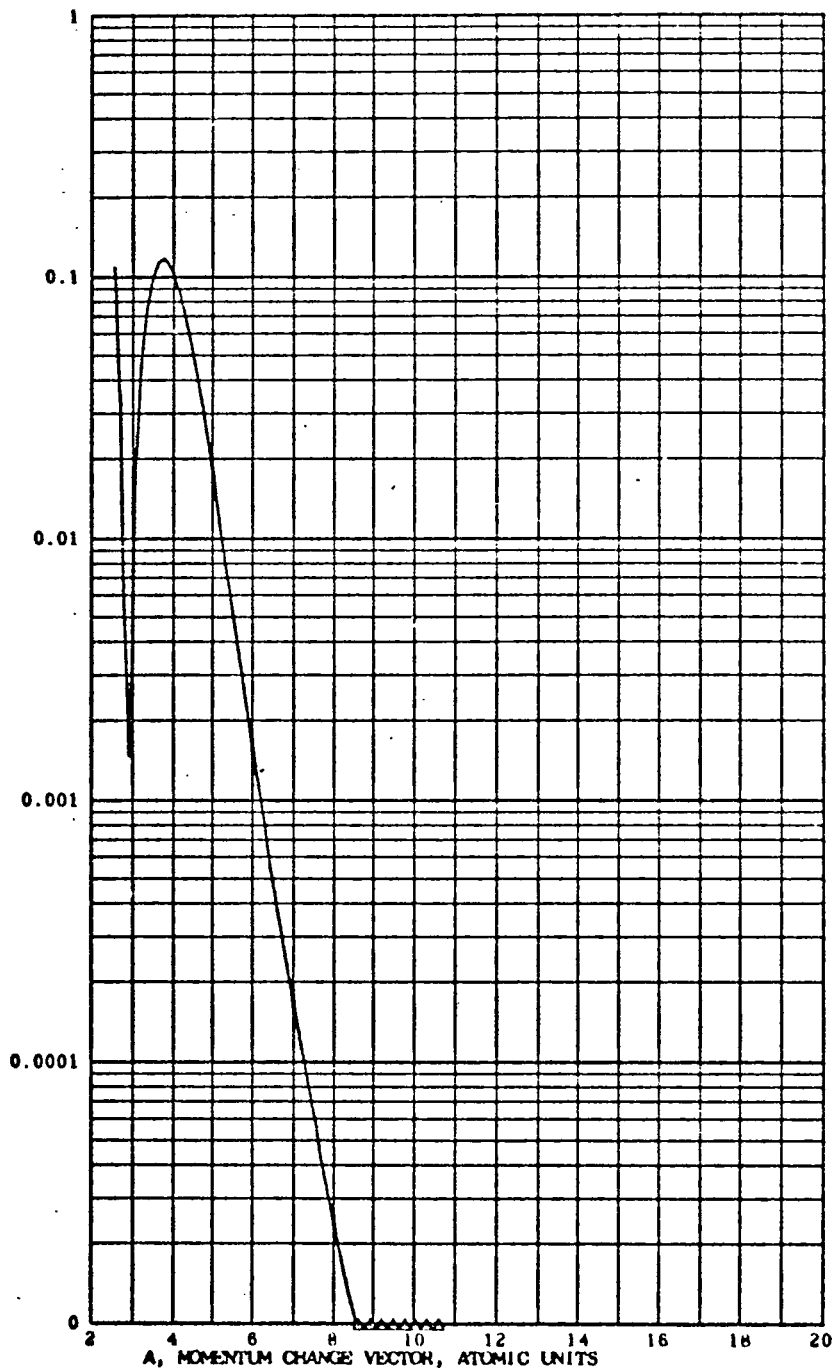
INCIDENT ENERGY = .12500+03

EJECTED ELECTRON ENERGY .26000+01

COS(THETA) = .10000+01

SCALE FACTOR =  $10^{+3}$

T  
O  
T  
A  
L  
L  
Y  
  
D  
I  
F  
F  
E  
R  
E  
N  
T  
I  
A  
L  
  
C  
R  
O  
S  
S  
  
S  
E  
C  
T  
I  
O  
N  
,  
  
U  
N  
I  
T  
S  
  
O  
F  
  
 $\pi \times 10^{-22}$



(35)

Figure B-3. - (Final State = 3s)

INCIDENT ENERGY= .50000+04

EJECTED ELECTRON ENERGY .56000+01

COS(THETA)= .10000+01

SCALE FACTOR=10\*\* 4

T  
O  
T  
A  
L  
L  
Y  
  
D  
I  
F  
F  
E  
R  
E  
N  
T  
I  
A  
L  
  
C  
R  
O  
S  
S  
  
S  
E  
C  
T  
I  
O  
N  
,  
  
U  
N  
I  
T  
S  
  
O  
F  
  
P  
I  
\*  
A  
0  
\*  
\*  
2

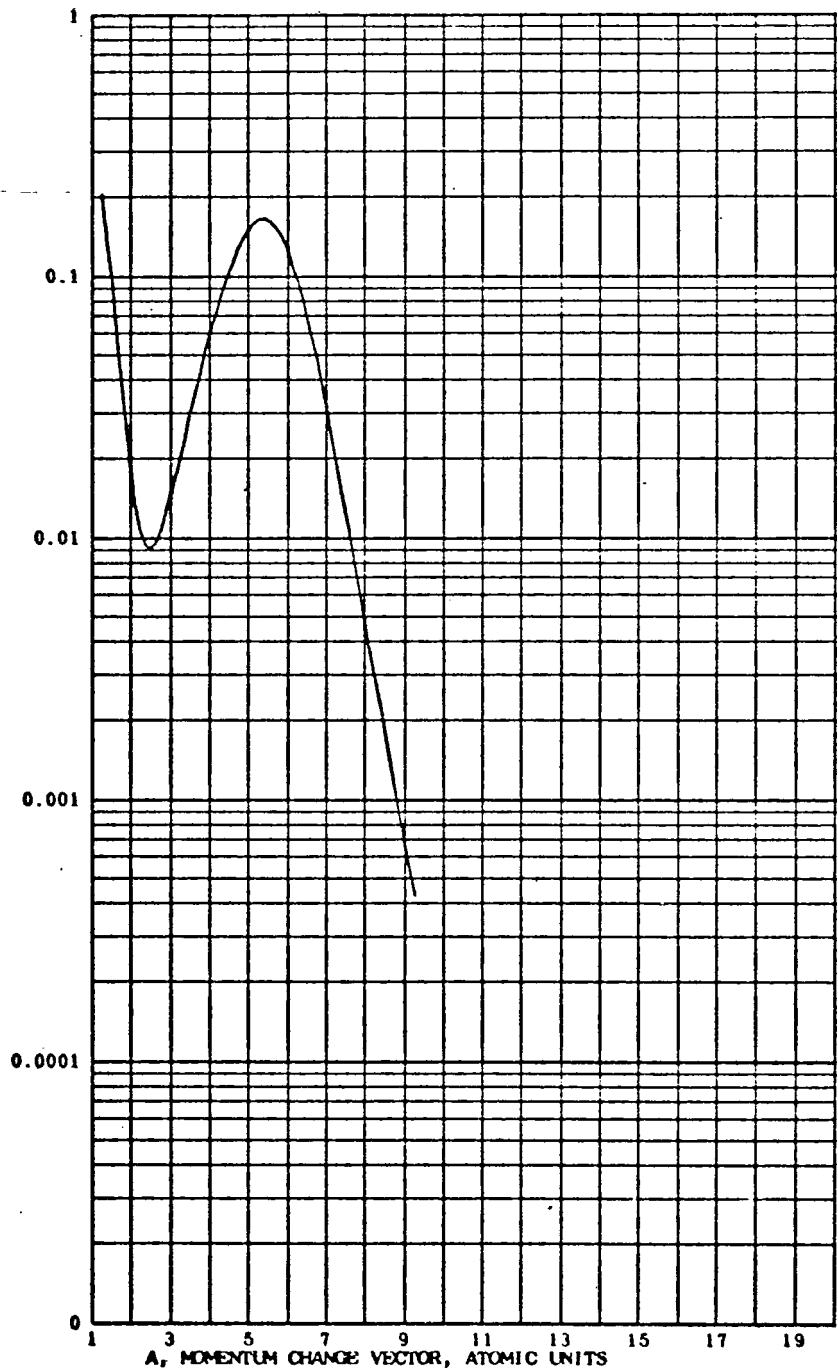


Figure B-4. - (Final State = 3p)

INCIDENT ENERGY = .50000+04  
 EJECTED ELECTRON ENERGY .55000+01  
 COS(THETA) = .10000+01

SCALE FACTOR =  $10^{-5}$ 

T  
T  
O  
T  
A  
L  
L  
Y  
  
D  
I  
F  
F  
E  
R  
E  
N  
T  
I  
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C  
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0  
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2

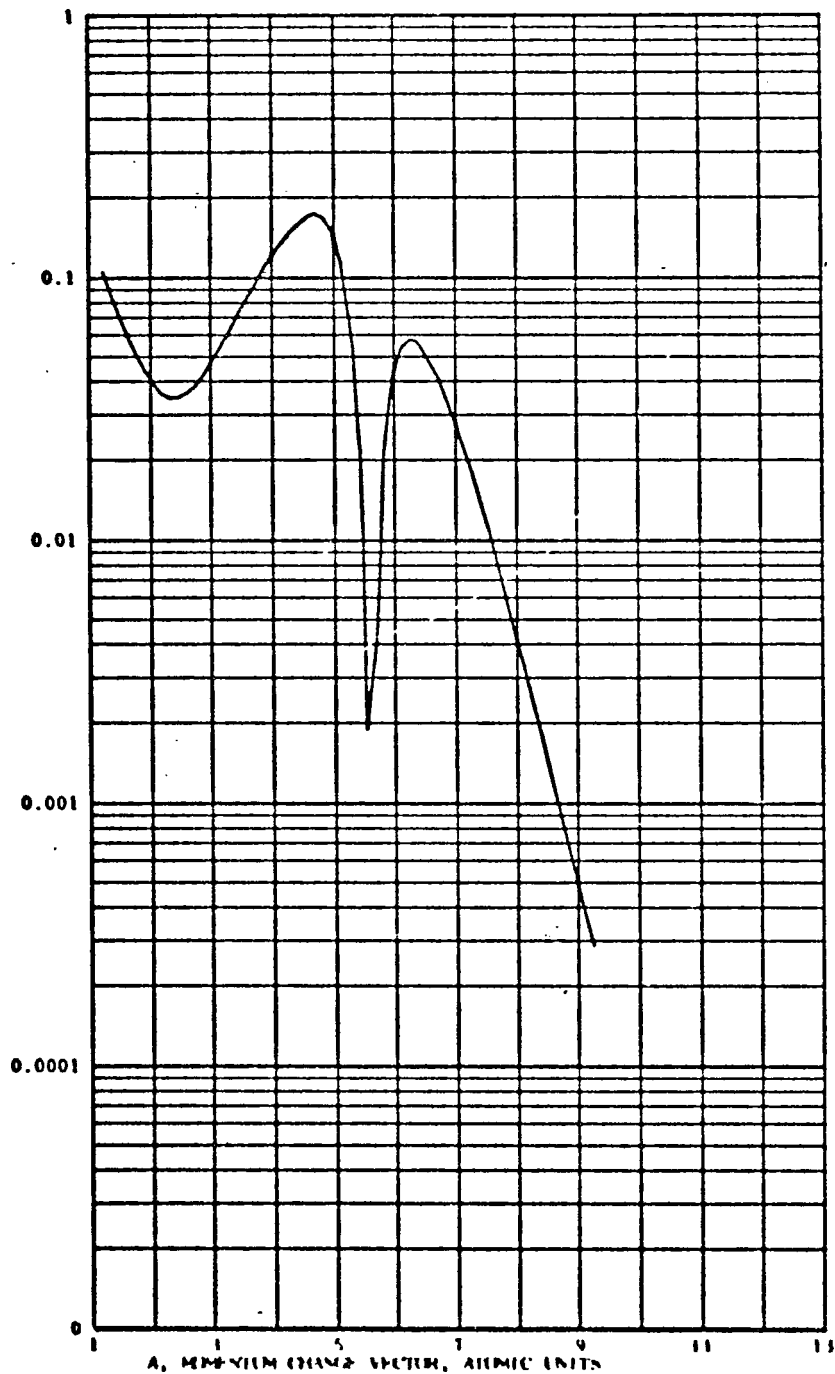
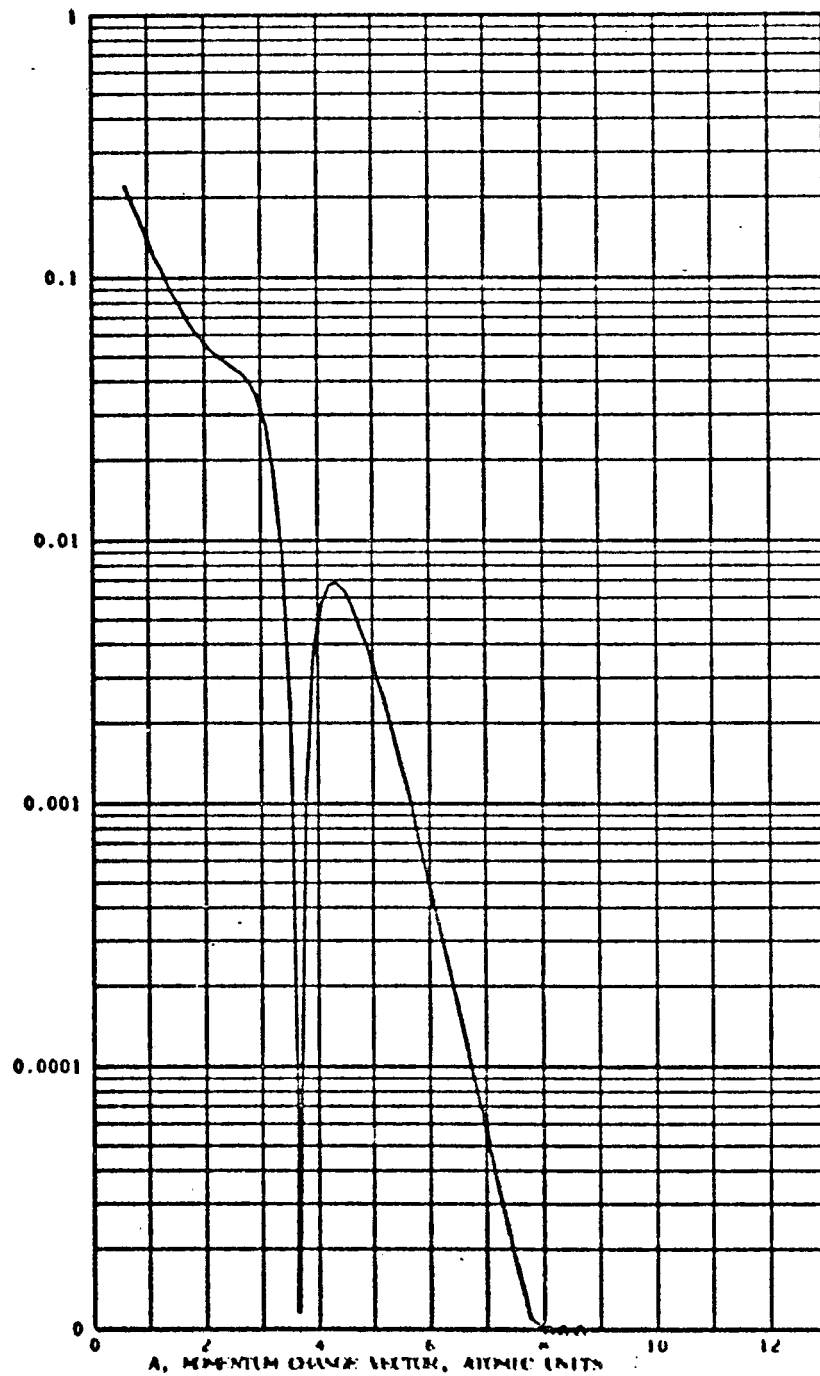


Figure B-5. - (Final State = 3p)

INCIDENT ENERGY = .50000+04  
 EJECTED ELECTRON ENERGY = .15000+01  
 COS(THETA) = .10000+01

SCALE FACTOR = 10\*\* 4

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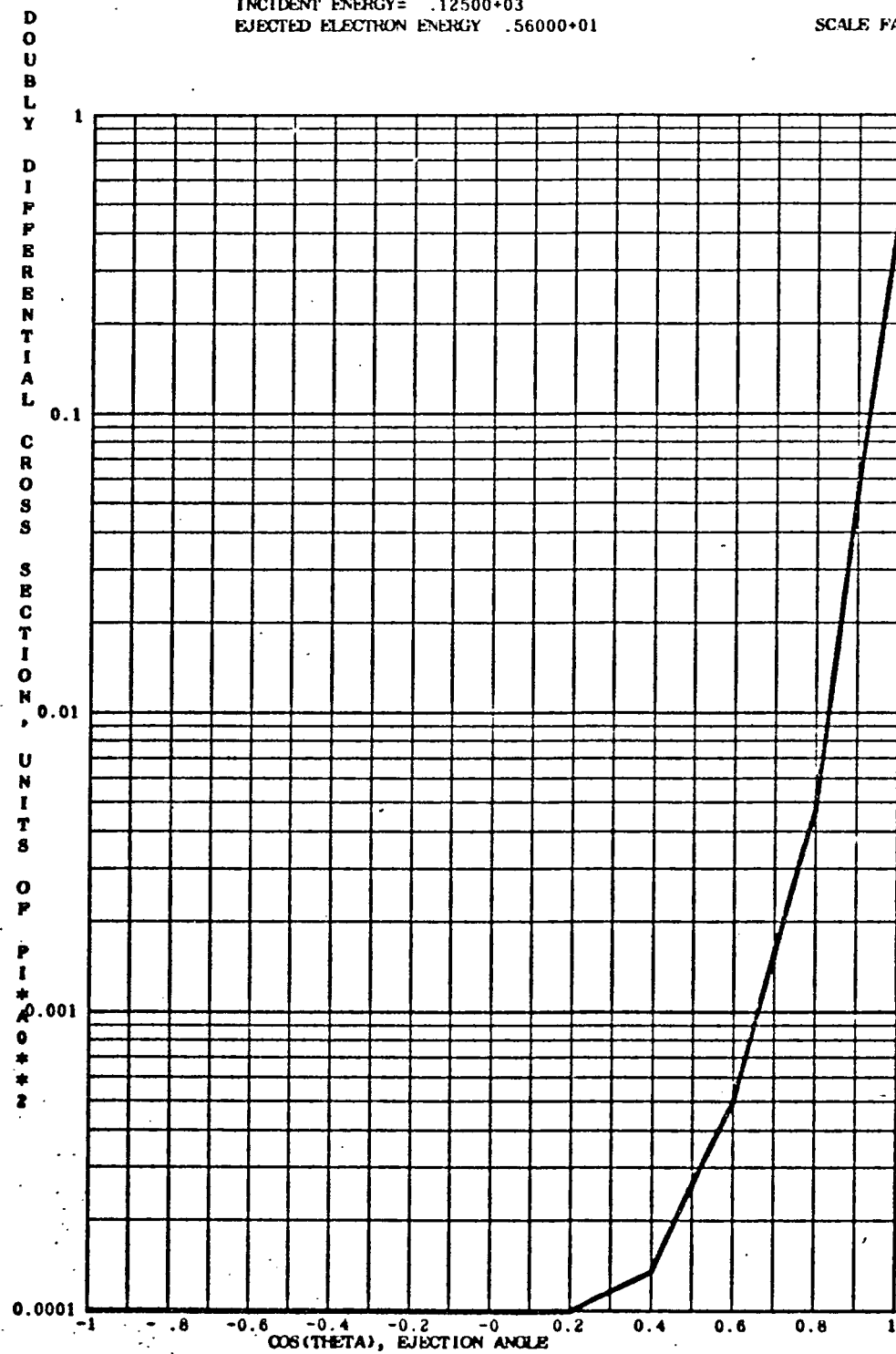


(38)

Figure B-6. - (Final State = 2p)

INCIDENT ENERGY= .12500+03  
EJECTED ELECTRON ENERGY .56000+01

SCALE FACTOR=10\*\*

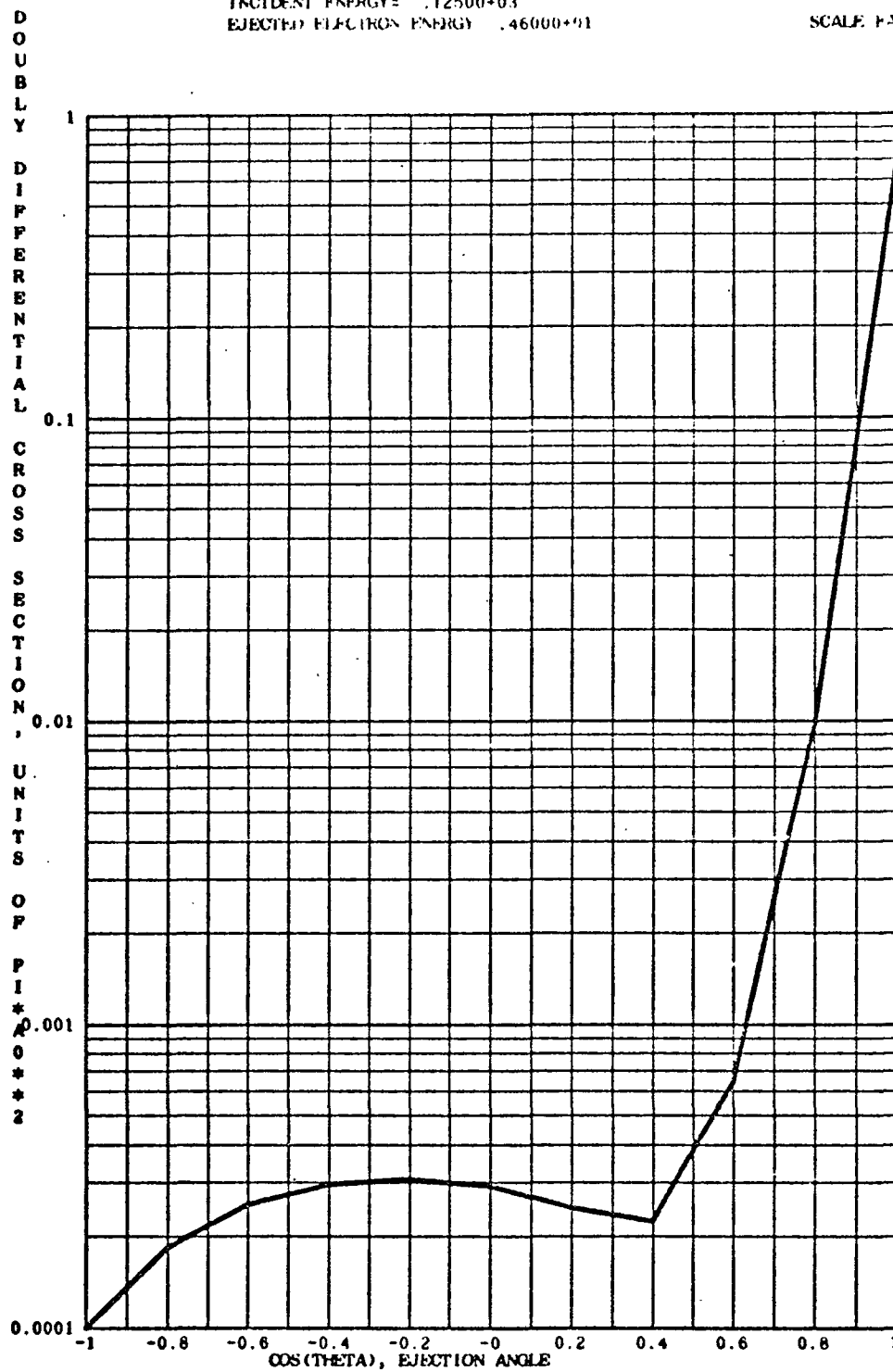


(39)

Figure B-7. - (Final State = 2p)

INCIDENT ENERGY = .12500+03  
EJECTED ELECTRON ENERGY .46000+01

SCALE FACTOR=10<sup>-4</sup>



(40)

Figure B-8. - (Final State = 2p)

INCIDENT ENERGY = .12500+03

EJECTED ELECTRON ENERGY .36000+01

SCALE FACTOR=10\*\* 4

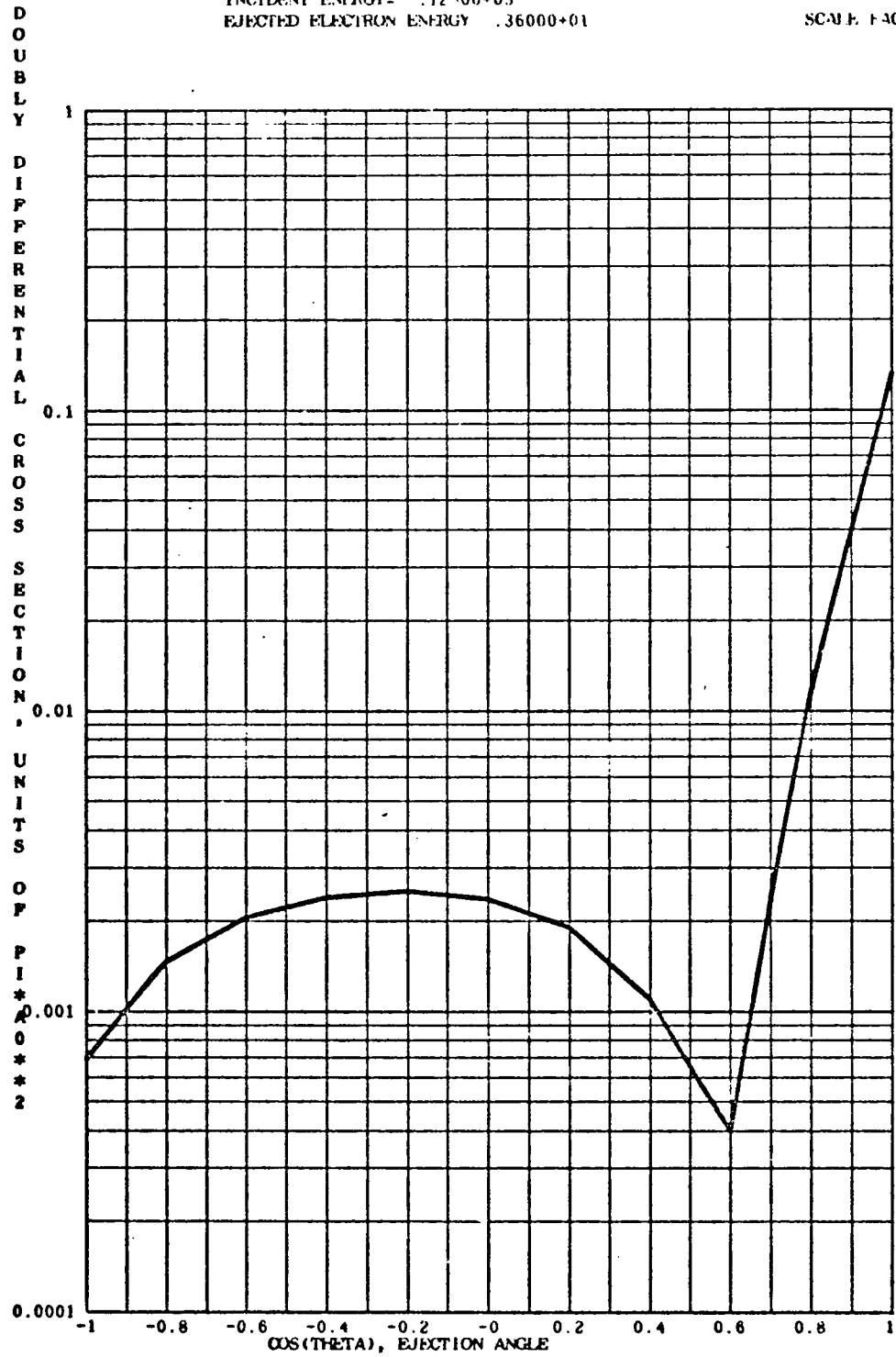


Figure B-9. - (Final State = 3p)

INCIDENT ENERGY = .50000+04  
 EJECTED ELECTRON ENERGY .55000+01

SCALE FACTOR = 10\*\* 5

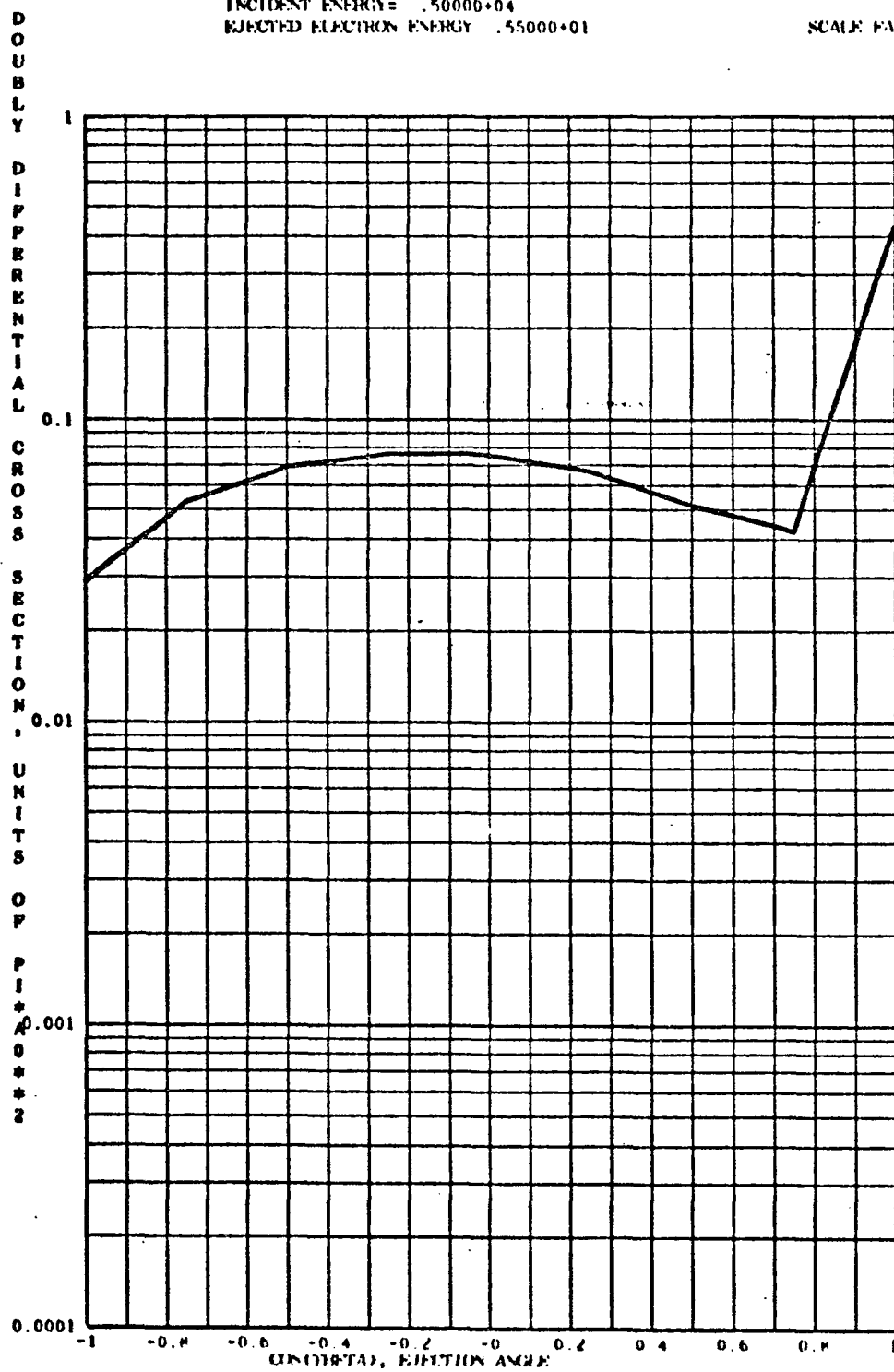




Figure B-10. - (Final State = 3p)

INCIDENT ENERGY = .12500+01  
 EJECTED ELECTRON ENERGY .55000+01

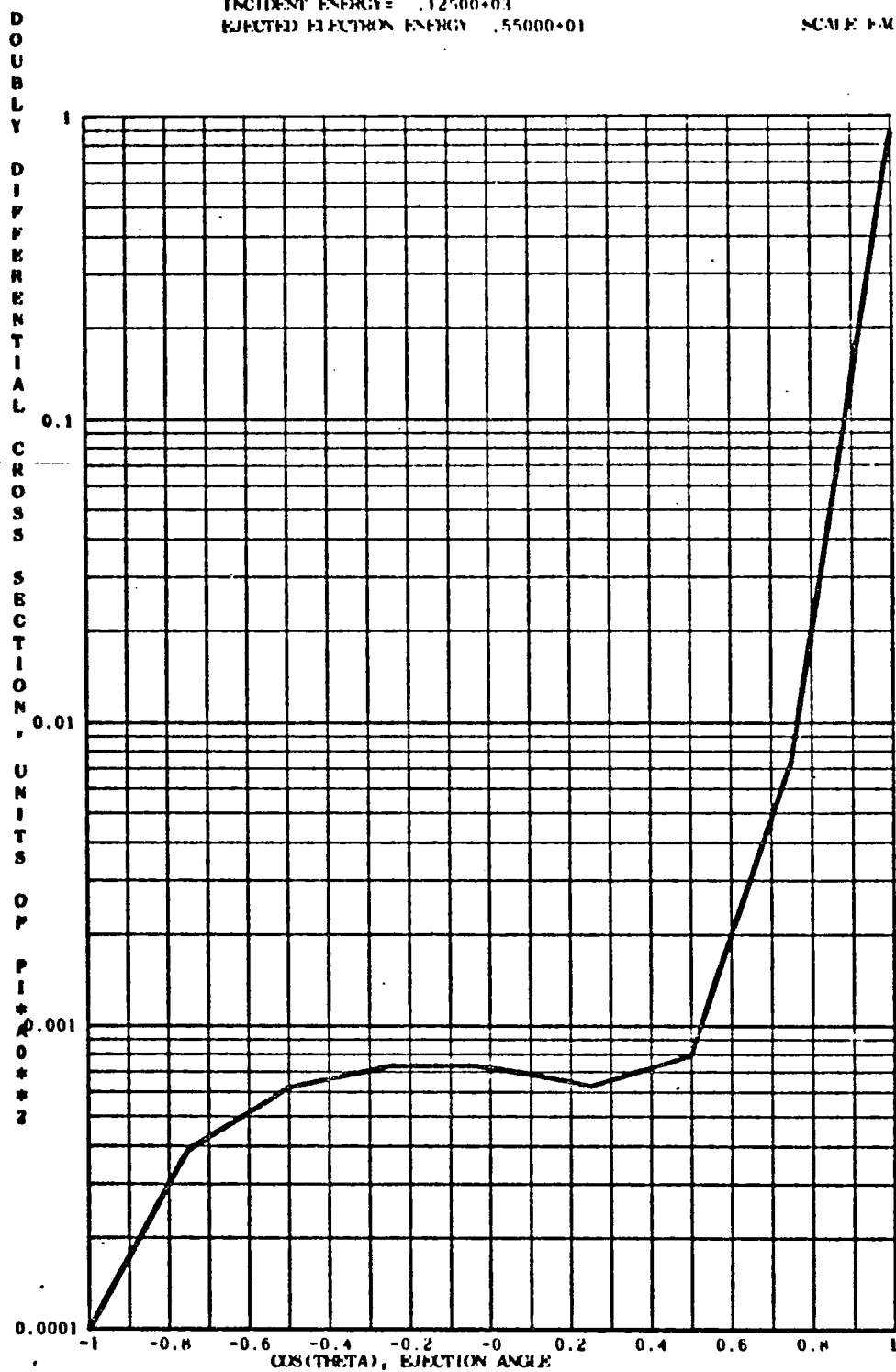
SCALE FACTOR =  $10^{+6}$ 

Figure B-11. - (Final State = .3p)

INCIDENT ENERGY = .12500+03  
 EJECTED ELECTRON ENERGY .35000+01

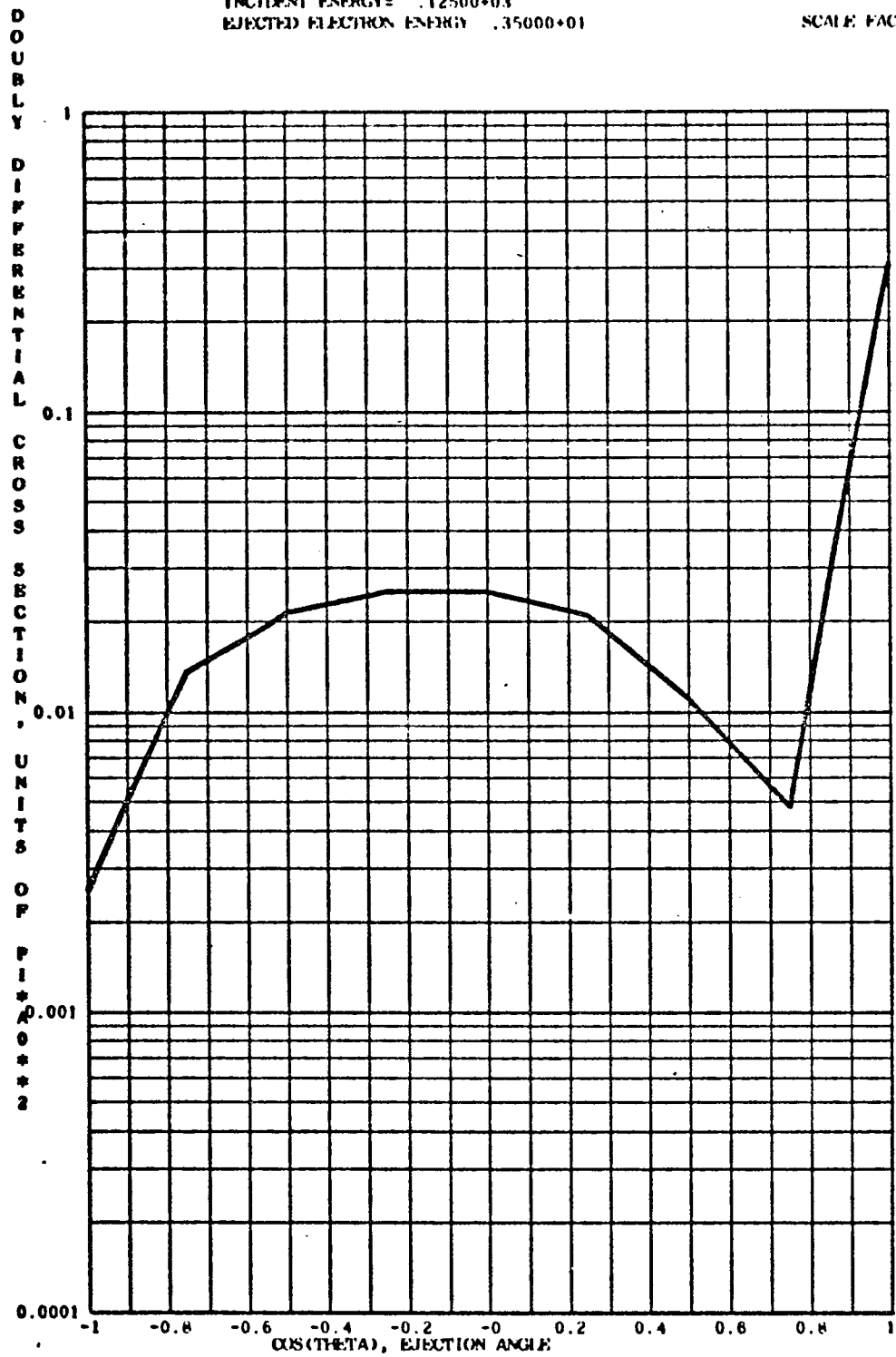
SCALE FACTOR =  $10^{**4}$ 

TABLE I. - PARAMETERS FOR INITIAL STATE WAVE FUNCTIONS

## I. Products of Normalized Hydrogen Wave Functions

N	$\lambda$	$\zeta$	$\omega$	$\alpha_1$	$\alpha_2$
1.529613	0	0	0	1.6875	1.6875

## II. Hartree-Fock, Green's Expansion

N	$\lambda$	$\zeta$	$\omega$	$\alpha_1$	$\alpha_2$
.252204	0	0	0	2.912	2.912
.4203400	0	0	0	2.912	1.456
.4203400	0	0	0	1.456	2.912
.7005700	0	0	0	1.456	1.456

## III. Correlated Wave Function, 12 Term

N	$\lambda$	$\zeta$	$\omega$	$\alpha_1$	$\alpha_2$
.6975873	0	0	0	1.85	1.85
.6975873	0	0	0	1.85	1.85
.2318076	0	1	0	1.85	1.85
.2318076	1	0	0	1.85	1.85
.3391472	0	2	0	1.85	1.85
.3391472	2	0	0	1.85	1.85
-.01831028	0	3	0	1.85	1.85
-.01831078	3	0	0	1.85	1.85
-.30262039	1	1	0	1.85	1.85
-.30262039	1	1	0	1.85	1.85
.03678389	1	2	0	1.85	1.85

## III. (Continued)

N	$\lambda$	$\zeta$	$\omega$	$\alpha_1$	$\alpha_2$
.03678389	2	1	0	1.85	1.85
-.59467608	1	1	1	1.85	1.85
-.59467608	1	1	1	1.85	1.85
.77032823	1	2	1	1.85	1.85
.77032823	2	1	1	1.85	1.85
-.08134807	1	3	1	1.85	1.85
-.08134807	3	1	1	1.85	1.85
-.00760124	1	4	1	1.85	1.85
-.00760124	4	1	1	1.85	1.85
-.32995764	2	2	1	1.85	1.85
-.32995764	2	2	1	1.85	1.85
.08318233	2	3	1	1.85	1.85
.08318233	3	2	1	1.85	1.85

TABLE II. - TABULATION OF CROSS SECTIONS

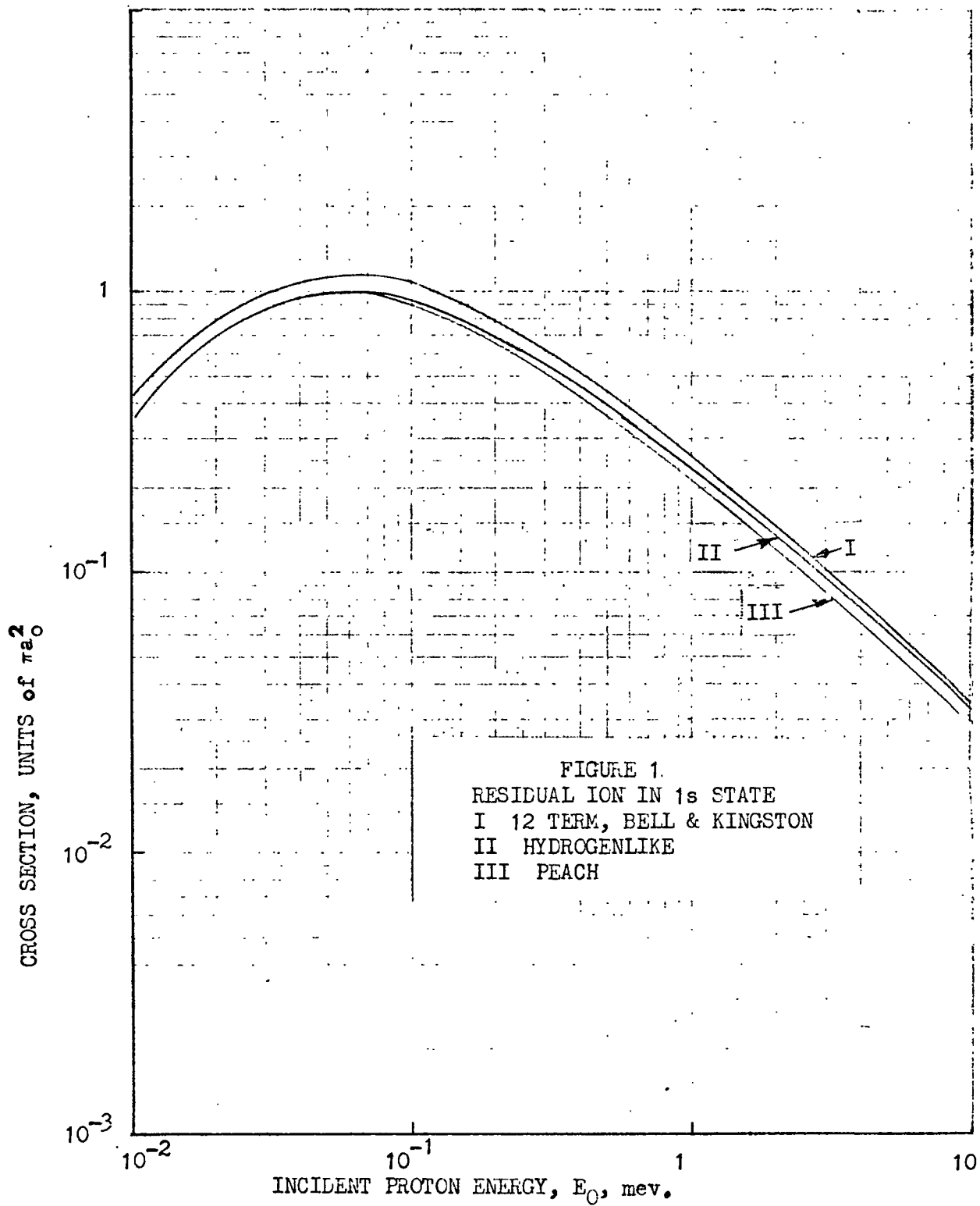
	$E_0$ , MEV	1S 12-TERM THIS WORK	1S BELL AND KINGSTON	1S HYDROGEN- LIKE MAPLETON	2S 12-TERM THIS WORK	2S HYDROGEN- LIKE MAPLETON	2P 12-TERM THIS WORK	2P HYDROGEN- LIKE MAPLETON	
	.0125			.456		.574x10 <sup>-4</sup>		.130x10 <sup>-3</sup>	
	.02229			.743		.246x10 <sup>-3</sup>		.670x10 <sup>-3</sup>	
	.03902	1.07		.953		.772x10 <sup>-3</sup>		.220x10 <sup>-2</sup>	
	.07109			.993		.194x10 <sup>-2</sup>	.356x10 <sup>-1</sup>	.519x10 <sup>-2</sup>	
	.100	1.08	1.07		.573x10 <sup>-2</sup>				
	.125			.867		.321x10 <sup>-2</sup>		.831x10 <sup>-2</sup>	
	.200	.798	.782		.690x10 <sup>-2</sup>				
	.2229			.659	.683x10 <sup>-2</sup>	.363x10 <sup>-2</sup>	.939x10 <sup>-1</sup>	.104x10 <sup>-1</sup>	
	.300	.622	.613						
	.3902			.465		.312x10 <sup>-2</sup>		.107x10 <sup>-1</sup>	
	.500		.428		.535x10 <sup>-2</sup>				
	.7109			.303		.227x10 <sup>-2</sup>	.109	.951x10 <sup>-2</sup>	
	1.250	.216		.196		.157x10 <sup>-2</sup>		.769x10 <sup>-2</sup>	
	2.229			.123	.199x10 <sup>-2</sup>	.103x10 <sup>-3</sup>	.881x10 <sup>-1</sup>	.577x10 <sup>-2</sup>	
	3.902			.778		.671x10 <sup>-3</sup>		.416x10 <sup>-2</sup>	
	5.0	.686x10 <sup>-1</sup>	.670x10 <sup>-1</sup>				.734x10 <sup>-1</sup>		
	10.0								

TABLE II. - TABULATION OF CROSS SECTIONS (continued)

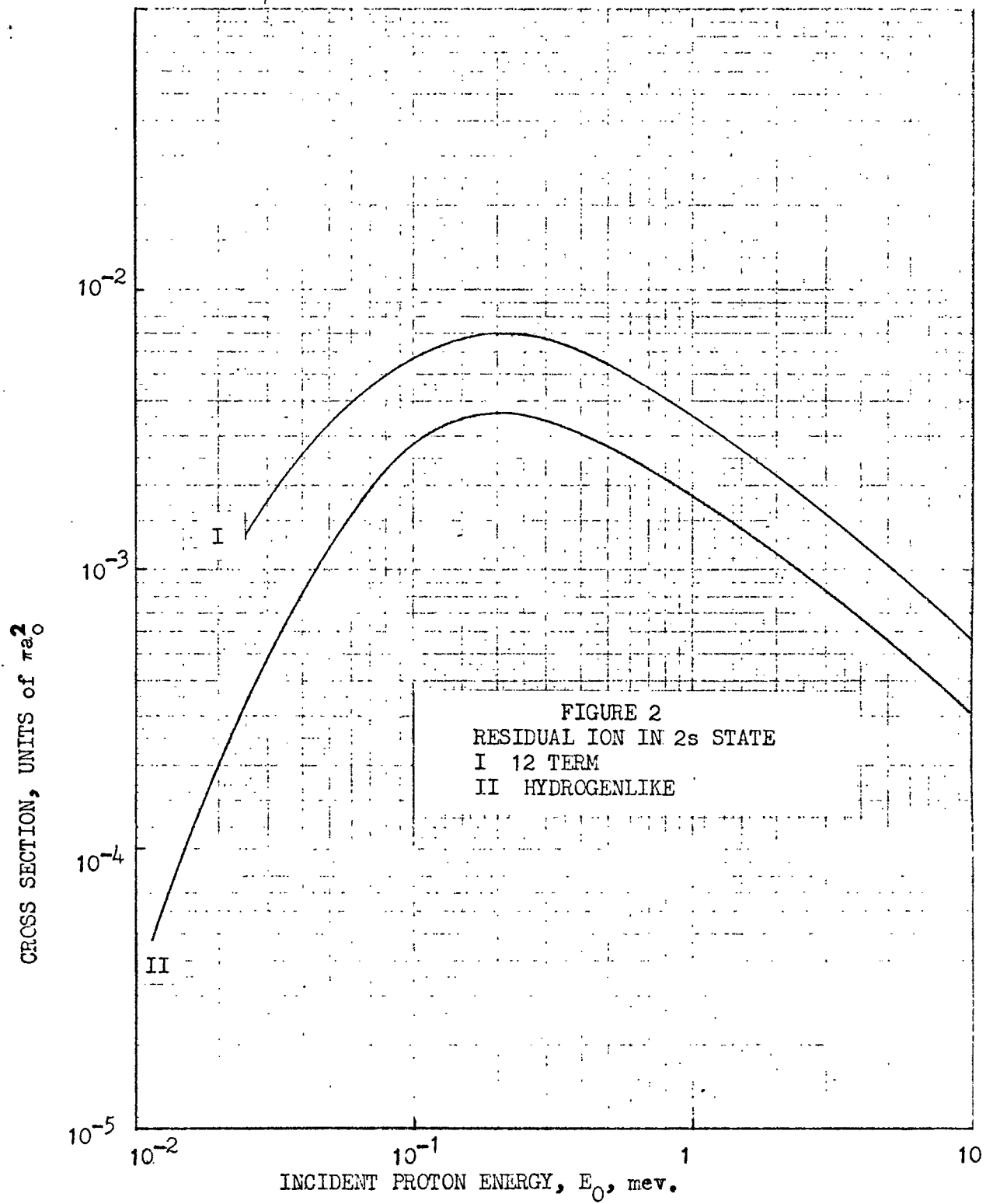
[illegible]

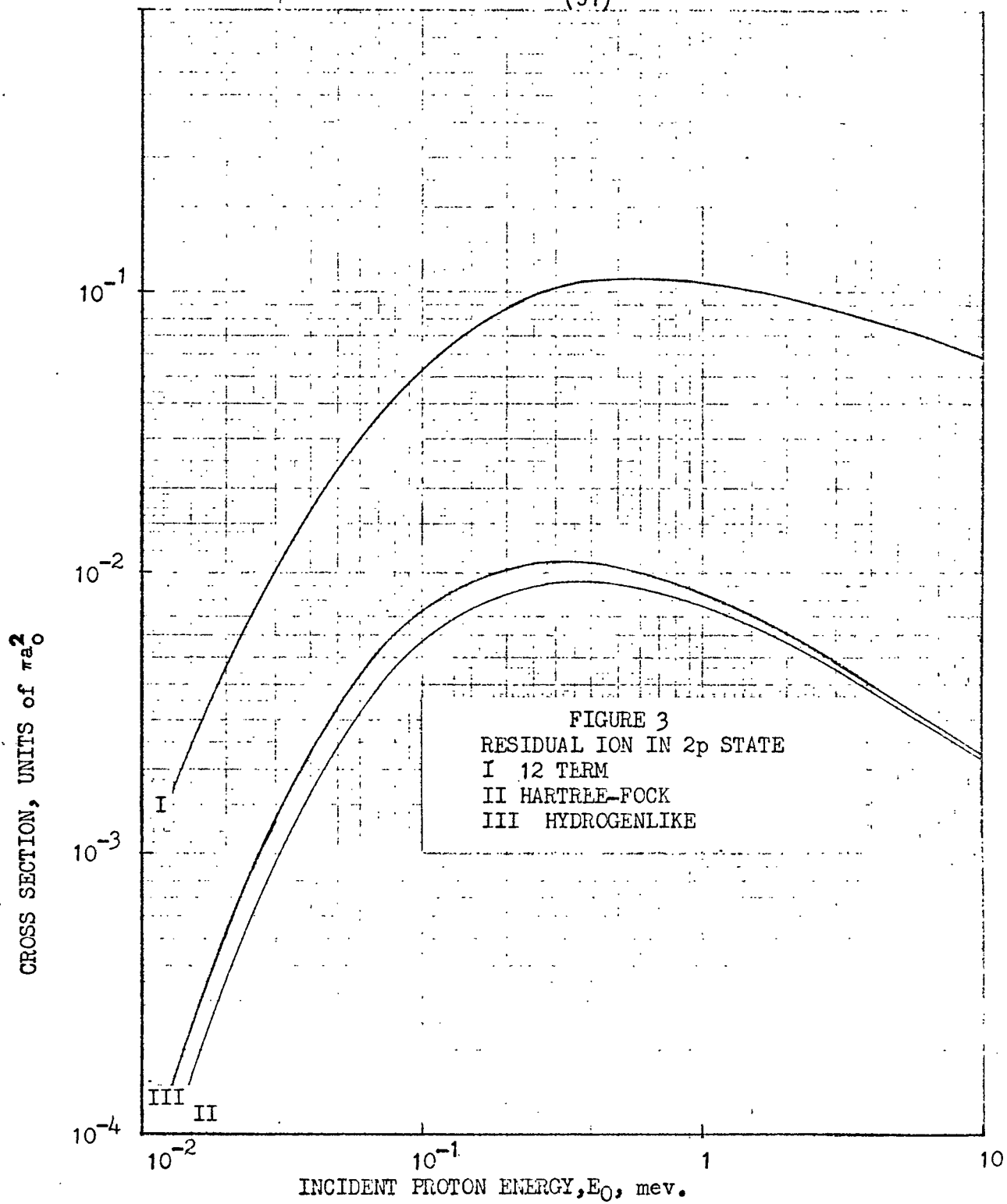
TABLE II. - TABULATION OF CROSS SECTIONS (concluded)

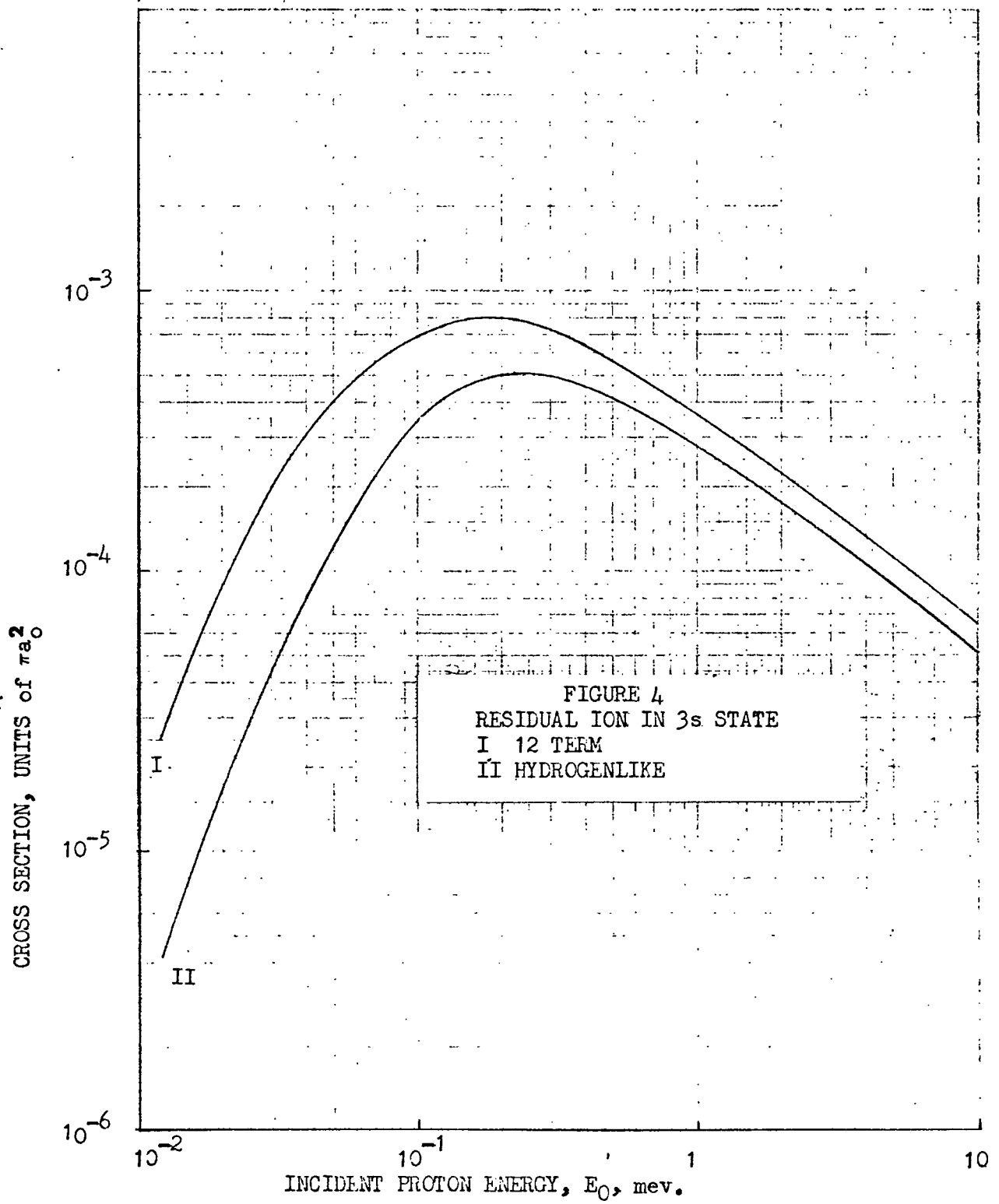
	$E_0$ , MEV	3P HARTREE- FOCK THIS WORK	3d 12-TERM THIS WORK	3d HYDROGEN- LIKE MAPLETON	3d HYDROGEN- LIKE THIS WORK	3d HARTREE FOCK THIS WORK	TOTAL A	TOTAL B	
	.0125	$.146 \times 10^{-4}$	$.461 \times 10^{-6}$	$.860 \times 10^{-6}$		$.602 \times 10^{-6}$			
	.02229	$.822 \times 10^{-4}$		$.788 \times 10^{-5}$	$.793 \times 10^{-5}$	$.536 \times 10^{-5}$			
	.03902	$.302 \times 10^{-3}$	$.317 \times 10^{-4}$	$.407 \times 10^{-4}$	$.410 \times 10^{-4}$	$.294 \times 10^{-4}$	1.095	1.077	
	.07109	$.782 \times 10^{-3}$		$.133 \times 10^{-3}$	$.135 \times 10^{-3}$	$.109 \times 10^{-4}$			
	.100						1.150	1.097	
	.125	$.128 \times 10^{-2}$	$.336 \times 10^{-3}$	$.250 \times 10^{-3}$	$.253 \times 10^{-3}$	$.233 \times 10^{-3}$			
	.200								
	.2229		$.522 \times 10^{-3}$	$.321 \times 10^{-3}$	$.324 \times 10^{-3}$	$.334 \times 10^{-3}$	.9690	.8710	
	.300								
	.3902	$.159 \times 10^{-2}$	$.576 \times 10^{-3}$	$.311 \times 10^{-3}$	$.313 \times 10^{-3}$	$.351 \times 10^{-3}$	.6581	.5390	
	.500								
	.7109		$.503 \times 10^{-3}$	$.244 \times 10^{-3}$	$.245 \times 10^{-3}$	$.294 \times 10^{-3}$			
	1.250	$.128 \times 10^{-2}$	$.381 \times 10^{-3}$	$.171 \times 10^{-3}$	$.172 \times 10^{-3}$	$.216 \times 10^{-3}$	.3433	.2281	
	2.229	$.977 \times 10^{-3}$	$.260 \times 10^{-3}$	$.110 \times 10^{-3}$	$.110 \times 10^{-3}$	$.143 \times 10^{-3}$	.2490		
	3.902	$.692 \times 10^{-3}$	$.169 \times 10^{-3}$	$.678 \times 10^{-4}$	$.680 \times 10^{-4}$	$.905 \times 10^{-4}$	.1850	.0881	
	5.0	$.475 \times 10^{-3}$					.1681		
	10.0	$.398 \times 10^{-3}$							

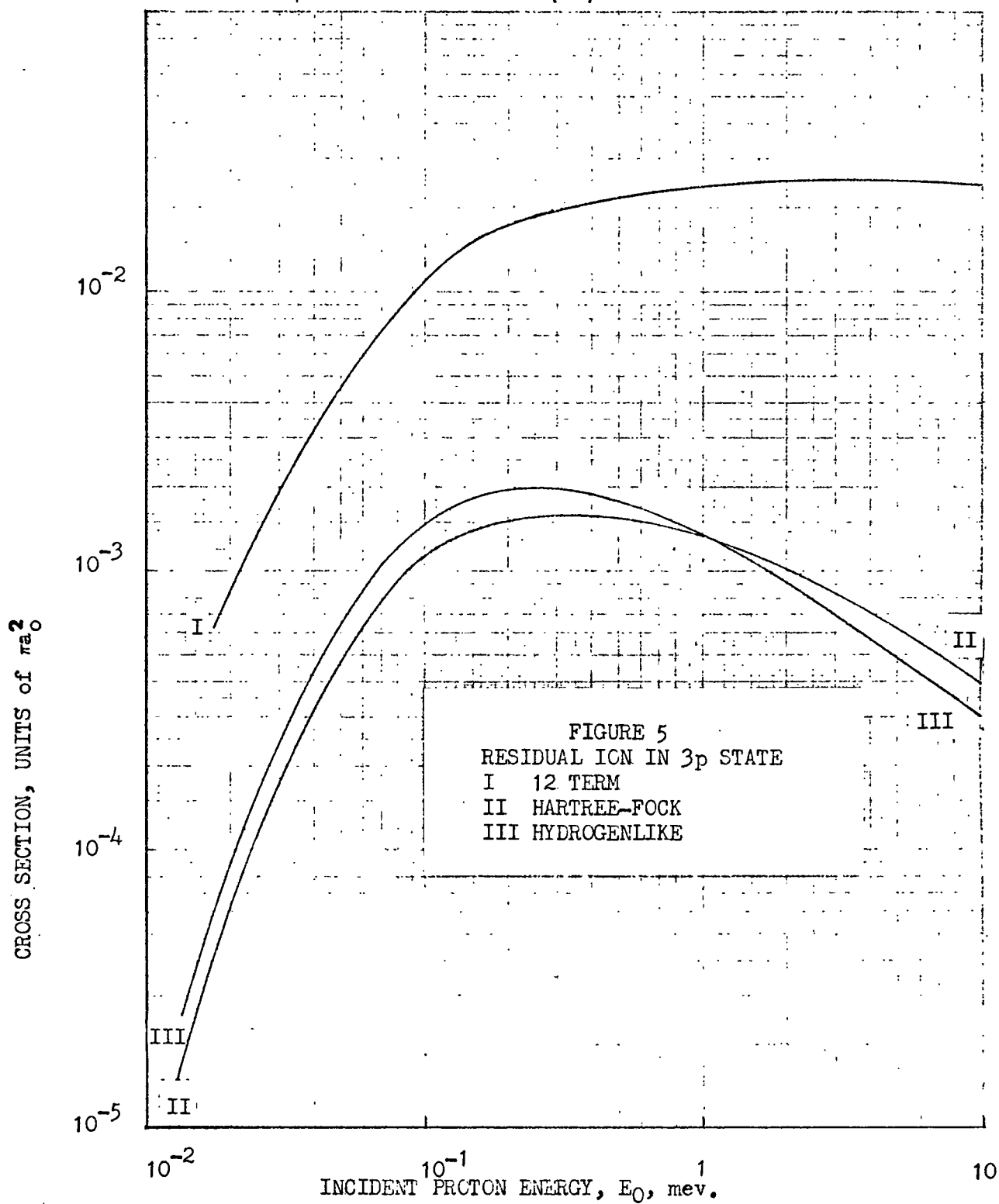


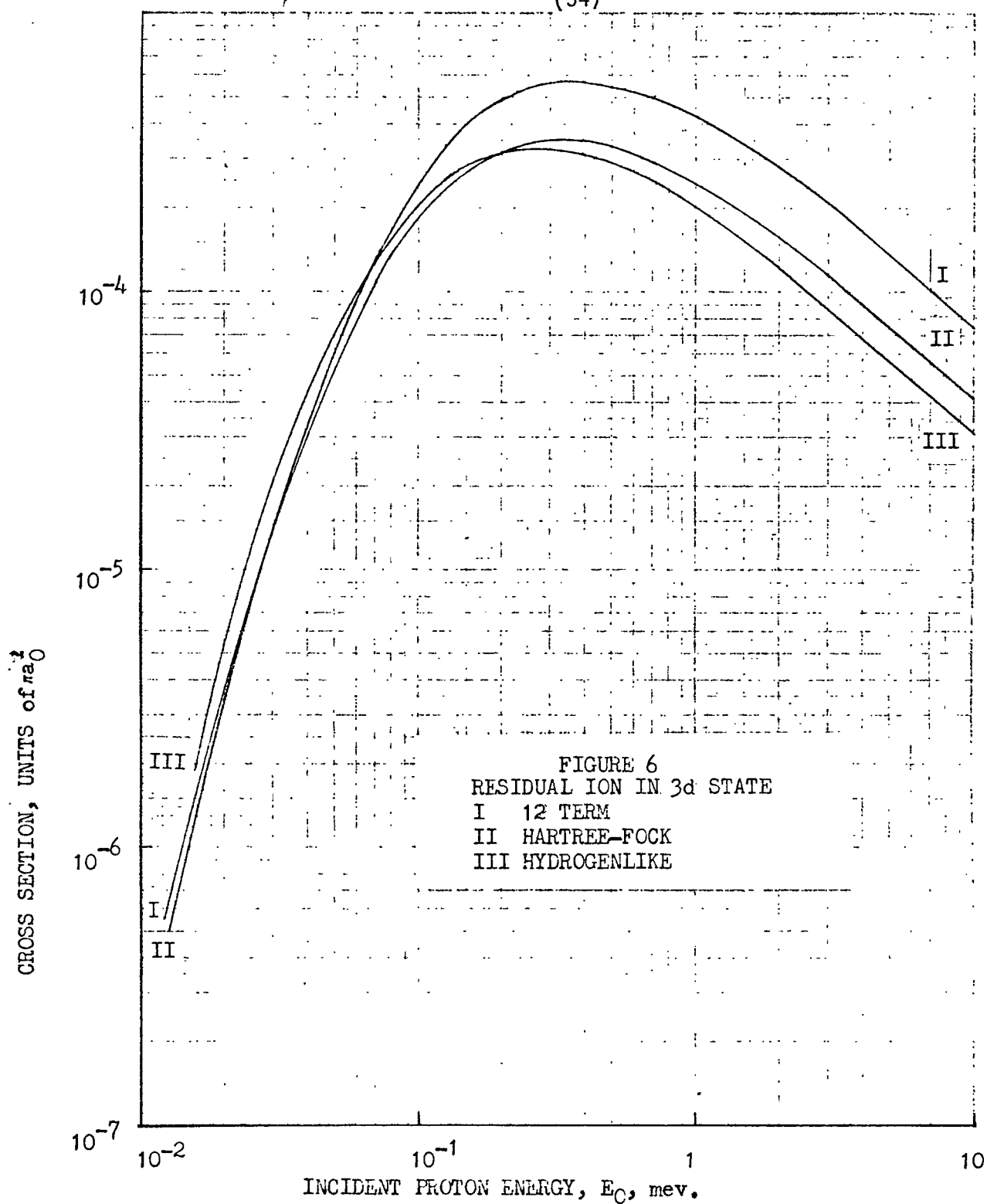


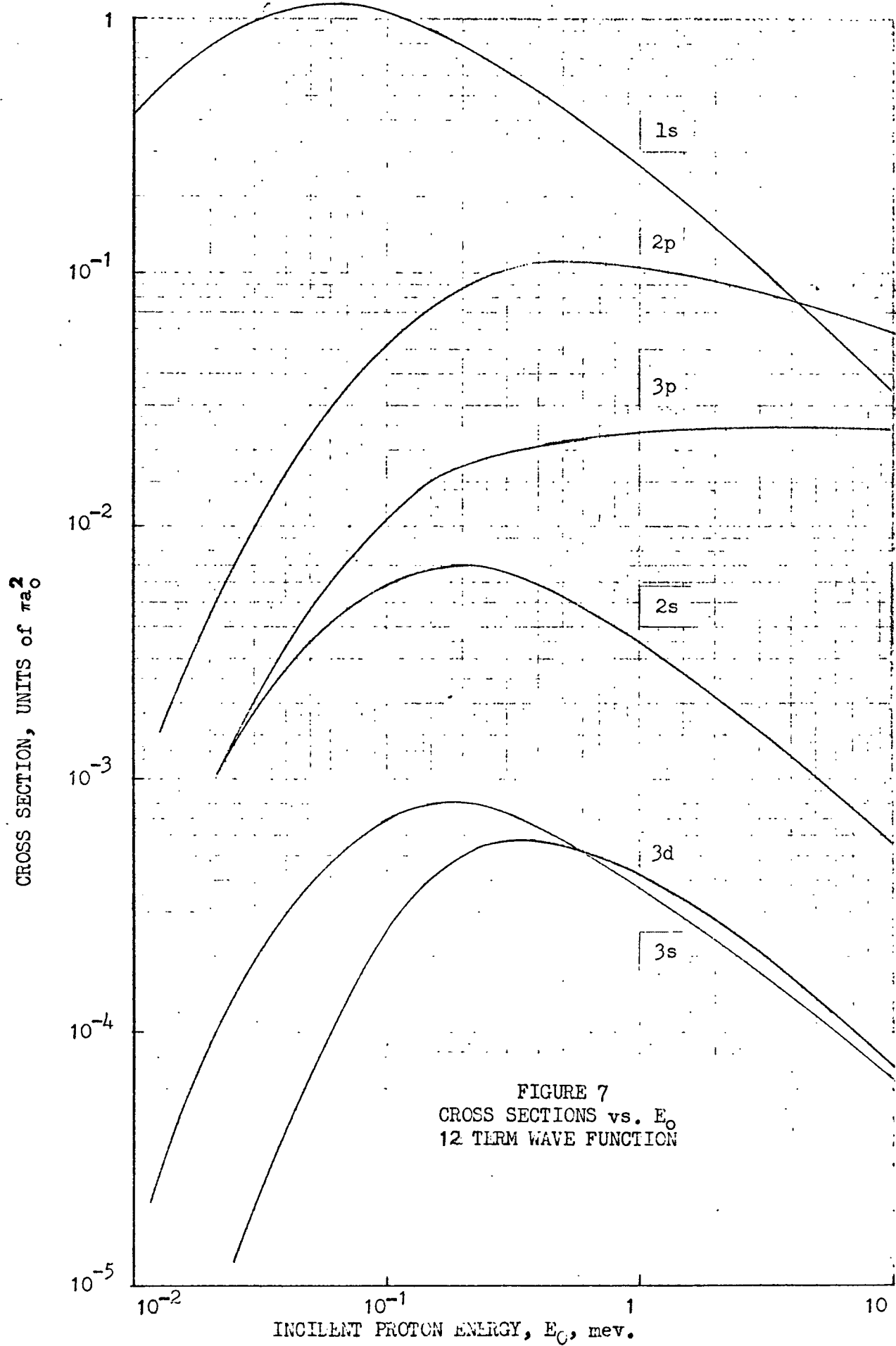


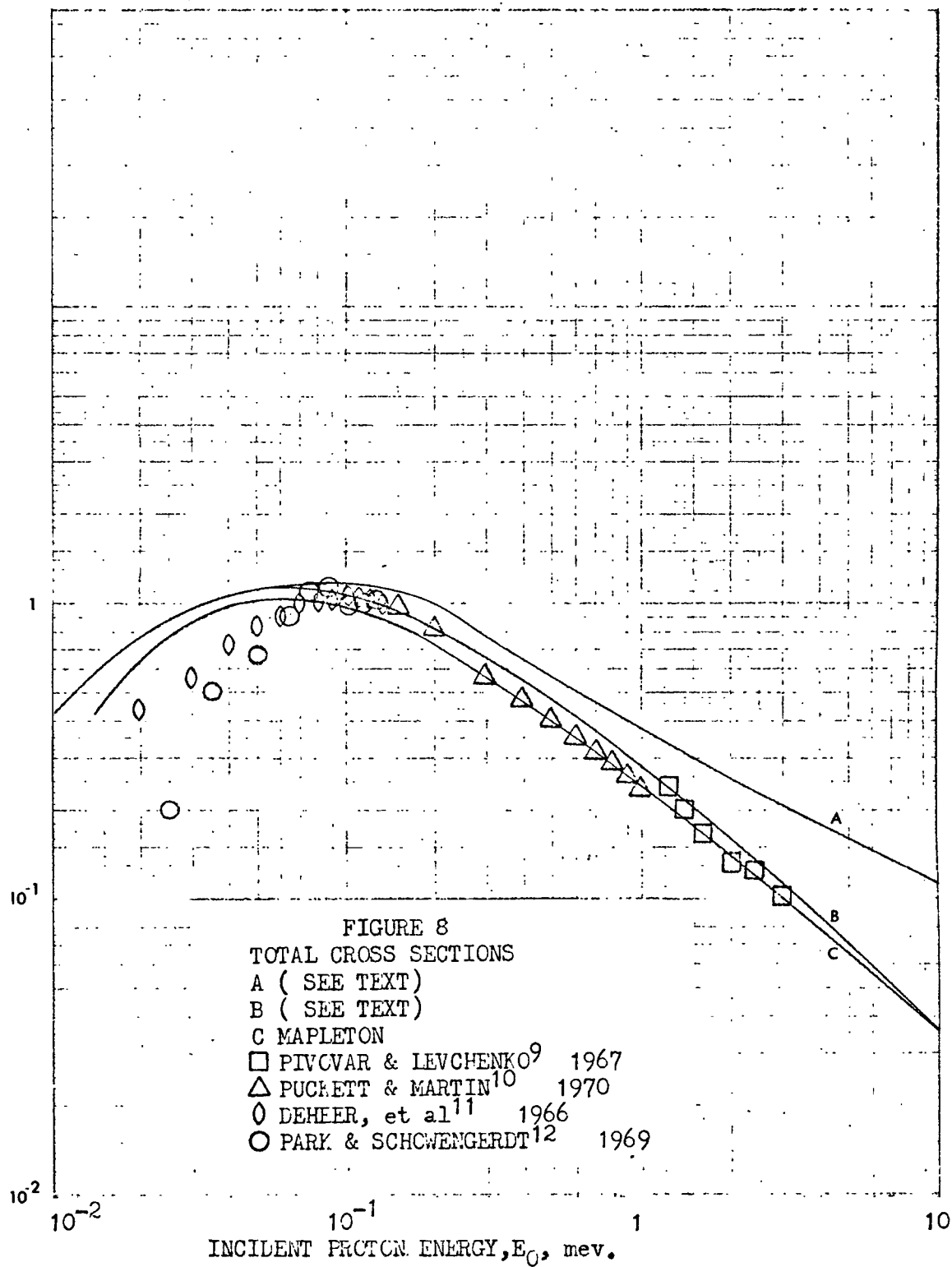










CROSS SECTION, UNITS OF  $a_0$ 

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