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F. D. Schowengerdt

John T. Park
Missouri University of Science and Technology, parkj@mst.edu

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Energy-Loss Spectra and Collision Cross Sections for Impact of 20–120-keV Positive Ions on Molecular Nitrogen*

F. D. Schowengerdt† and John T. Park
Physics Department, University of Missouri, Rolla, Missouri 65401
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Inelastic energy-loss spectra induced by impact of H^+, H_2^+, and Ar^+ on N_2 have been measured at incident ion energies of 20–120 keV, with an energy resolution of about 2 eV. Prominent peaks are observed at energy losses of 9.5 and 13.8 eV. The first of these is well resolved and is attributed to excitation of the Lyman-Birge-Hopfield (LBH) system of N_2. The peak at 13.8 eV is believed due primarily to excitation of the $b^1\pi_u$ band of the Worley-Jenkins series. The locations of these features on the energy-loss scale do not agree with results of the electron impact work of others and, in general, show trends with projectile velocity that are consistent with an assumed enhancement of excitation to higher vibrational states with the heavier particles. Collision cross sections for excitation of the two peaks are presented, as well as the total ionization cross section and the cross section for total inelastic processes in the case of proton impact.

I. INTRODUCTION

Collisions between energetic positive ions and molecular nitrogen have been studied since the early 1930's. Until now, studies of excitation in these collisions have been confined to detection and measurement of the optical emissions of the target molecules following ion impact. Thus, the range of transitions for which quantitative results could be obtained has been limited by their accessibility to optical methods.

Spectroscopic studies of ion-nitrogen molecule collisions have been carried out by many investigators.[1-12] Most of these studies have been concentrated on emissions from the $(B^2\Sigma_u^+ - X^2\Sigma_g^+)$ first negative bands of N_2^+, the $(C^3\pi_u - B^3\pi_g)$ second positive bands of N_2, and the Meinel Bands. Recently, Dahlberg *et al.*[8] reported the faint appearance of the optically forbidden $(a^1\pi_g - X^1\Sigma_g^+)$ Lyman-Birge-Hopfield (LBH) bands of N_2 following proton impact, but reported no cross sections for excitation into these bands.

Observations of auroral emissions from N_2 and N_2^+ have been reported by Vegard *et al.*,[13] Barbier and Williams,[14] and Clark and Belon,[15] among others. There is strong evidence that the solar-wind protons, which are thought to play a major role in auroral excitations, enter the earth's upper atmosphere at velocities comparable to those used in the present experiment. Branscomb *et al.*[16] list some of the arguments supporting this assertion; these arguments are based on observed time lapses between the appearance of solar flares and the occurrence of terrestrial aurora, the energy required for protons to penetrate to an observed altitude in the earth's atmosphere, and observations of Doppler-shifted Balmer lines in the aurora. In addition, recent rocket[17] measurements indicate solar proton energies of 30–240 keV at altitudes above 100 km, where the aurora are observed. Such studies indicate the importance of laboratory work on collisions between positive ions, especially protons, and molecular nitrogen in this energy range.

In the present experiment, a new approach is taken toward the study of excitation of N_2 by ions. Instead of observing a secondary product of the collision process, such as optical radiation, a direct measurement of the energy-loss spectra of the forward-scattered ion beam is undertaken. The energy-loss spectra is not affected by subsequent relaxation in the target and is due only to processes induced by the detected ions. Thus, excitation cross sections are obtained without complications from cascade effects, and it is assured that neutrals in the ion beam and secondary electrons in the collision chamber do not contribute to the results. By measuring the apparatus resolution function directly, in the absence of target gas, absolute cross sections can be obtained from the energy-loss spectra. Whereas the results of optical experiments are dependent on the calibration of detectors and on theoretical or experimental determination of transition probabilities, the present cross sections are independent of detector efficiencies and are not normalized to any other experiment or theory.

II. EXPERIMENTAL

A detailed description of the UMR heavy-ion energy-loss spectrometer has been published elsewhere.[18] A beam of ions from a Colutron source[19] is accelerated and focused on a collision chamber 6.29 cm in length. The forward-scattered beam is then mass-analyzed and decelerated

to 2 keV for energy analysis and detection. Energy analysis is accomplished by a 127° electrostatic analyzer.

During operation, the mass and energy analyses are both held fixed, while a small sweep voltage connected between the accelerator and decelerator high-voltage terminals is varied to obtain the energy-loss spectra. The collected current is measured by an electrometer, whose voltage output is fed through a servo arrangement to the Y axis of an X-Y recorder located at ground potential. The output of the sweep voltage is fed to the X axis by a similar arrangement. Thus, the raw data are obtained in the form of plots of collected ion currents versus energy losses. Auxiliary experiments are performed to assure that the currents are true functions of energy loss only (see Refs. 18 and 20).

The method of obtaining differential and total cross sections from the spectra has been discussed in a recent article.[20] The energy-loss spectrum $R(\xi)$ is a convolution of the apparatus resolution function $\Phi(\xi)$ (taken without gas in the collision chamber) and an experimental energy-loss differential cross section $d\bar{\sigma}/d\xi$; i. e.,

$$R(\xi) = ndx \int \Phi(\xi - \xi') \frac{d\bar{\sigma}}{d\xi}(\xi')\, d\xi' \quad ,$$

where ξ is a positive energy loss as measured from the most probable energy of the unscattered beam, and $d\bar{\sigma}/d\xi$ is taken to be the doubly-differential cross section (differential in energy loss and scattering angle), integrated over the acceptance angles of the apparatus; i. e.,

$$\frac{d\bar{\sigma}}{d\xi} = \int_{\Delta\Omega} \frac{d^2\sigma}{d\Omega d\xi}(\theta, \xi)\, d\Omega.$$

In studying H^+-He collisions, it was found that essentially all of the scattered beam could be accounted for, and, consequently, that the experimental differential cross section was equivalent to the true differential cross section integrated over all angles. This was due to the ineffectiveness of helium atoms in scattering protons through angles larger than those accepted by the apparatus (10^{-4} rad). In order for such scattering to be negligible, the following relation must hold:

$$\int R(\xi)\, d\xi \,/\, \int \Phi(\xi)\, d\xi + \sigma_c n\, dx \simeq 1, \qquad (1)$$

where $R(\xi)$ and $\Phi(\xi)$ are the energy-loss spectrum and resolution function, respectively; σ_c is the cross section for all charge-changing processes (the apparatus discriminates against any ion that changes charge); n is the number density of scatterers; and dx is the effective scattering path-length.

In case Eq. (1) does not hold, the loss of beam through large-angle scattering can be partially compensated for by dividing the measured cross sections by the left-hand side of (1). This correction assumes that the cross sections for elastic and inelastic scattering are independent of each other, an assumption which is reasonable for optically allowed transitions, but less so for forbidden transitions.

Total cross sections for a resolved peak are obtained by integrating over the peak in question and dividing by the area under the resolution curve. That is, if $R(\xi)$ drops nearly to zero on either side of a peak within an energy-loss interval $\Delta\xi_j$, the total cross section σ_j for processes contributing to the peak is given by

$$\sigma_j = \frac{1}{ndx}\left(\int_{\Delta\xi_j} R(\xi)\, d\xi \Big/ \int \Phi(\xi)\, d\xi \right). \qquad (2)$$

Since no experimental parameters, other than the target gas pressure, are changed between the times the two functions R and Φ are plotted, the cross sections are absolute and independent of detector efficiencies.

Systematic errors associated with this method are discussed in Ref. 20. In earlier experiments the pressure measurement, taken with a capacitance bridge manometer,[21] was calibrated against a McLeod gauge. Because of a sizeable (17%) discrepancy between the two, the capacitance manometer has since been returned to the factory for calibration. To avoid possible errors associated with the McLeod gauge, the manometer is now taken as the laboratory standard. The total systematic error in the present cross sections is believed to be less than ±20%, most of which is due to uncertainties in the pressure measurement and in the effects from large-angle scattering. Some idea of the magnitude of the large-angle scattering can be seen in Table I, where the measured quantities on the left-hand side of Eq. (1) are listed at different primary energies for the case of protons on nitrogen. The charge-exchange cross sections are from the data of Stier and Barnett.[22] All the cross sections reported in Secs. IV–VI have been divided by these quantities to correct for the scattering, as discussed above.

III. ENERGY-LOSS SPECTRA

Energy-loss spectra for H^+ on N_2 were obtained at target gas pressures ranging from 2×10^{-4} to 5×10^{-4} Torr ($n\,dx \simeq 4\times10^{13}$ to 10×10^{13} cm^{-2}) and at energies of from 20 to 120 keV in 10-keV increments. The target-gas-pressure range was chosen so as to fall in the region where the scattered intensities were linear with pressure.

TABLE I. Fraction of the total ion beam which was scatterd into the acceptance angle of the analyzer.

Incident proton energy (keV)	$\frac{\int R(\xi)\,d\xi}{\int \Phi(\xi)\,d\xi}$ [a]	σ_c (10^{-16} cm^2/atom)[b]	$\frac{\int R(\xi)\,d\xi}{\int \Phi(\xi)\,d\xi} + \sigma_c n\,dx$ [a]
20	0.84	4.0	0.88
30	0.95	2.9	0.98
40	0.91	2.1	0.95
50	0.93	1.6	0.95
60	0.96	1.2	0.97
70	0.94	1.0	0.95
80	0.92	0.7	0.92
90	0.99	0.6	0.99
100	1.0	0.5	1.0
110	0.99	0.3	0.99
120	0.96	0.2	0.96

[a]Averages over data obtained at four target gas pressures.
[b]From data of Stier and Barnett (Ref. 22).

Spectra for H_2^+ on N_2 were taken at the same pressures and over the same energy range, except in 20-keV increments. Ar^+ on N_2 spectra were taken at 50 keV. With each spectrum, a resolution curve was taken and the two were used together in eliminating background and calculating total cross sections.

An energy-loss spectrum for impact of 50-keV protons on N_2, at a pressure of 3×10^{-4} Torr, is shown in Fig. 1. The inelastic portion of the spectrum is shown at a gain 100 times that of the elastic peak. The elastic peak establishes the zero for the inelastic energy-loss scale.

The energy-loss scale was established, first, by careful calibration of the sweep voltage using two differential voltmeters and, second, from the location of a peak corresponding to the sum of the 1^1S-2^1S and 1^1S-2^1P transitions in the H^+-on-He spectrum. The first of these transitions occurs spectroscopically at 20.6 eV, the second at 21.2 eV. Because the two transitions cannot be separated with the present resolution, the calibration was done at a proton energy of 100 keV, where the contribution from the optically forbidden 2^1S state is expected to be small.

With this calibration, the first peak in the H^+ on N_2 spectrum occurs at 9.5 ± 0.2 eV; the second, and most prominent, occurs at 13.8 ± 0.3 eV. The uncertainties are an estimated $\pm2\%$ associated with the uncertainty in the location of the calibration peak in the helium spectrum.

Other features of the nitrogen spectrum are the ionization continuum and suggestions of some excited states of N_2^+.

A. 9.5-eV Peak

In the Appendix, the 9.5-eV peak is identified as arising primarily from excitation of the Lyman-Birge-Hopfield (LBH) bands of N_2. Herzberg[23] identifies these bands with the optically forbidden $X^1\Sigma_g^+$-$a^1\pi_g$ transition.

According to the potential energy curves of Gilmore,[24] the center of the LBH bands should occur at about 9.1 eV when the means of excitation are such that the Franck-Condon principle holds. In electron-impact work, close agreement is found with the 9.1-eV figure.[25–27] In the photoabsorption work of Tanaka,[28] the strongest band (3, 0) in the LBH progression appeared at $\lambda = 1353.8$ Å (9.11 eV), in agreement with both the Franck-Condon principle and the electron-impact spectra.

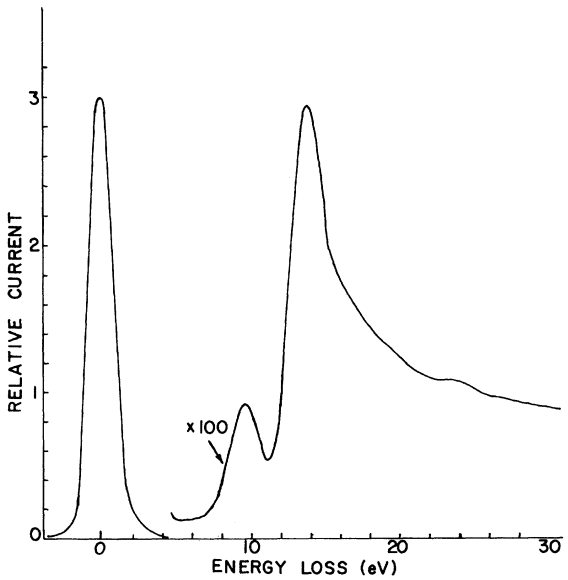

FIG. 1. Energy-loss spectrum for 50-keV protons on N_2 ($ndx = 6\times10^{13}$ cm^{-2}).

However, discrepancies between locations of other peaks in the photoabsorption and electron-impact spectra have been noted by Meyer *et al.*[29] and by Geiger and Stickel.[30]

The difference in location of the LBH peak in our spectra and of that in the photoabsorption and electron-impact spectra is outside the limits of accuracy in the present experiment. The shift could conceivably be due to any of three possibilities: (i) a calibration error in our energy-loss scale; (ii) unresolved peaks corresponding to higher energy losses; or (iii) enhancement of vibrational states higher than those expected from application of the Franck-Condon principle. The first of these is inconsistent with the location of the calibration peak in the H^+-He spectra (21.3 eV). That is, in order to account for the 0.4-eV shift in the LBH peak, the calibration peak would have to occur at 22.1 eV, a shift which is well within our limits of detection. The second possibility listed above is doubtful in view of the highly forbidden nature of the nearby states. None of the states lying within our limits of resolution has been observed with either electron or proton impact.[8,27] As to the third possibility, the observed shift could be accounted for if the most probable excited vibrational state is one for which $v'=5$ instead of $v'=3$, as predicted by the Franck-Condon principle[24] and observed in photoabsorption[28] and electron impact.[27] Because of the location of the equilibrium point of the $a^1\pi_g$ state relative to that of the ground state (see the potential energy curves of Gilmore[24]), the most probable excited vibrational quantum number depends strongly on internuclear separation and, therefore, on the effectiveness of a passing projectile in perturbing the internal motions of the N_2 molecule.

Vibrational enhancement by protons has been observed in other band systems of nitrogen by Fan[6] (3–350 keV) and by Branscomb *et al.*[16] (100 keV), although Sheridan and Clark[7] report little or no enhancement with 10- to 65-keV protons. Most recently, Moore and Doering[12] have found agreement with the Franck-Condon principle in relative intensities in the first negative bands when excited by ions of velocities greater than about 10^8 cm/sec. They report that below this velocity the relative population of higher vibrational states increased monotonically.

The studies discussed above indicate that vibration induced by protons in the velocity range of the present experiment ($2–5\times10^8$ cm/sec) is probably not sufficient to be detected in the first negative bands. However, the potential energy curve for the $B^2\Sigma_u^+$ state (first negative) is centered almost directly over that of the ground state of N_2 on the internuclear-separation-distance scale (see Ref. 24), while the potential energy curve for the $a^1\pi_g$ state (LBH) is centered at a somewhat larger value,[24] so that the Franck-Condon region intercepts the $a^1\pi_g$ curve over a portion where the slope of the latter is much steeper than that encountered in the case of the $B^2\Sigma_u^+$ curve. Because of this, a given change in internuclear separation in the N_2 molecule during the collision should show up as a more pronounced departure from the expected Franck-Condon intensities within the LBH system as compared to those within the first negative system.

In order to extend the range of results in the present experiment to lower ion velocities where we could expect significant vibrational enhancement, data were taken with H_2^+ and Ar^+ projectiles. A shift of the LBH peak toward higher energy losses, with decreasing projectile velocity, would indicate the expected vibrational enhancement. Energy-loss spectra for 50-keV H_2^+ and Ar^+ ions on N_2 are shown in Figs. 2 and 3. For H_2^+ at 50 keV, a shift of about 0.3 eV in the location of the LBH peak, and for Ar^+, about 0.7 eV, was noted, although in the latter case the second peak is not well resolved. (The peak at about 19 eV in the Ar^+ on N_2 spectrum is believed to be due to excitations of the lowest states of the Ar^+ ion.) These results appear to support the assumption that higher vibrational states are being excited by the slower-moving particles, although higher resolution is obviously needed for a full confirmation.

B. 13.8-eV Peak

There are many states of N_2 in the region 12–14 eV, most of which are the $^1\pi_u$ members of Worley's third series and the Worley-Jenkins series (see Mulliken,[31] for example). In high-resolution electron-impact spectra the $X^1\Sigma_g^+$ -

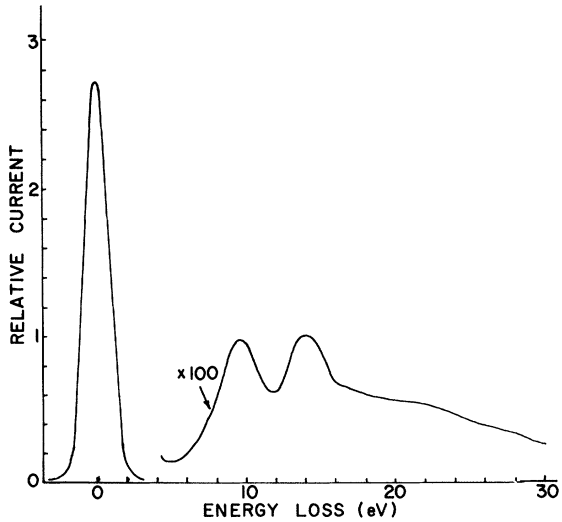

FIG. 2. Energy-loss spectrum for 50-keV H_2^+ ions on N_2 ($ndx=6\times10^{13}$ cm^{-2}).

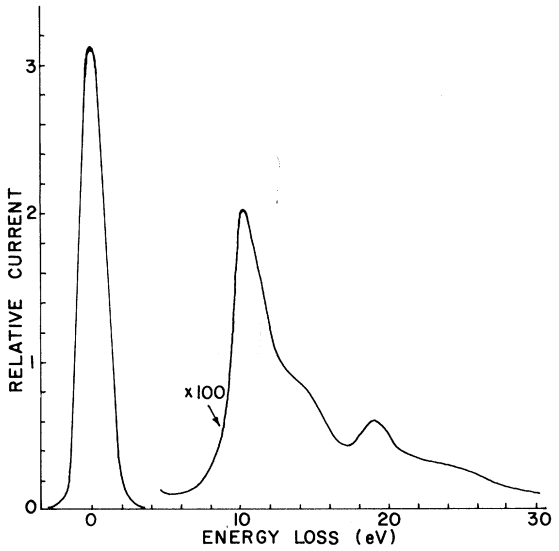

FIG. 3. Energy-loss spectrum for 50-keV Ar^+ ions on N_2 ($ndx = 6\times10^{13}$ cm^{-2}).

$b^1\pi_u$ bands are by far the most prominent of these for forward-scattered electrons at energies of 33 keV,[32] 200 eV,[27] and 35 eV.[26] The most intense peak observed in these studies corresponds to excitation of the $v'=3$ level of the $b^1\pi_u$ band at 12.76 eV (as opposed to the $v'=2$ level as observed in photoabsorption).[28]

When account is taken of the expected vibrational enhancement with protons, the $b^1\pi_u$ state fails within the 13.8-eV peak in our spectra. However, since the $^1\Sigma_u^+$ band at about 14 eV overlaps the $b^1\pi_u$ and is not resolved, the 13.8-eV peak probably contains significant contributions from both.

C. N_2^+ Excited States

In an energy-loss spectrum, simple ionization of the target molecule produces a continuum beginning at the ionization potential, while simultaneous excitation and ionization produces another continuum beginning at the potential required to simultaneously ionize the molecule and excite the molecular ion to the excited level.

In the energy-loss spectrum in Fig. 1, a change of slope is evident at an energy loss of just less than 16 eV, which marks the ground state of N_2^+. If only processes which do not involve a charge-changing process for the incident proton are considered, the excitation of the first negative band of N_2 is probably the result of the ionization of the N_2 molecule by the removal of a valence electron leaving the N_2^+ ion in the $B^2\Sigma_u^+$ excited state. Such a process would not produce any distinct features in the energy-loss spectrum. No features were seen at 19 eV (which corresponds approximately to the $B^2\Sigma_u^+$ state of the first negative system of the N_2^+), although a slight bump appeared at about 23 eV, the expected location of the $C^2\Sigma_u^+$ state.

IV. TOTAL EXCITATION CROSS SECTIONS

Total cross sections for excitation of the sum of the vibrational levels in the LBH bands by H^+ are shown in Fig. 4. These were obtained from Eq. (2) by integration over the 9.5-eV peak in the energy-loss spectra. The error bars are ± 1 standard deviation. There are no other measurements of the cross section for the LBH bands which are known to the authors. Dahlberg[8] has reported detecting faint emission from these lines, but gave no cross sections. The cross sections are about one order of magnitude less than the cross sections reported for the emissions in the N_2^+ first-negative-band system, which has been extensively studied.

The cross sections show an energy dependence that is characteristic of an optically forbidden transition. That is, they form a sharp maximum at a relatively low-impact energy and show an approximate $1/E$ dependence toward higher energies.

Total cross sections for the 13.8-eV peak are shown in Fig. 5. In marked contrast to those in Fig. 4, these cross sections show an energy dependence characteristic of optically allowed transitions.

V. TOTAL IONIZATION CROSS SECTIONS

Total gross ionization cross sections were obtained using Eq. (2), integrating from the energy loss corresponding to formation of N_2^+ to the end of the energy-loss spectrum. The results are

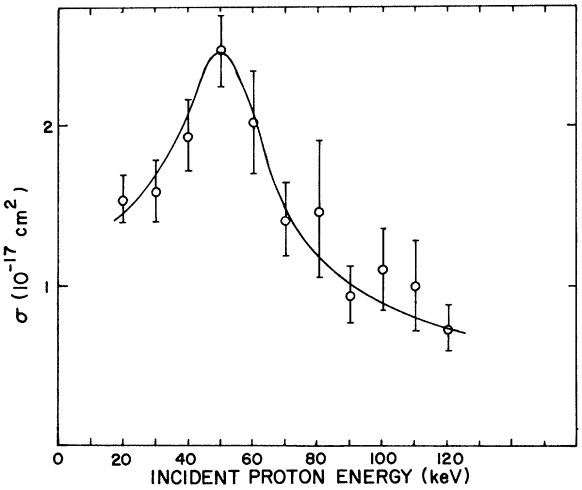

FIG. 4. Total cross section for excitation of the LBH system of N_2 by Protons.

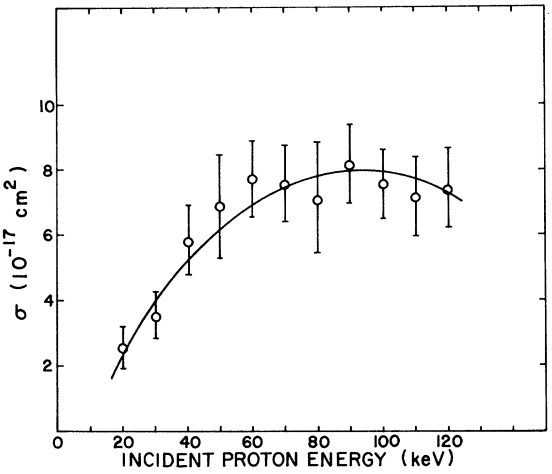

FIG. 5. Total cross section for excitation of the 13.8-eV peak of N_2 by protons.

shown in Fig. 6. These can be considered total cross sections for loss of energy greater than that required to remove a single electron from the N_2 target. They include processes such as simultaneous ionization and excitation, excitation of autoionizing levels, and double ionization. Shown also in Fig. 6 are data of DeHeer *et al.*,[33] Solov' ev *et al.*,[34] and Gordeev and Panov.[35] Since ionization is the only process for which we have other data with which to compare our results, the degree of agreement is some measure of the reliability of our other measurements. Agreement is good at the higher impact energies, but poor at energies below 50 keV. The discrepancies at lower energies could be due to incomplete accounting for loss of beam by scattering in our results. Such a situation would make our other reported cross sections low in this region, especially those for the forbidden LBH transition, due to the expected enhancement of this transition at larger scattering angles. As concerns the ionization cross sections, however, it should be pointed out that agreement among other investigators at energies below about 50 keV is not good. Of the extraneous processes that can affect ionization measurements by the conventional parallel-plate condensor methods, many become important at these low energies.[33] The cross section for charge exchange, for example, is comparable to that for ionization at these energies. Thus, elimination of charge-exchange effects in the parallel-plate method becomes difficult. As mentioned earlier, charge exchange does not affect measurements by the energy-loss method.

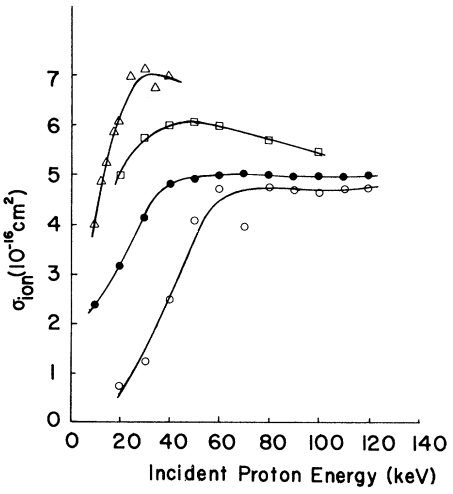

FIG. 6. Total ionization cross sections for ionization of N_2 by protons: open circle, present data; closed circle, De Heer *et al.* (Ref. 33); square, Solov'ev *et al.* (Ref. 34); and triangle, Gordeev and Panov (Ref. 35).

VI. TOTAL INELASTIC CROSS SECTIONS

Total cross sections for inelastic processes, not involving charge exchange, in collisions of H^+ with N_2 are shown in Fig. 7. These were obtained from Eq. (2) by integration over the entire inelastic portion of the energy-loss spectra. Included in these measurements are all excitations, gross ionization, and dissociation.

VII. DISCUSSION

With no adequate theory and no other known experimental data available for a comparison with our results, a complete evaluation is difficult at present. Proper determination of the relative intensities of vibrational levels in the LBH bands, for example, must await improved resolution. Mean-

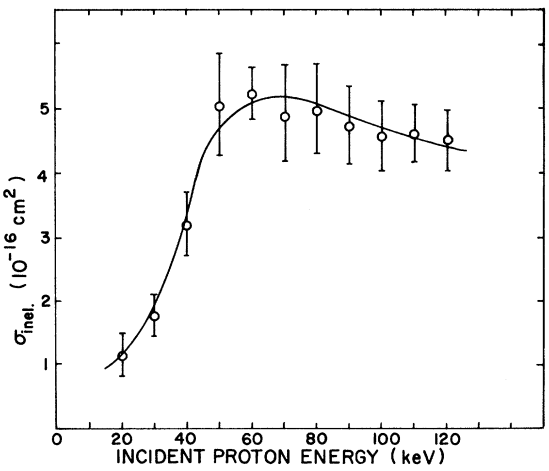

FIG. 7. Total cross section for inelastic processes in proton-N_2 collisions which do not involve charge exchange.

while, with the present 2-eV resolution, the most satisfactory explanation of the observed location of the 9.5-eV peak lies in an assumed vibrational enhancement within the LBH system.

Apart from this, a major result of the present study is a demonstration of the utility of the energy-loss spectrometry method in the study of forbidden transitions in heavy-particle collisions.

APPENDIX: IDENTIFICATION OF THE 9.5-eV PEAK

Using the spectroscopic measurements of Mulliken[31] and Wilkinson,[36] together with the potential energy curves of Gilmore,[24] we can list the well-established states which are within our 2-eV resolution of the 9.5-eV peak. These are

$$A^3\Sigma_u^+,\quad B^3\pi_u,\quad C^3\pi_u,\quad B'^3\Sigma_u^-,$$

$$a'^1\Sigma_u^-,\quad \omega^1\Delta_u,\quad \text{and } a^1\pi_g\ .$$

The first four cannot be reached from the ground state of N_2 by proton impact without violating the Wigner spin rule. The rule is expected to hold in the absence of perturbations from other states, which can produce a mixture of single and triplet terms within an otherwise pure triplet state. According to the spin-orbit coupling theory of Mulliken,[37] such a mixing occurs in the $C^3\pi_u$ state. Weak excitation of this state has been observed for proton impact by Dahlberg *et al.*[8] and by Thomas *et al.*[9] The cross sections for this state had a magnitude of 10^{-19}–10^{-20} cm^2 compared to cross sections of 10^{-17} cm^2 observed for the 9.5-eV peak in this experiment. Thomas *et al.*,[9] however, attribute their findings to excitation by secondary electrons formed in the collision chamber. If such is the case, these processes would not contribute to the observed proton energy-loss spectra in our experiment.

In electron-impact experiments below 200 eV, Lassettre *et al.*[27] and Hiedemann *et al.*[26] have observed excitation of the $C^3\pi_u$ state, although in these cases there is some question as to the relative importance of the singlet contribution as opposed to the contribution from electron spin-exchange effects. Excitation of the $C^3\pi_u$ is not observed in the higher-energy (25 keV) electron-impact work.[32] If the $C^3\pi_u$ is a mixture of singlet and triplet states, the cross section would not be expected to be strongly energy-dependent. The strong dependence on incident electron energy seems to support the hypothesis that the low-energy electron excitation of the $C^3\pi_u$ state is due to contributions from electron spin-exchange effects, which are not possible for incident protons. Lassettre *et al.*[27] have also noted that with electron impacts, electric quadrupole transitions, such as occur in the LBH bands, are much preferred over singlet-triplet transitions, even though the latter are weakly electric-dipole allowed.

Thus, we can expect no contributions to our spectra from the pure triplet states, with perhaps a slight contribution from the $C^3\pi_u$. Excitation of the $a'^1\Sigma_u^-$ state involves a Σ^+-Σ^- transition, which is forbidden for all orders of multipole radiation.

The $X^1\Sigma_g^+$-$\omega^1\Delta_u$ transition is dipole forbidden by virtue of a change of 2 in total orbital angular momentum quantum number. It is magnetic-dipole and electric-quadrupole forbidden because of a change in the over-all symmetry of the electronic wave functions with respect to a reflection about the midway point on the internuclear axis of the N_2 molecule ($g \rightarrow u$). Excitation of the $\omega^1\Delta_u$ state has not been observed with either electron or proton impact.

The $X^1\Sigma_g^+ \rightarrow a^1\pi_g$ transition (LBH) is allowed by magnetic dipole and electric quadrupole. Studies by others indicate that the transition occurs mainly through a magnetic-dipole interaction (see Lassettre *et al.*[27])

Thus, the $a^1\pi_g$ state can be reached from the ground state by a lower-order multipole transition than any of the other nearby states. The possible exception is the weak dipole transition to the perturbed $C^3\pi_u$ state discussed above. From the magnitude of the cross sections measured by others for excitation of this state, we can conclude that it contributes little to our energy-loss spectra. We can therefore identify the 9.5-eV peak with the $X^1\Sigma_g^+$-$a^1\pi_g$ transition.

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†Present address: Physics Dept., University of Nebraska, Lincoln, Neb.

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Many-Body Theory of the Elastic Scattering of Electrons from Atoms and Molecules

Barry Schneider*† and Howard S. Taylor†‡
Department of Chemistry, University of Southern California, Los Angeles, California 90007

and

Robert Yaris†
Department of Chemistry, Washington University, St. Louis, Missouri 63130
(Received 18 August 1969)

We present a method for calculating the elastic scattering of electrons from atoms and molecules using the many-body Green's-function techniques of Martin and Schwinger. The procedure involves the self-consistent solution of a pair of equations; one for the one-particle Green's function and the other for the response function of the target in the time-dependent Hartree-Fock approximation (random-phase approximation). That both equations are one-dimensional provides a great computational advantage over more conventional techniques. We discuss the physical nature of our approximation and a numerical scheme to implement our theoretical discussion.

I. INTRODUCTION

A. Historical

The problem of the elastic scattering of electrons from atoms and molecules has received considerable attention in the literature in the last few years, and a number of methods have been developed to handle the problem. Temkin[1–4] and Callaway[5] have used the "adiabatic" method to incorporate the distortions of the target by the incoming elec-