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CALCULATIONS OF ENERGY AND ANGULAR DISTRIBUTIONS OF ELECTRONS EJECTED FROM HELIUM BY 200- AND 300-keV PROTONS

by William J. B. Oldham, Jr.

Manned Spacecraft Center

Houston, Texas

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ABSTRACT

Doubly differential cross sections (ddcs) for ejection of secondary electrons of various energies at various angles from helium bombarded by 200- and 300-keV protons have been calculated and compared with the recent experimental results of Rudd, Sautter, and Bailey. The wave functions employed by Mapleton to calculate ionization cross sections are used in the Born approximation in a first calculation. In a second calculation, the Roothaan four-term wave function is used for the ground state of helium. The two calculated results differ very little. General agreement between theory and experiment for the ddcs is found, but discrepancies are noted in the forward and backward directions. Changing the ground-state wave function from the hydrogen-like to the Roothaan four-term wave function has very little effect on the ddcs.

CALCULATIONS OF ENERGY AND ANGULAR DISTRIBUTIONS OF ELECTRONS EJECTED FROM HELIUM BY 200- AND 300-keV PROTONS

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SUMMARY

Doubly differential cross sections for ejection of secondary electrons of various energies at various angles from helium bombarded by 200- and 300-keV protons have been calculated and compared with the recent experimental results of Rudd, Sautter, and Bailey. The wave functions employed by Mapleton to calculate ionization cross sections are used in the Born approximation in a first calculation. In a second calculation, the Roothaan four-term wave function is used for the ground state of helium. The two calculated results differ very little. General agreement between theory and experiment for the cross sections is found, but discrepancies are noted in the forward and backward directions.

INTRODUCTION

The cross sections for ejection of secondary electrons (with various energies and at various angles) from helium bombarded by 50-, 100-, and 150-keV protons have been determined theoretically and reported (ref. 1). From these cross sections, which may be termed doubly differential cross sections (ddcs), cross sections differential in ejection energy may be obtained by integrating the ddcs over the ejection angle. Cross sections for ionization are then obtained by integrating the differential cross sections over the energy of ejection. Several authors - Erskine (ref. 2), Dalgarno and McDowell (ref. 3), and Mapleton (ref. 4) - have published calculated values for the ionization cross sections, but, before the results given in reference 1 appeared, no theoretical results were available for the ddcs for comparison with experimentally determined ddcs. The Born approximation was utilized in reference 1, and products of hydrogen-like wave functions were used to approximate the wave functions of helium in both the ground state and the continuum states. The results of these calculations were compared with the experimental results of Rudd and Jorgensen (ref. 5). At the time reference 1 was published, the experimental results were given only at incident proton energies of 50-, 100-, and 150-keV. In these cases, the ddcs agreed in a general way with the experimental results, but discrepancies were noted, particularly in the forward and backward directions. Now experimental data at incident proton energies of 200- and 300-keV are available (ref. 6), and the Born approximation is more accurate at these levels.

The two purposes of this paper are:

1. To perform the calculations shown in reference 1 at the higher incident proton energies and to compare the results with the experimentally determined values.

2. To give the results of calculation of the ddcs using the four-term Roothaan ground-state wave function (ref. 7) for helium instead of the hydrogen-like wave function used in reference 1. The Roothaan wave function is determined by self-consistent field methods and agrees very well with the Hartree-Fock wave function.

The motivation for purpose (1) is that, since the Born approximation is a high-energy approximation, the results from (1) should agree with the experiment better than did the results given in reference 1. The reason for (2) is to determine the sensitivity of the ddcs to the choice of a ground-state wave function.

SYMBOLS

$\hat{A}$ momentum change vector of incident protons

a_0 radius of first Bohr orbit

$$C = \int \Phi_0^*\left(r_2\right) \phi\left(r_2\right) d\hat{r}_2$$

$$C_0 = \frac{2^{3/2} \mu Z_1^3}{\pi A^2} \int \phi_0^*\left(Z_3 \middle| r\right) e^{-Z_1 r} d\hat{r}$$

C_w defined by equation (19)

$E = \pi/2 - \tan^{-1}\left[\left(A^2 - k^2 + Z_1{}^2\right)\Big/2kZ_1\right]$

E_j energy of ejected electron

E_n final binding energy of helium atom

E_0 initial binding energy of helium atom

e electronic charge

$f = \left(k^2 - Z_1{}^2\right)\left(Z_1 - Z_3\right) - A^2\left(Z_1 + Z_3\right) + 2Z_3Ak \cos \theta$

F hypergeometric function

$f_0^{n,k}$ Born matrix element

G defined by equation (21)

$g = 2Z_1\left[k\left(Z_1 - Z_3\right) + Z_3A \cos \theta\right]$

$\hbar$ Planck's constant divided by 2π

I_D doubly differential cross section

J_0 Bessel function of order zero

$\hat{K}_n$ final proton wave vector

$\hat{K}_0$ initial proton wave vector

$\hat{k}$ vector of electron

$$L = \ln \frac{k^2 + A^2 + Z_1^2 - 2Ak \cos \theta}{\left[\left(A^2 - k^2 + Z_1^2\right)^2 + 4k^2 Z_1^2\right]^{1/2}}$$

ℓ	orbital angular momentum quantum number
$\hat{n}_0$	incident proton direction
$\hat{n}_1$	direction of proton scattering
$\hat{n}_2$	direction of electron ejection
$\hat{n}'$	direction of change of momentum of incident proton
n, s, p	electron states
$P_\ell(\cos \theta)$	Legendre polynomials
p	probability of ejecting an electron into the solid angle $d\omega$ with momentum between k and k + dk

$$R = \left(A^2 - k^2 + Z_1^2\right)^2 + 4k^2 Z_1^2$$

$\hat{r}$	radius vector
$\hat{r}_1$, $\hat{r}_2$	radius vectors of electrons 1 and 2

$$S = k^2 + A^2 + Z_1^2 - 2Ak \cos \theta$$

W_1	defined by equation (9)
W_2	defined by equation (10)
X, Z	spherical coordinates
Z	nuclear charge

$\alpha = E_j'/E_0$

β	constant
Γ	Gamma function
δ, ρ	spherical coordinate angles of scattered proton

$\eta = r(1 - \cos\theta)$

θ	angle between $\hat{r}$ and the direction of ejection
θ_k	angle between direction of ejection and momentum change vector
θ_r	angle between radius vector of ejected electron and momentum change vector
μ	reduced mass of the two-body system

$$\nu = \frac{Z_3}{2k} \ln\left[\frac{(k + A)^2 + Z_1^2}{(k - A)^2 + Z_1^2}\right]$$

Φ_0	Roothaan ground-state wave function of helium
ϕ_k	continuum wave function of hydrogen-like atom
ϕ_k^0	ϕ_k where $\ell = 0$
$\phi_0\left(Z_1 \middle| r\right)$	ground-state wave function of hydrogen-like atom of nuclear charge Z_1
χ	angle between momentum of ejected electron and incident proton direction
ψ_k	positive energy function for a Coulomb field of charge $-Z_3e$
$\psi_{k,n}$	wave function of the continuum state

ψ_0	ground-state wave function of helium
$d\Omega$	solid angle of scattered proton
$d\omega$	solid angle of electron ejection

THEORY

The probability p of ejecting an initially bound electron into the solid angle $d\omega$ with momentum between k and $k + dk$ and scattering the incident proton into the solid angle $d\Omega$ is

$$p = \left| f_0^{n,k} \right|^2 k^2 \, dk \, d\omega \, d\Omega \tag{1}$$

where $f_0^{n,k}$ is the Born matrix element for the transition from the ground state of helium to the continuum state with the bound electron in state n and the free electron with momentum k. If $\hat{r}_1$ and $\hat{r}_2$ are the position vectors of the two electrons, then, according to Mapleton (ref. 4),

$$f_0^{n,k} = \frac{4\mu e^2}{\hbar^2 A^2} \int \psi_{k,n}^* \left(\hat{r}_1, \hat{r}_2\right) e^{i\hat{A}\cdot\hat{r}_1} \psi_0\left(\hat{r}_1, \hat{r}_2\right) d\hat{r}_1 \, d\hat{r}_2 \tag{2}$$

where

μ	= reduced mass of the two-body system
ψ_0	= ground-state wave function of helium
$\psi_{k,n}^*$	= complex conjugate of the wave function of the continuum state
$\hat{A}$	= $\hat{K}_0 - \hat{K}_n$, where $\hat{K}_0$ and $\hat{K}_n$ are, respectively, the initial and final wave vectors of the proton in the center-of-mass system

e = electronic charge = 1

$\hbar$ = Planck's constant divided by 2π

Only final states in which the remaining bound electron is a 1s electron will be considered; hence, n will be dropped from the notation for the matrix element $f_0^{n,k}$. The justification for restricting the final-state bound electron to a 1s electron is found in reference 4, where calculated results are given for ionization cross sections in which the final-state bound electron is in the 1s, 2s, or 2p state. The cross sections for the latter two were found to be at least a factor of 100 less than the first one. Hence, ignoring the contribution such states make to the ddcs is probably justifiable.

For the ddcs I_D, equation (1) must be integrated over $d\Omega$, the solid angle of the scattered proton.

$$I_D = k^2 \int \left| f_0^k \right|^2 d\Omega \tag{3}$$

The calculations in reference 1 use the wave functions as stated in case III of reference 4, where the helium wave functions are approximated by products of normalized hydrogen-like wave functions. These wave functions are repeated here only for completeness. Thus,

$$\psi_{(1s)^2} = \psi_0 = \phi_0\left(Z_1 \middle| r_1\right) \phi_0\left(Z_1 \middle| r_2\right) \tag{4}$$

where $Z_1 = 1.6875$ and where ϕ_0 is the hydrogen ground-state wave function.

Then

$$\psi_{k,n}\left(\hat{r}_1, \hat{r}_2\right) = (1/\sqrt{2}) \left[\psi_k\left(Z_3 \middle| \hat{r}_1\right) \phi_n\left(Z_2 \middle| r_2\right) + \psi_k\left(Z_3 \middle| \hat{r}_2\right) \phi_n\left(Z_2 \middle| r_1\right)\right] \tag{5}$$

where ψ_k is the positive energy function for a Coulomb field of charge $-Z_3e$, and ϕ_n is the ground-state wave function of hydrogen with $Z_2 = 2$. To insure orthogonality of the initial and final states, Mapleton (ref. 4) let

$$\psi_k = \phi_k (1|r) - \phi_k{}^0 (1|r) + \phi_k{}^0 \left(Z_1\middle| r\right) \tag{6}$$

where

$$Z_1 = 1.6875$$

$$\phi_k^* \left(Z_3\middle| r\right) = \frac{1}{2\pi}\left[\frac{in}{1 - \exp(-i2\pi n)}\right]^{1/2} \frac{\exp(ikr)}{\Gamma(1 + n)}$$

$$\times \int_0^\infty J_0 \left[2(iku\eta)^{1/2}\right] \exp(-u)\, u^n\, du$$

$$= \frac{1}{2\pi\Gamma(n + 1)}\left[\frac{in}{1 - \exp(-i2\pi n)}\right]^{1/2} \exp(ikr)$$

$$\times \sum_{\ell=0}^{\infty} i^\ell\, \Gamma(\ell + 1 + n)\, (2kr)^\ell\, P_\ell(\cos\theta)$$

$$\times F(\ell + 1 + n,\ 2\ell + 2,\ -i2kr) \tag{7}$$

$$n = Z_3/ik$$

and

$$\eta = r(1 - \cos\theta)$$

where θ is the angle between r and the direction of ejection. Here, $\phi_k{}^0$ is the $\ell = 0$ part of ϕ_k.

If equations (4), (5), and (6) are substituted into equation (2) for the Born matrix element and the indicated integrations over $d\hat{r}_1$ and $d\hat{r}_2$ are carried out, the results can be written as follows:

$$f_0{}^k = C_0\left[W_1 - W_2(1) + W_2(1.6875)\right] \tag{8}$$

where

$$C_0 = \frac{2^{3/2}\mu Z_1{}^3}{\pi A^2} \int \phi_0^*\left(Z_3\middle|r\right)e^{-Z_1 r}\, d\hat{r}$$

$$Z_2 = 2$$

$$W_1 = \int \phi_k^*\left(Z_3\middle|r\right)e^{i\hat{A}\cdot\hat{r}}\, e^{-Z_1 r}\, d\hat{r}$$

$$W_2 = \int \phi_k^{*0}\left(Z_3\middle|r\right)e^{i\hat{A}\cdot\hat{r}}\, e^{-Z_1 r}\, d\hat{r}$$

The results of performing the integrations over $d\hat{r}$ for W_1 and W_2 are as follows:

$$W_1 = -4\left[\frac{Z_3/k}{1 - \exp\left(-i2\pi Z_3/k\right)}\right]^{1/2} \frac{f + ig}{S^2\, R^{1/2}} \exp\left[\frac{-Z_3}{k}\, E + i\left(\frac{Z_3}{k}\, L + E\right)\right] \tag{9}$$

$$W_2 = -\frac{2}{A}\left[\frac{Z_3/k}{1 - \exp\left(-2\pi Z_3/k\right)}\right]^{1/2}$$

$$\frac{\left[\left(A^2 - Z_1{}^2 - k^2\right)\sin\nu + 2Z_1 A\cos\nu\right]}{\left[(k + A)^2 + Z_1{}^2\right]\left[(k - A)^2 + Z_1{}^2\right]}\exp\left(-Z_3 E/k\right) \qquad (10)$$

where

$$f = \left(k^2 - Z_1{}^2\right)\left(Z_1 - Z_3\right) - A^2\left(Z_1 + Z_3\right) + 2Z_3 Ak\cos\theta$$

$$g = 2Z_1\left[k\left(Z_1 - Z_3\right) + Z_3 A\cos\theta\right]$$

$$E = \pi/2 - \tan^{-1}\left[\left(A^2 - k^2 + Z_1{}^2\right)/2kZ_1\right]$$

$$L = \ln\frac{k^2 + A^2 + Z_1{}^2 - 2\,Ak\cos\theta}{\left[\left(A^2 - k^2 + Z_1{}^2\right)^2 + 4k^2 Z_1{}^2\right]^{1/2}}$$

$$S = k^2 + A^2 + Z_1{}^2 - 2Ak\cos\theta$$

$$R = \left(A^2 - k^2 + Z_1{}^2\right)^2 + 4k^2 Z_1{}^2$$

$$\nu = \frac{Z_3}{2k}\ln\left[\frac{(k + A)^2 + Z_1{}^2}{(k - A)^2 + Z_1{}^2}\right]$$

and θ is the angle between $\hat{A}$ and $\hat{k}$. Now, I_D may be written as

$$I_D = C_0^2 k^2 \int \left| W_1 - W_2(1) + W_2(1.6875) \right|^2 d\Omega \tag{11}$$

To carry out the double integration over $d\Omega$ for I_D, the reference direction must be changed to a fixed direction in space. In this case, using the incident proton direction as a reference direction is most convenient. Suppose the electron is ejected in the direction $(\chi, 0)$ and the proton is scattered in the direction (δ, ρ), as shown in figure 1. If E_0 and E_n are the positive initial and final binding energies of the helium atom, then

$$A = (2\mu)^{1/2} \left\{ 2E_0 - E_j' - 2\left[\left(E_0 - E_j'\right)E_0\right]^{1/2} \cos\delta \right\}^{1/2} \tag{12}$$

where E_0 is the incident energy, and $E_j' = E_j + E_0 - E_n$ where E_j is the ejection energy of the electron. Also

$$\cos\theta = \frac{(2\mu)^{1/2}}{A}\left[\frac{\left(K_0 - K_n\cos\delta\right)}{(2\mu)^{1/2}}\cos\chi + \left(E_0 - E_j'\right)^{1/2}\sin\delta\sin\chi\cos\rho\right] \tag{13}$$

After using the conservation of energy and the binomial expansion in terms of the small quantity $\alpha = E_j'/E_0$, A can be written

$$A = \left(2\mu E_0\right)^{1/2}\left[2(2-\alpha)\sin^2(\delta/2) + \cos\delta\left(\frac{1}{4}\alpha^2 + \frac{1}{8}\alpha^3 + \ldots\right)\right]^{1/2} \tag{14}$$

and $\cos\theta$ can be written

$$\cos\theta = \frac{\left(2\mu E_0\right)^{1/2}}{A} \left\{ \left[2 \sin^2 (\delta/2) + \left(\frac{1}{2}\alpha + \frac{1}{8}\alpha^2 + \ldots \right) \cos\delta \right] \cos\chi \right.$$

$$\left. - \left[1 - \frac{1}{2}\alpha - \frac{1}{8}\alpha^2 - \frac{1}{16}\alpha^3 + \ldots \right] \sin\delta \sin\chi \cos\rho \right\} \tag{15}$$

The double integration indicated in equation (3) can now be carried out over δ and ρ. A computer program was written to perform these integrations for input parameters of E_0, E_j, and χ. Samples of results of these calculations are presented in figures 2 through 5, which also show the experimental results for comparison.

The calculation of the ddcs using the Roothaan ground-state wave function can be carried out with the procedure used above, except that $\phi_0\left(Z_1 \middle| r_1\right)$ in equation (4) is replaced by the Roothaan ground-state wave function:

$$\Phi_0 = \beta_1 e^{-\alpha_1 r} + \beta_2 r e^{-\alpha_1 r} + \beta_3 e^{-\alpha_2 r} + \beta_4 r e^{-\alpha_2 r} \tag{16}$$

with

$\beta_1 = 0.429299$

$\beta_2 = 0.110917$

$\beta_3 = 1.47974$

$\beta_4 = -0.169854$

$\alpha_1 = 3.0$

$\alpha_2 = 1.4$

However, this change greatly increases the work and the numerical computation. The Born matrix element is now

$$f_0^k = \frac{4\mu C}{A^2} \int \phi_k^*\left(Z_3 \middle| r\right) e^{i\hat{A}\cdot\hat{r}} \, \Phi_0(r) \, d\hat{r} \tag{17}$$

where

$$C = \int \Phi_0^*\left(r_2\right) \phi\left(r_2\right) d\hat{r}_2$$

and $\phi(r)$ is the ground-state wave function of hydrogen with $Z = 2$.

Since $\Phi_0(r)$ is the sum of four terms, the Born matrix element in equation (17) can be written as the sum of four integrals. From observation of the form $\Phi_0(r)$, f_0^k can then be written in terms of W_1 of equation (9) and $\partial W_1/\partial Z_1$.

$$f_0^k = \frac{4\mu C}{A^2} \left[\beta_1 W_1(3, 1) - \beta_2 \frac{\partial W_1}{\partial Z_1} (3, 1) + \beta_3 W_1(1.4, 1) - \beta_4 \frac{\partial W_1}{\partial Z_1} (1.4, 1) \right] \tag{18}$$

Here, $W_1\left(Z_1, Z_3\right)$ refers to equation (9) with W_1 considered as a function of the parameters Z_1 and Z_3. In the first two terms of equation (18), $Z_1 = \alpha_1$, and in the second two terms $Z_1 = \alpha_2$. Hence, most of the integration for f_0^k has already been carried out. The derivative of W_1 with respect to Z_1 is tedious, but straightforward, to carry out. Introducing

$$C_w = -4 \left[\frac{Z_3/k}{1 - \exp\left(-2\pi Z_3/k\right)} \right]^{1/2} \tag{19}$$

then gives

$$\frac{\partial W_1}{\partial Z_1} = W_1 \left[i \frac{Z_3}{k} \frac{\partial L(Z_1)}{\partial Z_1} + \left(i - \frac{Z_3}{k} \right) \frac{\partial E(Z_1)}{\partial Z_1} \right] + \frac{C_w \exp\left[-Z_3 E(Z_1)/k\right]}{S^3(Z_1) R^{3/2}(Z_1)}$$

$$\times \exp\left\{ i \left[\frac{Z_3}{k} L(Z_1) + E(Z_1) \right] \right\} \left\{ S(Z_1) R(Z_1) \left[\frac{\partial f(Z_1)}{\partial Z_1} \right.\right.$$

$$\left.\left. + i \frac{\partial g(Z_1)}{\partial Z_1} \right] - G(Z_1) \right\} \tag{20}$$

with

$$G(Z_1) = \left[f(Z_1) + i\, g(Z_1) \right] \left[4Z_1 R(Z_1) + \frac{S(Z_1)}{2} \frac{\partial R(Z_1)}{\partial Z_1} \right] \tag{21}$$

The noted derivatives are as follows:

$$\frac{\partial f(Z_1)}{\partial Z_1} = k^2 - A^2 - 3Z_1{}^2 + 2Z_1 Z_3 \tag{22}$$

$$\frac{\partial g(Z_1)}{\partial Z_1} = \frac{g(Z_1)}{Z_1} + 2kZ_1 \tag{23}$$

$$\frac{\partial L\left(Z_1\right)}{\partial Z_1} = \frac{2Z_1}{R\left(Z_1\right)S\left(Z_1\right)}\left[R\left(Z_1\right) - \left(A^2 + Z_1{}^2 + k^2\right)S\left(Z_1\right)\right] \tag{24}$$

$$\frac{\partial S\left(Z_1\right)}{\partial Z_1} = 2Z_1 \tag{25}$$

$$\frac{\partial E\left(Z_1\right)}{\partial Z_1} = \frac{-2k}{R\left(Z_1\right)}\left(Z_1{}^2 - A^2 + k^2\right) \tag{26}$$

$$\frac{\partial R\left(Z_1\right)}{\partial Z_1} = 4Z_1\left(A^2 + Z_1{}^2 + k^2\right) \tag{27}$$

Now, I_D can be found by carrying out the double integration over the proton scattering angle as before. Some results are shown in figures 2 through 5 for comparison with the experiment and also with the first calculation.

RESULTS AND DISCUSSION

The theoretical results are in general agreement with the experimental results (see figs. 2 through 5), but discrepancies occur in the forward and backward directions. Also noted is that the agreement between theory and experiment improves for ejection angles less than 90° as the ejection energy increases, but agreement seems to worsen for angles greater than 90°. It is probably noteworthy that the results for 300-keV incident protons are neither significantly better nor worse than the same results for 150-keV protons as given in reference 1, except for one aspect: for a fixed ejection energy, the theory predicts a maximum value of the ddcs (considered as a function of ejection angle) whose location depends on the ejection energy and always occurs between 0° and 90°. The experiment always shows an absolute maximum in the forward direction or at 0°. Only at high incident proton energies and high electron ejection energies does the experiment show a relative maximum to match the theoretically predicted maximum. Even at these higher proton and electron energies, the experimental results sharply increase again to an absolute maximum in the forward direction, but the theory predicts decreases in this region. The reason for this discrepancy is not known. It seems likely that this discrepancy is due to error in wave functions or errors inherent in the Born approximation.

CONCLUDING REMARKS

As shown by these calculations, changing the ground-state wave function from the hydrogen-like to the Roothaan four-term wave function has very little effect on the ddcs. This is disappointing, considering the extra labor involved in using the Roothaan ground-state wave function instead of the hydrogen-like wave function. However, it does indicate that for future calculations the simpler wave function may be used.

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National Aeronautics and Space Administration
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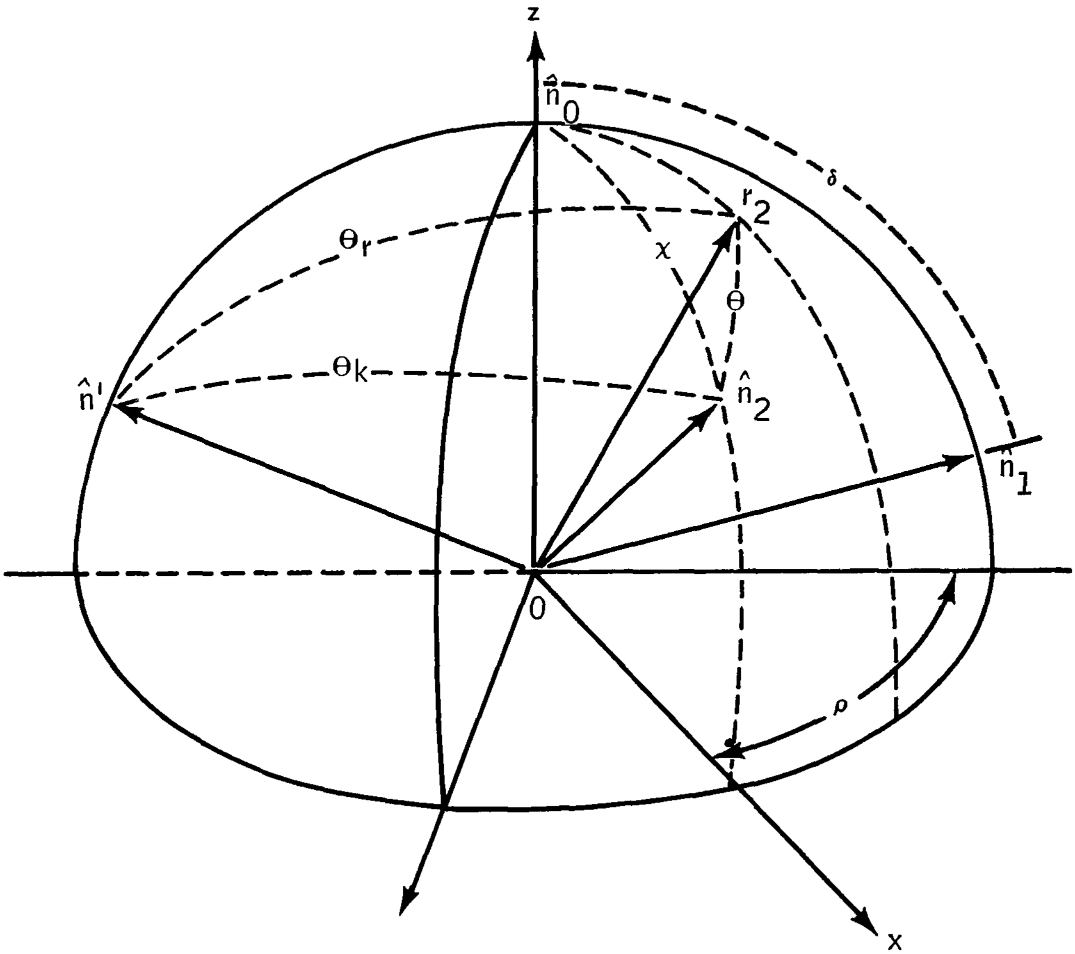

$\hat{n}_0$ direction of incidence; $\hat{n}_1$ direction of scattering; $\hat{n}_2$ direction of ejection; $\hat{n}'$ direction of change of momentum of incident proton

Figure 1. - Directions of the incident and scattered particles.

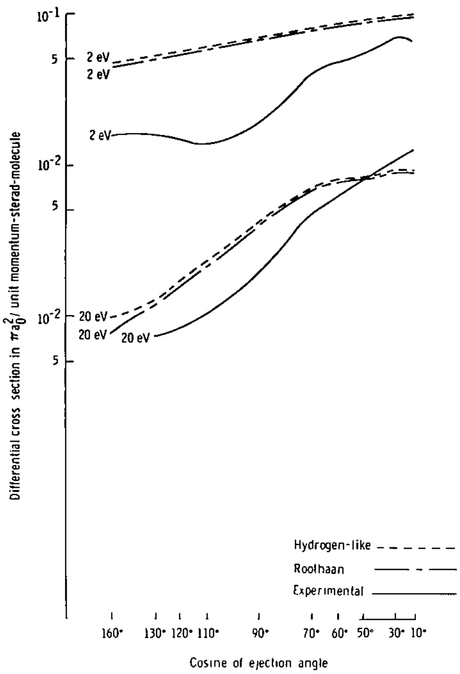

Figure 2. - Differential cross section for production of secondary electrons by 200-keV protons I.

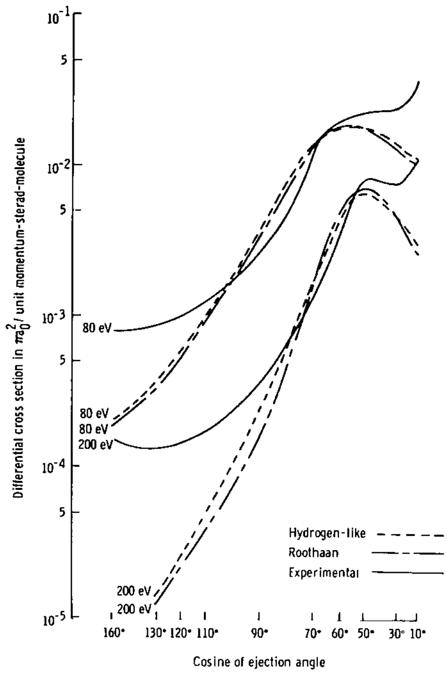

Figure 3. - Differential cross section for production of secondary electrons by 200-keV protons II.

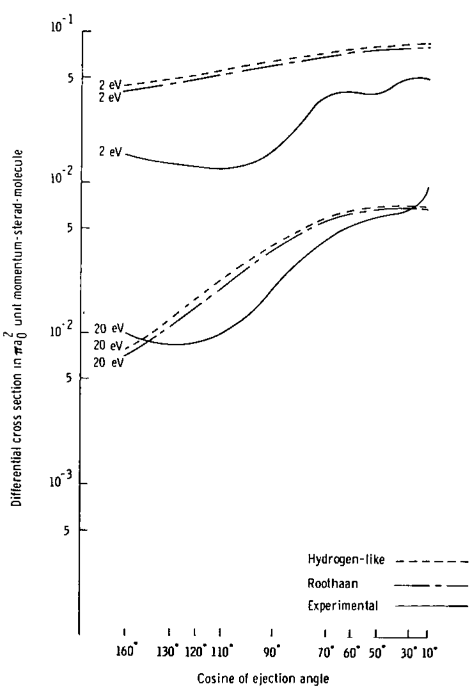

Figure 4. - Differential cross section for production of secondary electrons by 300-keV protons I.

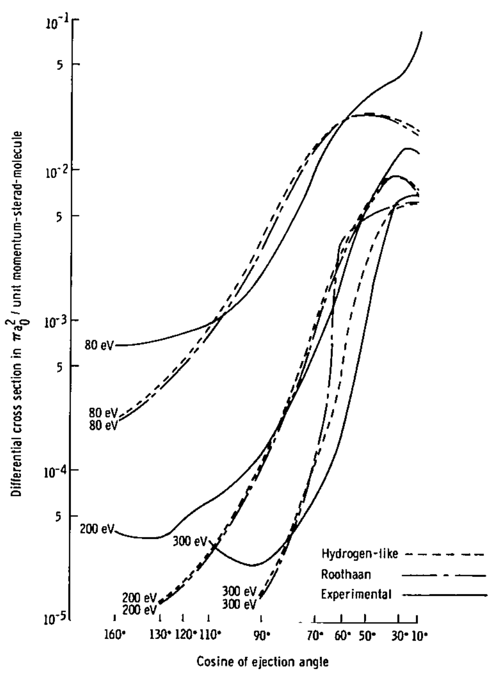

Figure 5. - Differential cross section for production of secondary electrons by 300-keV protons II.

"The aeronautical and space activities of the United States shall be conducted so as to contribute . . . to the expansion of human knowledge of phenomena in the atmosphere and space. The Administration shall provide for the widest practicable and appropriate dissemination of information concerning its activities and the results thereof."

—NATIONAL AERONAUTICS AND SPACE ACT OF 1958

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