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TECHNICAL NOTE

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VARIATIONAL APPROACH TO THE CALCULATION OF CHARGE

EXCHANGE CROSS SECTIONS FOR

ADIABATIC COLLISIONS

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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SUMMARY

Cross sections for the reaction $H^+ + H(1s) \rightarrow H(1s) + H^+$ are calculated for incident particle energies between 10 ev and 2250 ev using an impact parameter method. The required electronic energy levels were found by varying one parameter in the molecular ion wave function at every value of proton separation. The resulting cross sections are compared with those obtained using more accurate wave functions and with experimental data.

INTRODUCTION

Interest in charge exchange cross sections has increased in recent years because of their usefulness in explaining the presence of certain ions in the upper atmosphere and because of their application to ion beam techniques. Methods for calculating cross sections were described by Bates, Massey, and Stewart (ref. 1). Their "perturbed stationary state" (PSS) method was used by Dalgarno and Yadav (ref. 2) to calculate cross sections for the resonant reaction $H^+ + H(1s) \rightarrow H(1s) + H^+$ at energies too low for use of the Born approximation. Exact molecular ion wave functions were used in the calculation. For analogous reactions among larger atoms, exact wave functions are not available. Approximate wave functions with three variable parameters were used by Moiseiwitsch (ref. 3) to calculate cross sections for the reaction $He^+ + He \rightarrow He + He^+$, but the parameters were optimized only for infinite separation of the nuclei.

In order to examine the errors introduced by the use of approximate wave functions, calculations of cross sections for the reaction $H^+ + H(1s) \rightarrow H(1s) + H^+$ were performed at the Ames Research Center by means of the impact parameter method of reference 1, using hydrogen-like wave functions with a variable parameter. In this method as in the PSS method, the adiabatic approximation is used; that is, it is assumed that the nuclei move much more slowly than the electron, so that the latter can be described by stationary state wave functions which must be determined for each internuclear distance. For a hydrogen molecular ion only one parameter is needed to obtain a fairly good approximation to the wave

function (ref. 4). An algebraic expression for this parameter in terms of the particle separation has been obtained by using the variational principle, and the resulting energy eigenvalues were used in conjunction with the equations of reference 1 to obtain cross sections for the reaction $H^+ + H(1s) \rightarrow H(1s) + H^+$ for incident particle energies between 10 ev and 2250 ev. The calculations were programmed for the IBM 709 computer by Miss Marilyn A. Myers.

SYMBOLS

a	proton moving in the laboratory frame of reference
b	proton stationary in the laboratory frame of reference
e	base of natural logarithms
e_-	charge on an electron
E	initial kinetic energy of proton a
E_O	ground state energy of the electron in a hydrogen atom
$\hbar$	Planck's constant divided by 2π
H	Hamiltonian operator
i	$\sqrt{-1}$
m	mass of the electron
Q	charge exchange cross section
r_a	distance from electron to proton a
r_b	distance from electron to proton b
R	distance between protons a and b
$R_c(\rho)$	distance of closest approach of protons a and b
t	time
$v(R)$	relative velocity of protons a and b
$v(\infty)$	relative velocity of protons a and b at infinite separation
X^+	symmetric wave function
X^-	antisymmetric wave function

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β   variational parameter in equation (4)

ϵ^+ energy eigenvalue of the symmetric state

ϵ^- energy eigenvalue of the antisymmetric state

$\zeta(\rho)$ phase shift defined in equation (3)

ρ   distance of closest approach of protons a and b assuming that their
        paths are undeviated in the encounter

ψ   wave function of the electron

ANALYSIS AND DISCUSSION

Consider a proton a approaching a second proton b at constant speed,
initially directed along a straight line whose closest distance to proton b is
ρ as shown in the sketch. An electron e_- is originally in the 1s state of
system a. Its distance from proton a is r_a, from proton b, r_b. Since
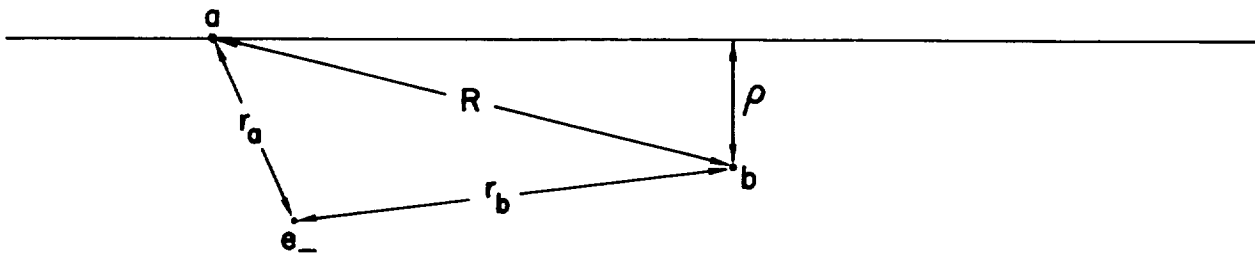
protons a and b are identical, the electronic wave function must be symmetric
or antisymmetric with respect to interchange of the two protons. Let X^+ be an
appropriate symmetric wave function, X^- an antisymmetric wave function, and let
the initial wave function of the system be $(1/\sqrt{2})$ $(X^+ + X^-)\exp[-(i/\hbar)E_0 t]$. After
the collision the electronic wave function is (ref. 1):

$$\psi = \frac{1}{\sqrt{2}} \left\{ X^+ \exp\left[\frac{-i}{\hbar} \int_{-\infty}^{+\infty} (\epsilon^+ - E_0)dt \right] + X^- \exp\left[\frac{-i}{\hbar} \int_{-\infty}^{+\infty} (\epsilon^- - E_0)dt \right] \right\} \exp\left(\frac{-i}{\hbar} E_0 t \right) \quad (1)$$

in the approximation that there are no transitions to higher states, where E_0
is the ground state energy of the electron at infinite separation of the protons,
ϵ^+ is the ground state energy of the symmetric state, ϵ^- is the ground state
energy of the antisymmetric state. The cross section for charge exchange is
(ref. 1)

$$Q = 2\pi \int_0^\infty \rho \, \sin^2 \zeta(\rho) d\rho \qquad (2)$$

where

$$\zeta(\rho) = \frac{1}{\hbar} \int_{R_c(\rho)}^\infty \frac{\epsilon^- - \epsilon^+}{v(R)} \left[1 - \frac{v^2(\infty)\rho^2}{v^2(R)R^2} \right]^{-1/2} dR \qquad (3)$$

where $v(R)$ is the relative velocity of the two protons, and $R_c(\rho)$ is the distance of closest approach. Moiseiwitsch (ref. 3) used the further approximations $v(R) = v(\infty)$ and $R_c(\rho) = \rho$ which we shall use for the case of hydrogen.

The symmetric and antisymmetric spatial wave functions used in our calculations are, respectively,

$$X^+ = \frac{1}{\sqrt{\pi}} \left(e^{-\beta r_a} + e^{-\beta r_b} \right) \quad \text{and} \quad X^- = \frac{1}{\sqrt{\pi}} \left(e^{-\beta r_a} - e^{-\beta r_b} \right) \qquad (4)$$

where β is the variational parameter. Inserting these into the expression for the initial wave function shows that the electron was assumed to be originally in a 1s state near proton a. The energy eigenvalues for the symmetric and antisymmetric states are, respectively,

$$\epsilon^+ = \frac{\int X^+ H X^+ \, d\tau}{\int X^+ X^+ \, d\tau} \quad \text{and} \quad \epsilon^- = \frac{\int X^- H X^- \, d\tau}{\int X^- X^- \, d\tau} \qquad (5)$$

where

$$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{e_-^2}{r_a} - \frac{e_-^2}{r_b} + \frac{e_-^2}{R}$$

is the Hamiltonian operator for the electron in a hydrogen molecular ion, m is the electron mass, e_- is the electron charge, $d\tau$ is the increment of volume, and the integrations are carried out over all space. Evaluation of the integrals is simple except where r_a and r_b appear together in the integrand. In the latter case it is convenient to use confocal elliptic coordinates (ref. 4). The integrals of equation (5) are separately minimized with respect to β to determine ϵ^+ and ϵ^- in terms of R. The integrations for $\zeta(\rho)$ were carried out on an IBM 709 computer for many values of ρ. These values were then used in the integration for Q at several values of $v(\infty)$.

A plot of the energy eigenvalues of the symmetric and antisymmetric states is shown in figure 1. Plots of the integrand of equation (2) appear in figures 2 and 3. The error in assuming $R_c(\rho) = \rho$ in equation (3) may be estimated by noting that the ϵ^+ curve determines the classical limit of proximity of the protons. Contributions to Q for smaller values of ρ should be omitted. However, figures 2 and 3 show that these are very small anyway. In fact, the contribution is only 1 percent at 10 ev and gets smaller for higher

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energies. At higher energies the effect of assuming $v(R)$ constant is mainly to ignore the slowing down of the protons when they are very close ($\rho < 1$). Figure 3 shows that for small ρ the resulting change in $\zeta(\rho)$ would make little difference, since the integrand is very small. This is not the case at low energies where the velocities are changing by a significant fraction at several Bohr radii. Thus the calculation is not made below 10 ev. Ferguson (ref. 5) finds that consideration of momentum transfer of the electron (neglected in our approximation) reduces the cross section by 5 percent at 2000 ev and by larger amounts at higher energies, so our calculation was not extended much above 2000 ev.

The resonant charge exchange cross sections obtained using the variational wave functions are shown in the following table at various incident particle energies E:

E (ev)	$v(\infty)(10^6$ cm per second)	$Q\ (10^{-16}$cm$^2)$
10	4.38	38.5
40	8.76	30.4
100	13.84	25.6
160	17.51	23.3
250	21.9	21.3
1000	43.8	15.3
2250	65.7	12.2

They are compared with those of reference 2 and with the experimental results of Stebbings, Smith, and Fite (ref. 6) in figure 4. The good agreement between these results and those obtained by more exact calculations suggests that the variational method may be applied with satisfactory results to more complicated atoms.

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REFERENCES

1. Bates, D. R., Massey, H. S. W., and Stewart, A. L.: Inelastic Collisions Between Atoms. I. General Theoretical Considerations. Proc. Roy. Soc. A216, 1953, p. 437.

2. Dalgarno, A., and Yadav, H. N.: Electron Capture II: Resonance Capture From Hydrogen Atoms by Slow Protons. Proc. Phys. Soc. A66, 1953, p. 173.

3. Moiseiwitsch, B. L.: Interaction Energy and Charge Exchange Between Helium Atoms and Ions. Proc. Phys. Soc. A69, 1956, p. 653.

4. Pauling, L., and Wilson, E. B., Jr.: Introduction to Quantum Mechanics. McGraw-Hill Book Company, Inc., New York and London, 1935.

5. Ferguson, A. F.: Resonance Charge Transfer Between $H(1s)$ and H^+ Calculated by Means of an Approximation Based on an Expansion in Molecular Eigenfunctions. Proc. Roy. Soc. A264, 1961, p. 540.

6. Stebbings, R. F., Smith, A. C. H., and Fite, W. L.: Charge Transfer in Collisions Involving Symmetric and Asymmetric Resonance. Preprint GA-2783, General Atomic, Div. of General Dynamics, Jan. 1962.
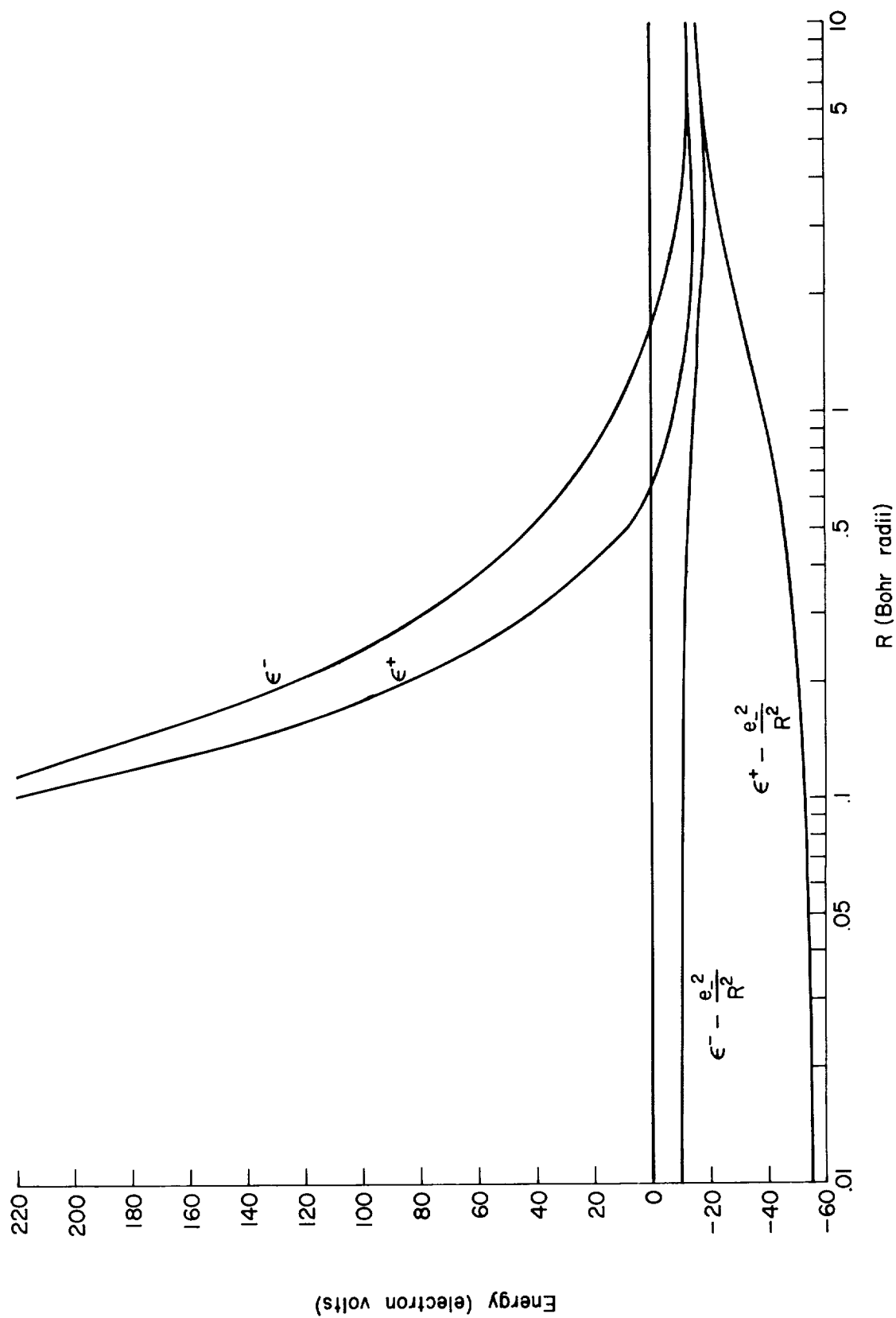
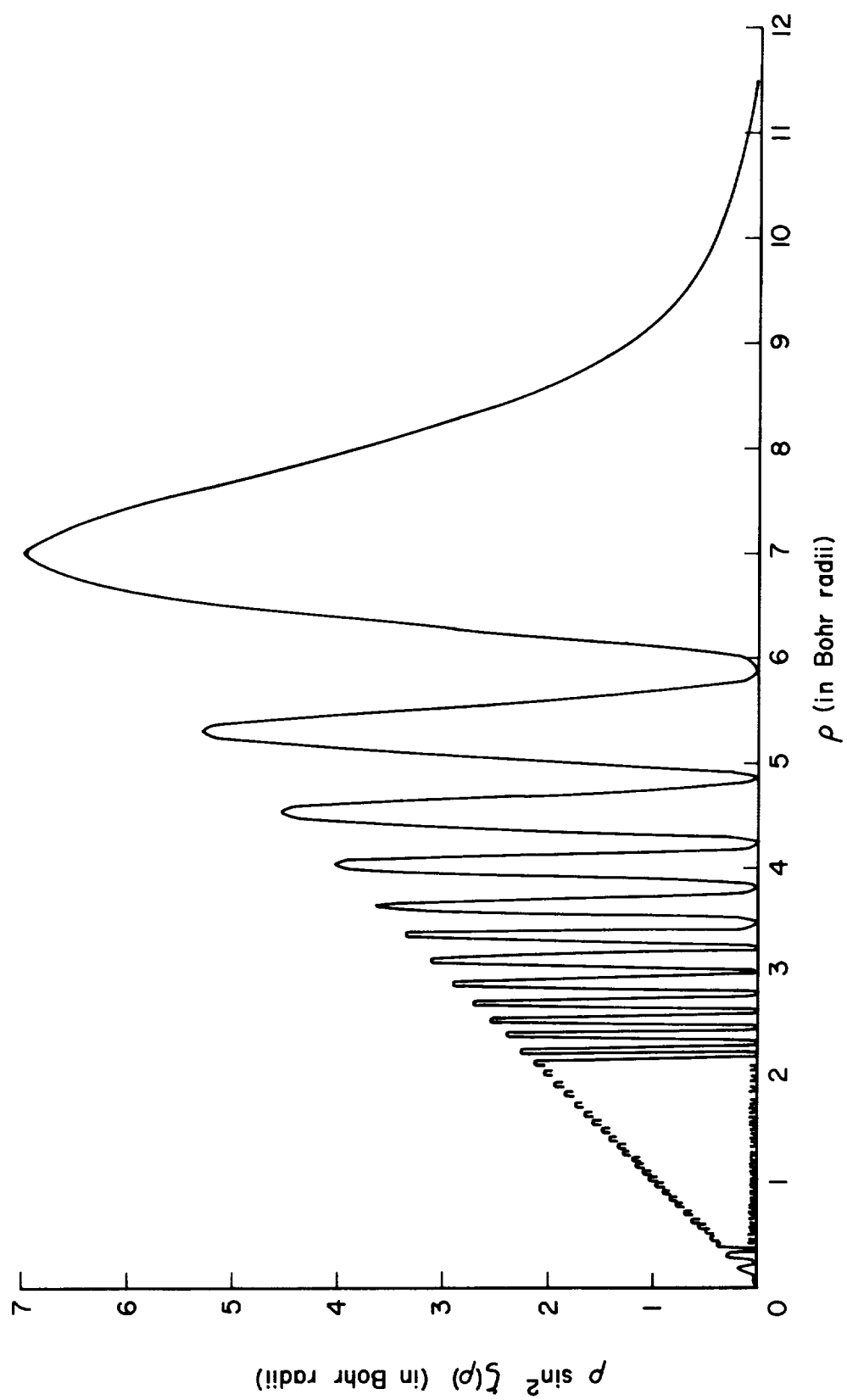Figure 1.- Interaction energy versus proton separation.

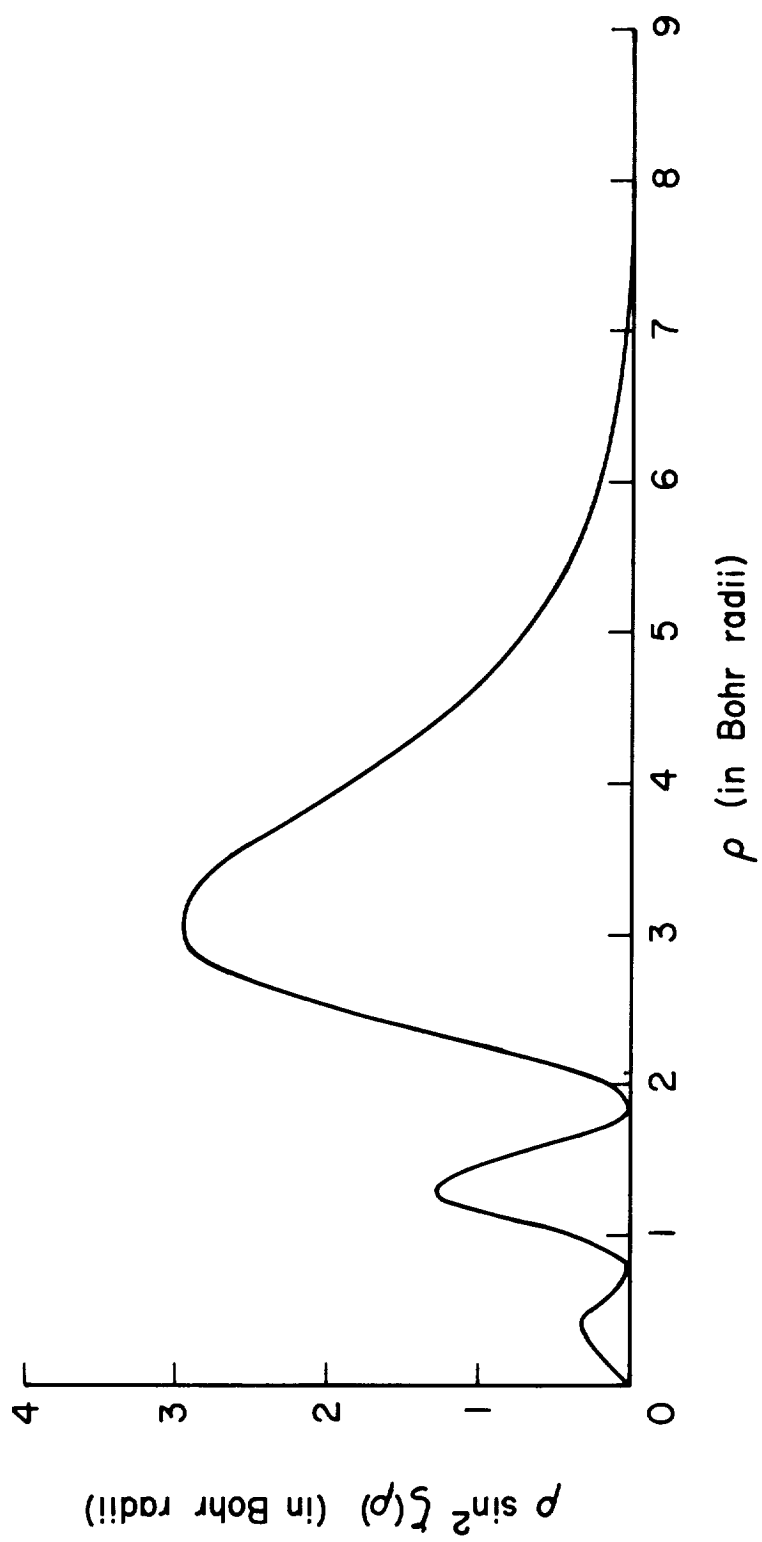Figure 2.- $\rho \sin^2 \zeta(\rho)$ versus ρ at $E = 10$ ev.

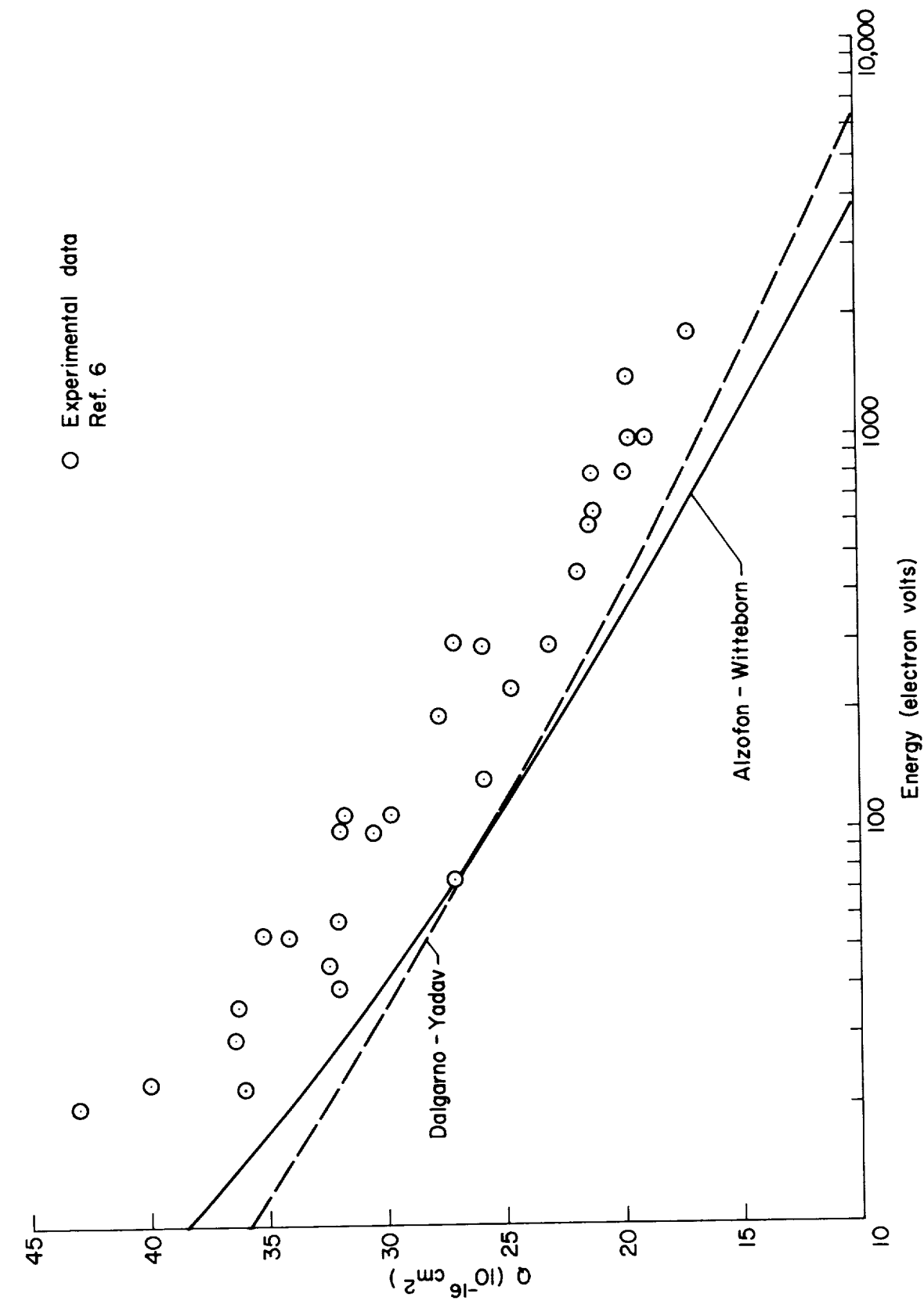Figure 3.- $\rho \sin^2 \zeta(\rho)$ versus ρ at E = 2250 ev.

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Figure 4.- Cross section versus energy for reaction $H(1s) + H^+ \rightarrow H^+ + H(1s)$.