Comparison of Electron and Proton Ionization Data with the Born Approximation Predictions*

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A comparison is made of the experimental ionization cross sections for protons and electrons incident at the same velocity of relative motion on helium, neon, argon, hydrogen, nitrogen, oxygen, and carbon monoxide. For a given target gas, the Born approximation predicts the proton and electron cross sections to be equal at the same velocity of relative motion, provided the velocity is sufficiently high. This prediction is shown to hold for the above gases at electron energies greater than about 300 ev. The corresponding proton energy is 552 kev.

The experimental cross sections as functions of energy for incident protons on these gases have been fitted to the theoretical expression of Bethe to obtain empirical values of the several parameters. For the case of hydrogen, these are in satisfactory agreement with the theoretical values obtained by Bethe. Similar comparisons cannot be made for the other gases since numerical values for these quantities have not yet been calculated from theory. It is demonstrated that the proton ionization data can be fitted to the Born approximation to a lower projectile velocity than can the corresponding electron data.

I. INTRODUCTION

A THEORETICAL treatment of the high-energy ionization process has been given by Bethe,[1] who used the Born approximation and hydrogen-like electron wave functions. Bethe showed that for high impact velocity v, the cross section for ionization from the nl shell is

$$Q_{nl}{}^{i}=\frac{2\pi\epsilon^4Z'^2}{mv^2}\frac{c_{nl}Z_{nl}}{|E_{nl}|}\log(2mv^2/C_{nl}), \qquad (1)$$

where ϵ is the electronic charge, Z' is the ion charge number, m is the electronic mass, Z_{nl} is the number of electrons in the nl shell, E_{nl} is the ionization energy of that shell, and C_{nl} is a quantity of the order of the energy of an electron in the nl shell. c_{nl} is a reduced electron matrix element. Theoretical values of C_{nl} and c_{nl} were computed by Bethe for the case of hydrogen and are utilized in the comparisons which follow in Sec. III. The approximations used in this calculation have only a limited range of validity, so it is necessary to compare experimental results with the theoretical predictions in order to determine under what conditions the treatment is valid. Such comparisons will permit extrapolation into unmeasured regions and may provide a means of comparing various experimental measurements.

In the limit of sufficiently high energy, the Born approximation[1] predicts the total cross section for proton ionization to be the same as that for electrons at the same velocity of relative motion. This has also been pointed out by Mott and Massey,[2] Bates and Griffing,[3] Mapleton,[4] and others. Thus a comparison of measured proton and electron data at sufficiently high energy should indicate any wide discrepancy in the experimental data for these two types of ionization.

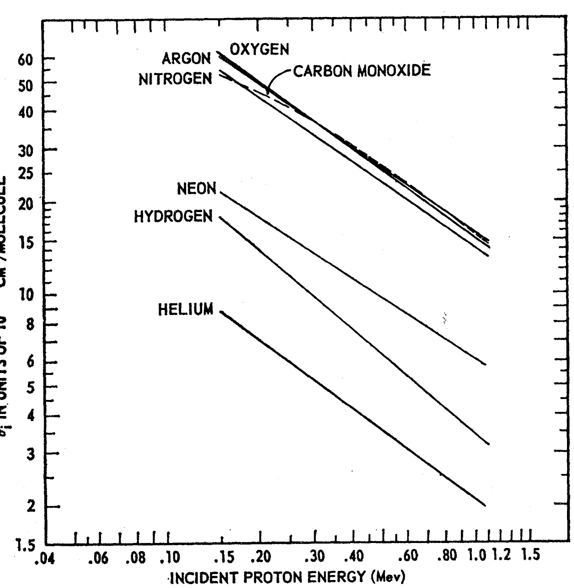

FIG. 1. Gross ionization cross sections for protons incident on helium, neon, argon, molecular hydrogen, molecular nitrogen, molecular oxygen, and carbon monoxide.

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[1] H. Bethe, Ann. Phys. **5**, 325 (1930).

[2] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, New York, 1952), pp. 247, 271.

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[4] R. A. Mapleton, Phys. Rev. **109**, 1166 (1958).

We have recently measured the cross sections for ionization of helium, neon, argon, hydrogen, nitrogen, oxygen, and carbon monoxide by protons at 20 values of energy over the range 0.15–1.1 Mev.[5,6] A summary of these results is shown in Fig. 1. For clarity, only the lines which were fitted to the experimental data are shown, the individual data points being omitted. The data were fitted by least-squares procedures described in the appendix, and the results thus obtained are tabulated there in order to make available more accurate values for the cross sections than can be obtained from Fig. 1. From the least-squares analysis, the data were found to be self-consistent to within 0.3%, indicating the relative cross sections to be determined to within the same degree of accuracy. Thus these data are sufficiently accurate and in an appropriate energy range so that comparisons with electron ionization data and with the predictions of

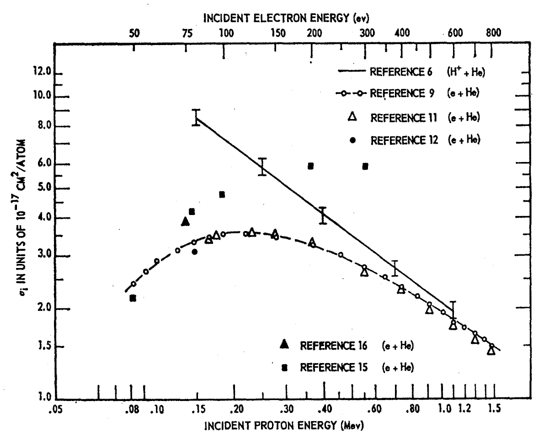

FIG. 2. Comparison of experimental gross ionization cross sections for protons and electrons of equal velocity incident on helium.

the Born approximation can be made. A comparison of the present proton ionization results with those obtained by other investigators[7,8] at energies up to 0.18 Mev has already been presented.[5,6]

II. COMPARISON OF ELECTRON AND PROTON DATA

The electron data available at a sufficiently high energy for comparison to proton data are limited in quantity and were obtained, for the most part, several decades ago. The bulk of these data are, however,

[5] J. W. Hooper, E. W. McDaniel, D. W. Martin, and D. S. Harmer, Phys. Rev. **121**, 1123 (1961).

[6] E. W. McDaniel, J. W. Hooper, D. W. Martin, and D. S. Harmer, *Proceedings of the Fifth International Conference on Ionization Phenomena in Gases*, Munich, 1961 (North Holland Publishing Company, Amsterdam, 1962), Vol. I, p. 60.

[7] V. V. Afrosimov, R. N. Il'in, and N. V. Fedorenko, Soviet Phys.—JETP **7**, 968 (1958); J. Exptl. Theoret. Phys. (USSR) **34**, 1398 (1958).

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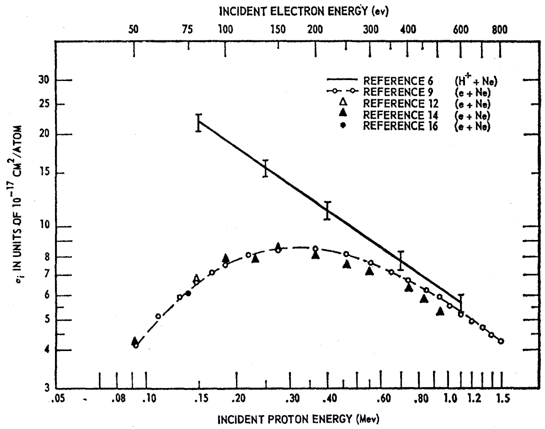

FIG. 3. Comparison of experimental gross ionization cross sections for protons and electrons of equal velocity incident on neon.

generally accepted as reliable. Data from the following sources appear in Figs. 2 through 8, along with the proton ionization cross sections obtained by the present authors[5,6]: Smith[9] for the gases He, Ne, A; Tate and Smith[10] for N_2, H_2, O_2, CO; Harrison[11] for H_2, He; Tozer and Craggs[12] for A, Ne, He; Bleakney[13,14] for Ne, A, H_2; Compton and Van Voorhis[15] for H_2, He; and Lampe, Franklin, and Field[16] for He, Ne, A, H_2, N_2, CO, O_2. It should be pointed out that the error flags on the proton data curves do not represent the actual data points but are intended to represent the

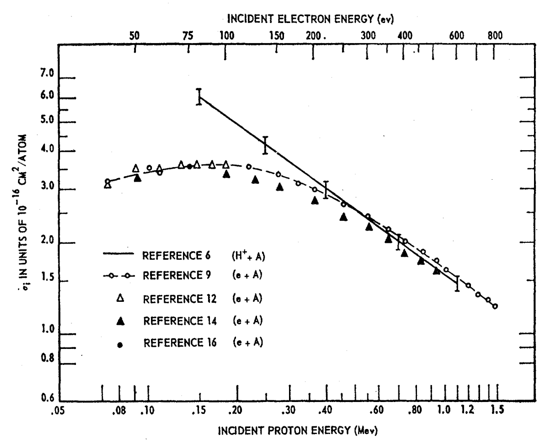

FIG. 4. Comparison of experimental gross ionization cross sections for protons and electrons of equal velocity incident on argon.

[9] P. T. Smith, Phys. Rev. **36**, 1293 (1930).

[10] J. T. Tate and P. T. Smith, Phys. Rev. **39**, 270 (1932).

[11] H. Harrison, Ph.D. thesis (Catholic University Press, Washington, D. C., 1956).

[12] B. A. Tozer and J. D. Craggs, J. Electronics and Control **8**, 103 (1960).

[13] W. Bleakney, Phys. Rev. **35**, 1180 (1930).

[14] W. Bleakney, Phys. Rev. **36**, 1303 (1930).

[15] K. T. Compton and C. C. Van Voorhis, Phys. Rev. **26**, 436 (1925).

[16] F. W. Lampe, J. L. Franklin, and F. H. Field, J. Am. Chem. Soc. **79**, 6129 (1957).

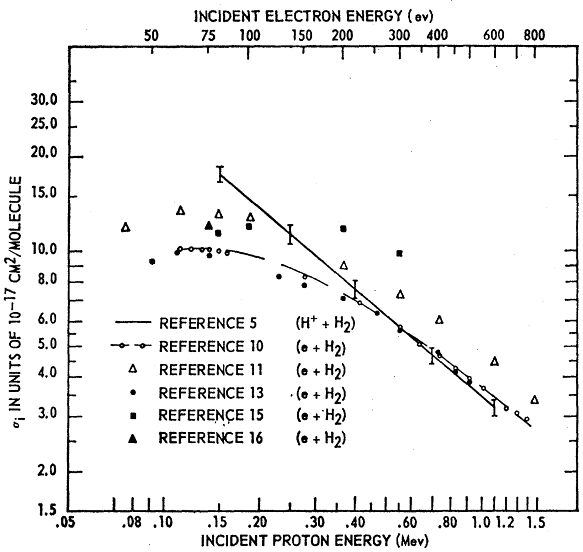

FIG. 5. Comparison of experimental gross ionization cross sections for protons and electrons of equal velocity incident on molecular hydrogen.

maximum possible shift in absolute magnitude of the cross sections that could occur from combined systematic pressure and energy calibration errors. These shifts would be the same for all gases, the relative magnitudes being accurate to within 0.3% (see Table II, appendix).

There is excellent agreement between the cross sections obtained with incident electrons and with incident protons of the same velocity for the target gases helium, neon, argon, nitrogen, oxygen, and carbon monoxide above 0.6 Mev. There is also good agreement for the molecular hydrogen case if only the data of Tate and Smith,[10] Bleakney,[13] and Tozer and Craggs[12] are considered. The cross sections obtained by Harrison,[11] and by Compton and Van Voorhis[15] lie somewhat above the result obtained with incident protons.

An additional feature of comparison which is not apparent from Figs. 6 and 8 is that according to the data of Tate and Smith the electron cross sections for nitrogen and carbon monoxide are equal at high energy whereas the proton results were found to be unequal by about 12%. The electron results lie between the proton results for the two gases and are within the limits of the stated maximum experimental uncertainties for the proton measurements on both gases. However, it does not seem likely that the proton experimental errors could be such as to lead to the observed displacement of the curves since, as it was pointed out in reference 6, the $\pm 6\%$ possible experimental error is believed to be largely systematic and the relative cross sections are believed to be accurate to $\pm 0.3\%$.

The composite results indicate that the equality of cross sections predicted by the Born approximation for electrons and protons of the same velocity is verified, for the gases investigated, for electron energies greater than about 300 ev. The corresponding proton energy is 552 kev.

III. COMPARISON OF PROTON DATA WITH THEORY

A. Bethe's Calculation

In the energy range in which the Born approximation is valid, the observed ionization cross section should vary with incident particle velocity as in Eq. (1). In the actual case, the total ionization is the sum of the contributions from each of the nl shells. It is known that the predominant contribution comes from outer shell ionization,[1] and thus we shall consider only one term like Eq. (1) in our analysis. The experimental proton ionization data have been fitted by a least-squares procedure to Eq. (1), and empirical values of the parameters have been determined (see Table III, appendix).

For the hydrogen atom, Bethe[1] has calculated the appropriate values of c_{nl} and C_{nl}. With these values, the cross section for fast proton ionization of hydrogen atoms becomes

$$Q^i = (2\pi\epsilon^4 \times 0.285/|E_0|E')\log(2E'/0.048|E_0|), \quad (2)$$

in which $E'=2Em/M$, E and M being the incident proton energy and mass, respectively, and E_0 is the ionization energy. For comparison of this result with hydrogen molecule ionization, it is assumed that the hydrogen molecule is equivalent to two hydrogen atoms in high-energy collisions with the exception that the ionization potential, E_0, must be taken to be that of the molecule.[5] Thus two electrons are available for ionization ($Z_{nl}=2$ for the molecule). If the parameters from the least-squares fit are substituted into equation 2, the "best" values of E_0 may be obtained. From the linear factor, E_0 is 16.3 ± 0.4 ev, and from the log factor, E_0 is 13.0 ± 2.5 ev, in surprisingly good agreement with the measured electron ionization threshold,

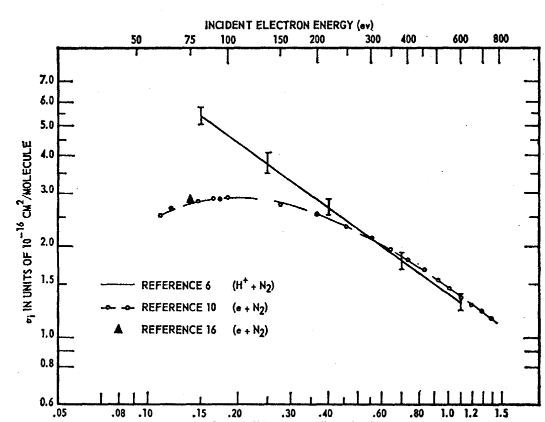

FIG. 6. Comparison of experimental gross ionization cross sections for protons and electrons of equal velocity incident on molecular nitrogen.

TABLE I. Values for the parameters appearing in Bethe's theory, as derived from a least-squares fit of experimental proton ionization data to the theoretical expression. E_0 is the observed threshold for electron ionization, and all energies are in electron volts.

	He	Ne	A	H_2	N_2	O_2	CO
C_{nl}	15.0	39.0	30.6	0.62	29.8	14.7	46.4
$E_{nl}/c_{nl}Z_{nl}$	29.0	8.1	3.3	28.6	3.7	4.0	3.0
E_0	24.5	21.5	15.7	15.6	15.5	12.5	14.1

E_0, of 15.6 ev. The larger uncertainty in the value of E_0 derived from the log factor arises from the uncertainty in the least-squares fit of the more slowly varying factor over a limited range of change of the independent variable, E.

For the other gases detailed calculations of c_{nl} and C_{nl}/E_{nl} are not available. However, the values listed in Table I for C_{nl} and $E_{nl}/c_{nl}Z_{nl}$, derived from the least-squares fit, appear to be of the right order of magnitude. If detailed calculations become available these values may be used for comparisons similar to that for hydrogen.

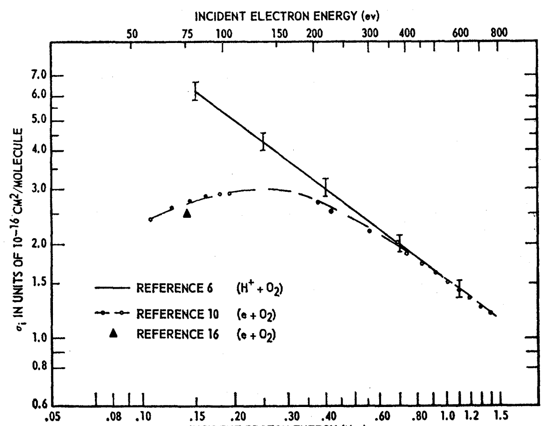

FIG. 7. Comparison of experimental gross ionization cross sections for protons and electrons of equal velocity incident on molecular oxygen.

B. Other Calculations

Mapleton[4] has made theoretical calculations in the Born approximation of the cross sections for ionization and simultaneous ionization and excitation of helium by protons. Three different cases were treated, corresponding to different assumptions about the electronic wave function. The dashed line in Fig. 9 represents Mapleton's result for case III, which he believed to be the most realistic of the three. There is satisfactory agreement with the experimental results in the energy range above approximately 400 kev, as can be seen from Fig. 9.

Ionization cross sections for α-particle impact and electron impact on helium have been calculated by Erskine[17] through an application of the Born approximation. Mapleton has demonstrated that it is possible to scale the α-particle results to those for protons if particles with equal velocities of relative motion are considered. Translation of Erskine's results to the proton case leads to close agreement with Mapleton's case III. It is also significant to note that Erskine's results for electron impact on helium are in close agreement with the experimental cross sections determined from the data of Smith.[9] This cross-correlation leads to added confidence in the experimental results for protons incident on helium obtained in this research.[6]

Theoretical calculations for hydrogen atom ionization by protons have been made by Bates and Griffing.[3] A comparison of their results with the hydrogen molecule ionization data has been made by a scaling procedure described in reference 5. Excellent agreement between theory and experiment was obtained for energies greater than 0.15 Mev.

The cross section for ionization of lithium by fast electrons and protons has also been calculated.[18] At the present time, no experimental data are available for comparison with this computation.

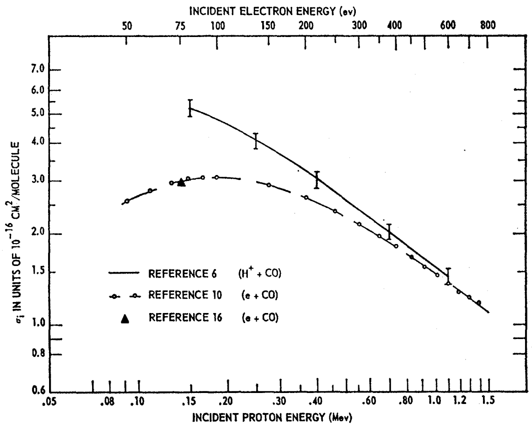

FIG. 8. Comparison of experimental gross ionization cross sections for protons and electrons of equal velocity incident on carbon monoxide.

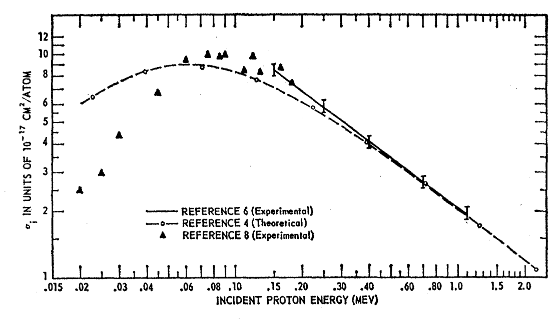

FIG. 9. Comparison of experimental and theoretical gross ionization cross sections for protons incident on helium.

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[18] M. R. C. McDowell and G. Peach, Phys. Rev. **121**, 1383 (1961).

The excellent agreement between the experimental data and theoretical predictions indicates that the approximations used in deriving Eqs. (1) and (2) have a wide range of validity for proton ionization. The proton data appear to agree with the Born approximation to lower incident particle velocities than do the corresponding electron data. This agreement is reasonable since the assumptions made by Bethe[1] concerning the momentum distribution of the ejected electron in the derivation of Eq. (1) should hold to a lower incident particle velocity for protons than for electrons.

APPENDIX

Data Fitting by Least-Squares Analysis

The experimental results[5,6] indicate that for all our target gases except carbon monoxide the proton data give a good straight-line fit on a log-log plot so that the gross ionization cross section appears to vary with energy as E^{-C} over the range investigated. This energy dependence applies in the case of CO for energies above about 0.4 Mev. The experimental data were fitted by a least-squares procedure to the function: $\sigma_i = A \times E^{-C}$ cm²/molecule. Since this is a nonlinear function of the parameter C, the least-squares method is not directly applicable. The procedure of linearization by using the log of the function has the disadvantage of placing an undue bias on data points at one end of the range. It can be shown, in general, that each point should be weighted according to the variance of the point in order that the proper significance of each point be considered in the least-squares procedure. If, instead of the log linearization, the function is expanded in a Taylor's series about the mean "best" value of the coefficients, this new function can be appropriately weighted by the variances of the individual points. Only the first two terms of the expansion need be used if good estimates of the values of A and C are available. A simple iterative least-squares procedure can then be used, in which trial values of A and C are used in the calculation. After solution of the equations, these values are replaced by the ones calculated and the equations are resolved, until the values of the coefficients are unchanged for the required number of significant figures. The method was programed for the Burroughs 220 computer of the Rich Electronic Computer Center of the Georgia Institute of Technology.

TABLE II. Values of the constants A and C in the equation, $\sigma_i = AE^{-C}$ for the gross proton ionization cross section in the range of incident proton energies from 0.15 to 1.10 Mev. E is the numerical value of the energy in Mev, and σ_i is in units of 10^{-17} cm²/molecule.

Gas	A ($\times 10^{-17}$ cm²/molecule)	C
He	2.073±0.005	0.755±0.003
Ne	5.883±0.013	0.687±0.003
Ar	15.59 ±0.03	0.712±0.003
H_2	3.433±0.009	0.864±0.004
N_2	14.20 ±0.03	0.704±0.003
O_2	15.26 ±0.11	0.747±0.007
CO[a]	15.47 ±0.05	0.733±0.009

[a] The straight-line relationship holds only above 0.4 Mev for this case.

TABLE III. Values of the constants A and B in the equation $\sigma_i = (A/E)\ln BE$ for the gross proton ionization cross section from the best fit to experimental data for incident proton energies in the range from 0.15 to 1.10 Mev. E is in units of Mev and σ_i in units of 10^{-17} cm²/molecule.

Gas	$A\left(\times 10^{-17}\ \frac{\text{cm}^2\text{-Mev}}{\text{molecule}}\right)$	$\ln B$	$B\left(\frac{1}{\text{Mev}}\right)$
He	0.4132±0.008	4.974±0.09	144.6± 13
Ne	1.470 ±0.008	4.017±0.02	55.6± 1.1
Ar	3.616 ±0.08	4.261±0.08	70.9± 6.0
H_2	0.4191±0.01	8.160±0.19	3500 ±667
N_2	3.257 ±0.07	4.287±0.08	72.8± 5.8
O_2	3.006 ±0.10	4.993±0.14	147.4± 21
CO	4.040 ±0.04	3.844±0.03	46.7± 1.4

The value of the cross section obtained at each energy was the average of many individual measurements, and a reliable estimate of the variance could be obtained from these data. The values of the coefficients were obtained from the least-squares procedure with the appropriate weighting, and thus the error estimates obtained reflect the true random errors of the measurements. From Table II it can be seen that the error estimates of the coefficients are quite small, and hence the relative cross sections are known quite accurately. Systematic errors due to uncertainties in the calibration of the McLeod gauge or of the proton energy would affect the magnitude of A but leave C unchanged. This effect is the same for all measurements. Hence a larger error estimate is shown on the graphical representations of the data than is shown in the calculated coefficients in Table II. This represents the maximum error estimate from combined systematic errors in the measurements.

The Born approximation predicts that in the high-energy limit the ionization cross section should vary as[1]

$$\sigma_i = (A/E)\ln BE, \tag{3}$$

where B is inversely proportional to the average energy of ionization and A is related to other constants and parameters of the system. The values of the parameters obtained by a least-squares fit of the data to the above equation are shown in Table III.