

THE SPACE ENVIRONMENT: 100 TO 500 KILOMETERS
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This work is a summary of a series of studies in theoretical aeronomy carried out at the University of Florida in collaboration with Drs. V. A. Dulock, now at Louisiana State University at New Orleans; C. E. Watson, now at the University of Texas; A. T. Jusick, now at Stetson University; R. S. Stolarski, now at the University of Michigan; and S. K. Dutta and L. R. Peterson, still at the University of Florida, and with Professor Charles A. Barth, formerly of Jet Propulsion Laboratories and now at the University of Colorado.

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INTRODUCTION

It is impossible in one hour to cover all aspects of the earth's environment from 100 to 500 kilometers. I will concentrate my attention mainly on those aspects of the space environment which have been the concern of a research program in theoretical aeronomy which has been underway at the University of Florida for several years.

In this program, in addition to collaborations with postdoctoral associates and graduate students, there has been an extensive collaboration with Professor Charles A. Barth, now at the University of Colorado.

The development of rockets, one of the great engineering achievements of this century, has literally and figuratively added new dimensions to the science of astronomy. It is likely that the rocket vehicle represents the greatest advance in astronomical instrumentation since the invention of the telescope. Rockets were first exploited for astronomical studies shortly after World War II by Tousey, Freidman, Johnson, Hinterregger and others who equipped V-2 rockets with spectroscopes. These men found it possible from a vantage point above the earth's ozone layer to study the sun's emissions at ultraviolet wavelengths much shorter than 3000 Å, the limit of ground observations. Since then the emissions of the sun have been studied at wavelengths down to the 1Å⁰ region.

About five or six years ago a number of investigators, William Fastie, John Hopkins, Charles Barth (then at Jet Propulsion Laboratories), Wallace of Kitt Peak, and one or two others turned rocket spectrometers to look at the emissions of the earth's atmosphere itself. This development, which is still in its infancy, undoubtedly will have an impact upon aeronomy (the study of the upper atmospheres of the earth and planets) as great as the impact of the rocket upon astronomy.

My own personal involvement with aeronomy began eight years ago and with the particular topic of my talk some four years ago when I spent a month as a consultant at the Jet Propulsion Laboratory consulting for Dr. Charles A. Barth. He posed the question "How many kilorayleighs of Lyman-Birge-Hopfield emissions can I expect if I fly my rocket spectrometer into an IBC III aurora?"

Well! by starting with the old consultmanship ploy "That's a very penetrating question," I managed to strike up a long conversation during the course of which I found the meaning of a few terms, specifically kilorayleigh, Lyman-Birge-Hopfield emissions and an IBC III aurora. Roughly speaking, a kilorayleigh is the emission rate of 10⁹ photons/cm² sec by a column. Lyman-Birge-Hopfield emissions are an ultraviolet radiation of N₂. An IBC III aurora is one whose intensity is equivalent to that of the light of a full moon.

After these hints I did some intensive homework on auroral studies which, as it turns out, is a subject many centuries old. While doing so, it became clear that an answer to

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Barth's question could be given if one knew the probabilities (or cross sections) for all the possible atomic and molecular excitation processes which take place when an incoming stream of electrons or protons encounters the earth's atmosphere. Since we have known the fundamental laws governing the physics of the atom and molecule for about 40 years, I thought I would have no difficulty in finding the needed numbers. To my great surprise, after studying intensively the experimental and theoretical literature on atomic and molecular cross sections, I found that practically none of the numbers needed were available. Almost no calculational work had been done with important atmospheric gases such as nitrogen. From the progress to date, I estimated that it would take some ten to twenty years to carry out rigorous calculations of these properties. On the other hand, my needs and those of the average physicist concerned with the space applications are so urgent that one could hardly wait for such a development. What seems to be needed for the development of aeronomy is a marriage of atomic and space physics in which both disciplines made some compromises for the sake of going forward together. I felt so strongly about this that, together with a collaborator I wrote a book about the marriage of atomic and space physics⁶.

Returning to the specific topic at hand, it occurred to me that a semi-quantitative answer to Barth's question could be given if a reasonably detailed set of cross sections for exciting the various states of molecular nitrogen and its ions could be pieced together. Accordingly, we assembled an empirical set of 11 excitation and ionization cross sections for N_2 using whatever bits and pieces of data we could scrape together. The states involved in this calculation are shown in Figure 1.

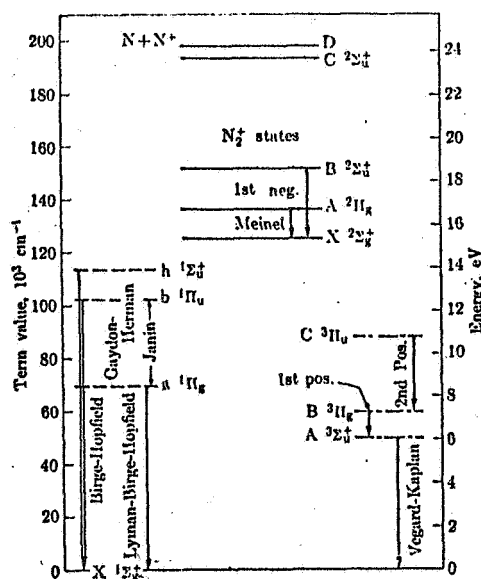


Fig. (1) Energy Levels of N_2 and N_2^+ .

The assembled set of cross sections are given in Figure 2.

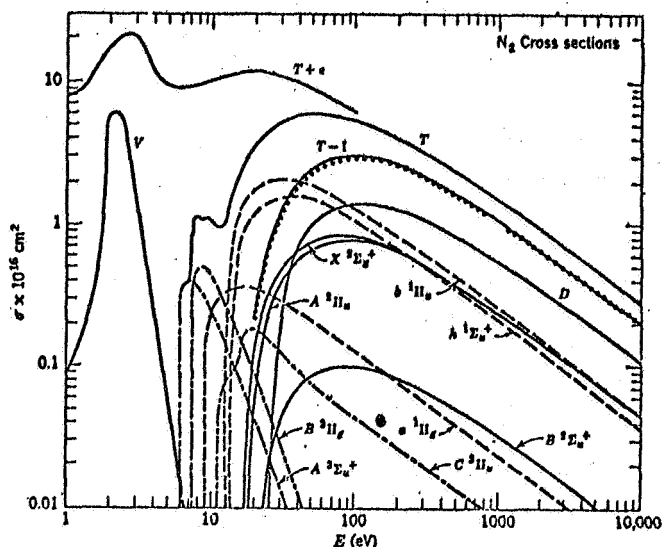


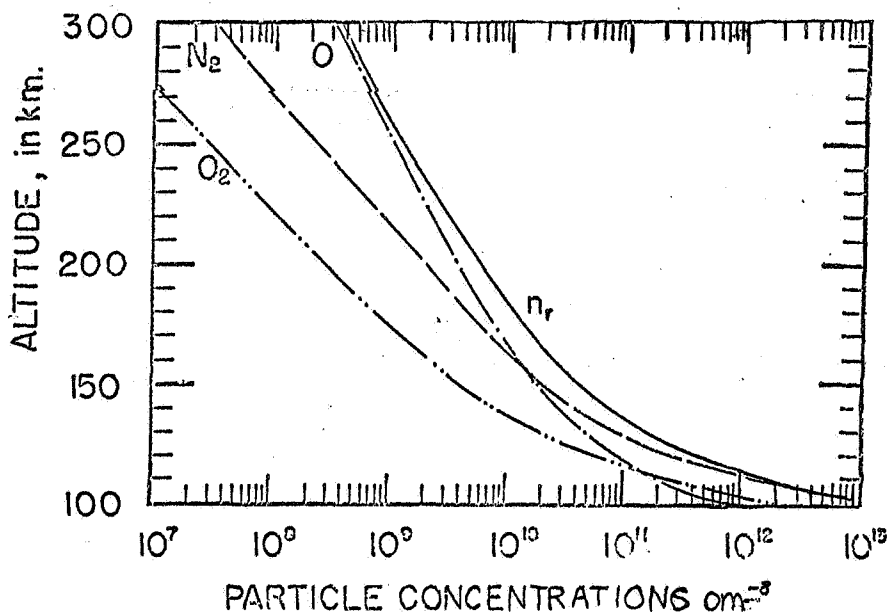
Fig. (2) Electron Impact Cross Sections of N_2

With these cross sections as input, I carried out approximate energy loss calculations to find out what states of N_2 were populated by the degradation of a 30 keV electron in N_2 . Barth followed this with estimates of the photons released in the decay of these states and estimates of the relative intensities of the many nitrogen emissions when we normalized the 3914 Å line to that of an IBC III aurora. This study by Green and Barth led to some very interesting conclusions. It showed that even though we assumed that 30 keV electrons were incident our attention was immediately focused upon very low energy electrons (below 50 eV). Thus current cross sections indicate that as a high energy electron slows down, it loses energy mostly by ionization collisions. In such collisions the average of about 60 e. v. is lost in each encounter. Of this, only fifteen e. v. are expended in pulling the electron from the molecule. The balance (45 e. v.) goes to the secondary electron created in the ionization process. Accordingly, as the primary electron slows down, 3/4 of its energy is pumped into low energy electrons. Accordingly one must know the cross sections for these low energy secondaries to calculate their energy degradation in order to determine the ultimate disposition of the incident energy.

A second major consequence of this first calculation was the discovery that there are important allowed transitions in N_2 which had been completely ignored in the auroral literature which, via the secondary electron mechanism absorb much of the energy of incoming auroral electrons. Indeed, our calculations suggested these transitions would give rise to the most intense auroral lines if one were equipped with instruments that could detect radiations below 1000 Å.

This first effort stimulated quite a bit of interest and has served as an heuristic guide toward further efforts to understand upper atmospheric phenomena initiated by energetic electrons. Indeed, for the past three years we have penetrated much more deeply into this field, and I would like to indicate briefly the nature of our second generation efforts.

It was clear that to go further we would have to compile all the known information with respect to the important species N₂, O₂ and O which are the most predominant species in the 100 to 500 kilometer region.



To do a better job than our first effort, it was necessary to have a more systematic approach to the determination of electron impact cross sections for N_2 , O_2 and O and other atmospheric species of importance. Accordingly, an overall study and comparison was made of all semi-empirical cross section methods¹⁰.

Having made this survey, I selected the Bethe-Born quantum mechanical concept of generalized oscillator strengths as the basis of detailed system for estimating cross sections. The choice was based upon my background as a nuclear physicist, a field which depends almost entirely upon quantum mechanical scattering calculations. Thus began an intensive series of efforts to arrive at cross sections for atmospheric species.

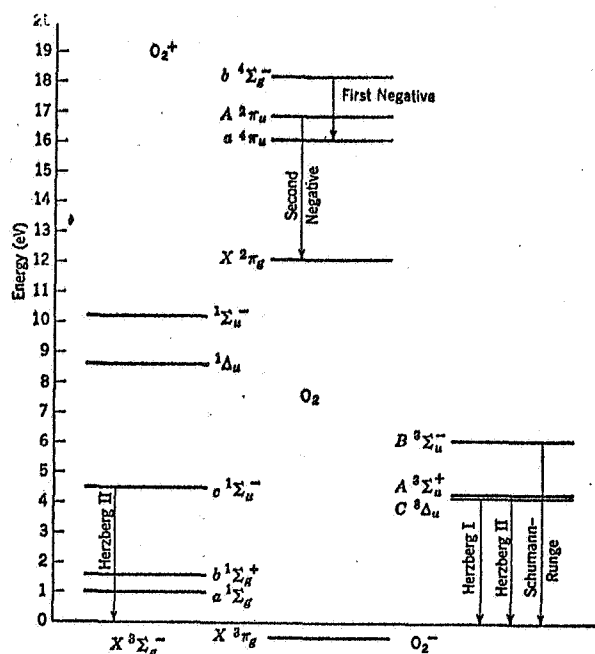
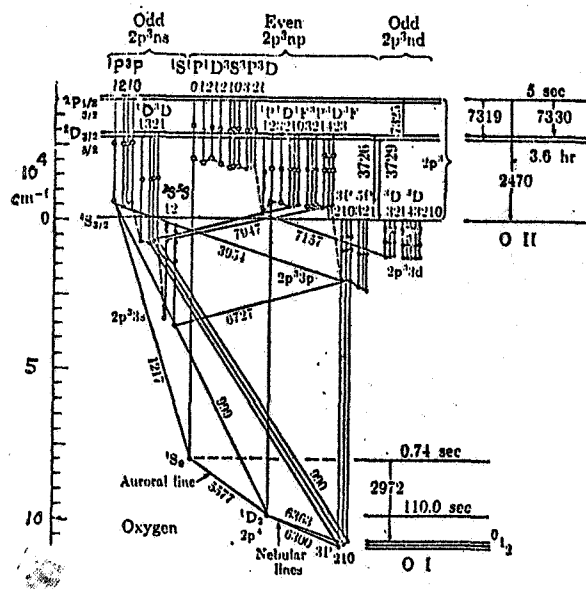


Fig. (4) Energy Levels of O_2 from The Middle Ultraviolet, A.E.S.
Green, Ed., Wiley, 1966.⁹

Fig. (3) N_2 , O_2 , and O concentrations of
H₂H₂S₂ model.

Fig. (5) Energy Levels of O from Atomic and Space Physics, A.E.S. Green and P.J. Wyatt, Addison Wesley, 1965. 6



To gain an insight as to how to modify the Born approximation at low energies, we made an intensive study of helium which has been subjected to more theoretical and experimental investigations than for any other substance. By doing so we developed what we believe to be a fairly good semi-empirical cross section estimating system in which optical cross sections represent the most important ingredient in the adjustment process. We used this system along with all available experimental data to determine a set of cross sections for N_2 , O_2 and O .

With the aid of this set of cross sections we embarked upon a second generation set of aurora calculations considering all the loss processes going on at a representative altitude in the upper atmosphere (150 kilometers). This I might say is where the astronauts have been flying. According to an atmospheric model which we assumed, there is approximately 45% N_2 to 45% O and 10% O_2 at this altitude. Assuming this mixture, Dr. Stolarski, in connection with his Ph.D. thesis study, solved the energy loss problem in considerable detail. The primary electron was assumed to have one of four possible energies, 30 keV, 10 keV, 1 keV and 0.1 keV. For these energies the energy deposited by the primaries, all the secondaries, tertiaries, etc. to the last generation were calculated. The populations of 150 states of N_2 , O and O_2 were considered and the intensities of the important emissions of N_2 , O_2 and O calculated.

One of the major objectives of this second generation auroral study was to determine whether from observation of spectral distribution analysis of observed photons we could infer the relative intensities of the incident electrons. An indication of the results will be given later.

The final study which has been completed to date considers the varying atmospheric constituents in the domain above 100 kilometers using the abundances given by the representative atmospheric model of Hinterreger, Hall and Schmitke (H.H.S.) (see Fig. 3). Together with Professor Barth and Dr. Stolarski we have calculated the altitude dependence of various spectral lines of N_2 , O and O_2 excited by photoelectrons of the dayglow. Here the hard ultraviolet emissions of the sun ionize the upper atmospheric atoms and molecules. The study of these ions and the altitude dependence of their concentrations is the concern of ionospheric physicists. The calculation of ionospheric ion production rates using a detailed assembly of photon cross sections for N_2 , O and O_2 has been carried out by Hinterreger, Hall and Schmitke. Our work builds upon this work but treats the question of what happens to the photoelectrons which are released when these ions are created. We have a number of other studies underway which employ our semi-empirical cross sections, but these will not be

reported on here. Let us now go into some of the detailed technical considerations involved in airglow, auroral and ionospheric calculation important to an understanding of the 100-500 kilometer region.

2. Semi-Empirical Cross Sections

We let E denote the incident electron energy and W denote the energy loss by that electron in a collision with an atom or molecule (see Fig. 6a). Here the loss W corresponds to the excitation energy of a discrete state of the target molecule and $E_f = E - W$ is the final electron energy. If the energy loss is above the ionization threshold (I) (see Fig. 6b), W represents a continuum of excitation states starting at the ionization threshold and going upward. Here $W = I + E_s$ which I is the energy necessary to pull the electron out of the atom and E_s is the energy of the secondary electron. If we could put tags on the primary and secondary electrons, then the range of possible secondary electron energies would extend from 0 if $W = I$ to $E - I$ if all the incident energy were lost in one collision. However, since the measurement of the energy is the only tag we can put on the primary and secondary electrons we assign $(E-I)/2$ as the maximum secondary electron energy and $W_m = (E+I)/2$ as the corresponding maximum energy loss.

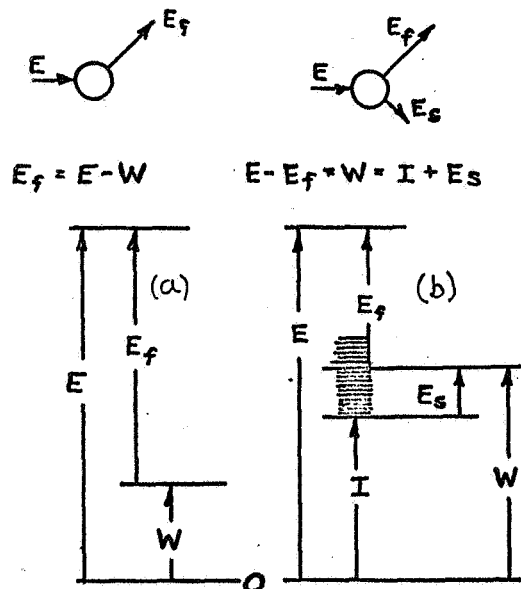


Fig. (6) Energy Relationships a) Excitation. b) Ionization.

Physicists characterize the probability of a collisional process by assigning an effective area to every discrete excitation. This is a matter of convenience and is a carry over from gunnery experience where a large target is easy to hit and a small target difficult or less probable. Thus the cross section is the effective area presented by a target molecule for any particular process to incident particle. An experimental arrangement for assigning excitation cross sections is shown in Fig. 7. The

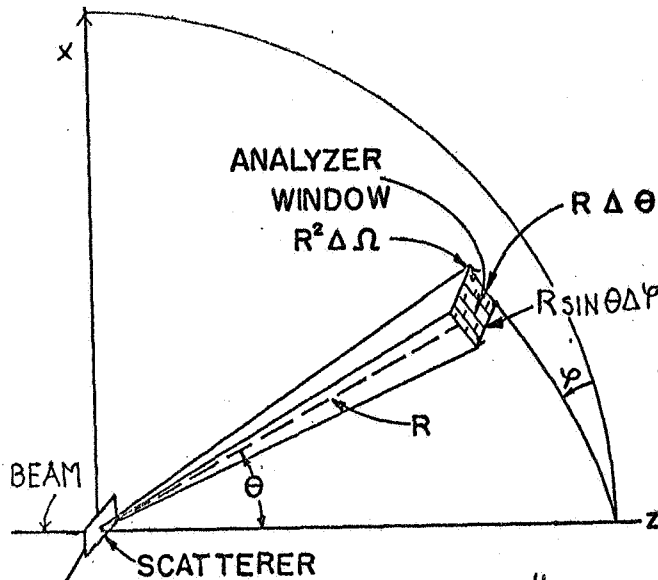


Fig. (7) Scattering Arrangement "

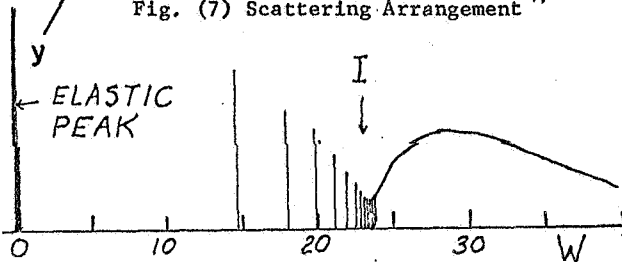


Fig. (8) Electron Spectrum from Analyzer

electrons scattered into the window (area $R^2 \Delta \Omega$) are energy analyzed and counted (see Fig. 8) to determine Δn_j , the number of electrons per unit area per unit time which lose the energy W_j and which go into the solid angle $\Delta \Omega$. Then the differential cross section $\sigma_j(\theta, \varphi)$ is an area defined by

$$\sigma_j(\theta, \varphi) = \Delta n_j / I N_s \Delta \Omega \quad (1)$$

Here N_s is the number of scatterers per unit area in the beam, I is the incident number of electrons per unit area per unit time. By dividing I and N_s we obtain from the measured outgoing electron flux with energy loss W_j an experimental number which represents an area associated with a collision between a single incident particle and a single scatterer. This is how one measures a differential cross section.

To measure a total cross section we integrate $\sigma_j(\theta, \varphi)$ over all possible angles. Thus the total excitation cross section is given by

$$\begin{aligned} \sigma_j(E) &= \int_0^\pi \int_0^{2\pi} \sigma_j(\theta, \varphi) \sin \theta d\theta d\varphi \\ &= 2\pi \int_0^\pi \sigma_j(\theta, \varphi) \sin \theta d\theta \end{aligned} \quad (2)$$

The last form takes advantage of the fact that scattering is usually symmetric with respect to the angle φ . Thus for various incident electron energies one has only to measure the observed angular distribution of the scattered particles with respect to the angle θ in one plane to establish the total cross section for an inelastic process. It is these cross sections which are the most important quantities needed in energy loss calculations. Conceptually, they could be determined simply by varying the incident energy E , the angle θ and the band pass of the energy analyzer.

Experimental observations indicate that excitation cross sections when studied with low resolution have shapes which can be characterized by simple analytical functions. A particularly simple and useful form is

$$\begin{aligned} \sigma_j(E) &= \frac{g_0 A}{W^2} \left(1 - \frac{W}{E}\right)^\nu \left(\frac{W}{E}\right)^\Omega \\ &\quad \frac{g_0 A}{W^2} \sum_s a_s \left(\frac{W}{E}\right)^{\Omega_s}, \quad \sum a_s = 0 \end{aligned} \quad (3)$$

where $g_0 = \pi a_0^2 (2R_e)^2 = 6.51 \times 10^{-14} \text{ cm}^2 \text{ ev}^2$. Here a_0 , the Bohr radius, $2R_e = 27.12 \text{ eV}$ is the atomic unit of energy; A is a parameter which fixes the overall magnitude of the cross section, and ν is a parameter which determines the rise of the cross section above the threshold W and Ω a parameter which determines the fall of the cross section at high energies. The second form is approximately equivalent. We have fitted this and a closely related functional form to a host of theoretical models and a large variety of experimental observations and have found that it can usually fit the theory or data to 5% accuracy for a large range of energies. If theoretical or experimental data is available, it is simple to fix the parameters of Eq. 3. We plot the data on log-log paper. Then the asymptotic slope gives Ω . The location of the peak then is determined by ν and the magnitude of the peak determines A .

For ionization cross sections we may use the same analytic form for $S(E, W) = d\sigma/dW$ as for discrete transitions but allow $A(W)$ to depend upon W . If we use $A(W) = A_0 (I/W)^p$, the total ionization cross section is given by

$$\begin{aligned} \sigma_i(E) &= g_0 A_0 I^p \int_I^{W_m} \frac{dW}{W^{2+p}} \sum_s a_s \left(\frac{W}{E}\right)^{\Omega_s} \\ &= g_0 A_0 I^p \sum_s \frac{a_s}{E^{\Omega_s + 1}} \left[1 - \left(\frac{2I}{E+I}\right)^{\Omega_s} \right] \end{aligned} \quad (4)$$

where $\Theta_s = 1 + p - \Omega_s$.

These empirical representations of $\sigma_j(E)$ and $S(E,W)$ are very useful if experimental data is available to adjust the parameters. Unfortunately, at this time we cannot find a complete set of data for any atomic or molecular system. Accordingly, it is necessary for the purposes of detailed degradation studies to develop semi-empirical cross section systems which make use of theoretical considerations or the systematics of the known experimental information to extract electron impact cross sections.

Various semi-empirical attempts to organize cross sections have been summarized recently.^{10,12} One of the predominant semi-empirical schools¹³ essentially chooses the classical mechanical approach of J. J. Thompson's 1912 paper as a point of departure.

In our work at the University of Florida, the wave mechanical approach of Born's 1926 and Bethe's 1930 papers are taken as the basic point of departure. The history of the last 40 years should make it unnecessary to defend the wave-mechanics vs. classical mechanics as a suitable approach to the description of atomic phenomena. Thus our concentration has been to adapt quantum mechanical models into a convenient analytic framework for inferring cross section curves from fragmentary experimental data. The primary strength of the approach is that the shape parameters η and ν conform to certain simple rules and the most important parameter A may be related to f_0 , the optical oscillator strengths determined from photon impact studies on the same substance. Furthermore, this quantity may also be determined from theoretical calculations of optical oscillator strengths which are somewhat simpler to carry out than calculations of electron impact cross sections. We shall refer to cross sections inferred from such theoretical framework, but later represented in a simple analytic form as semi-empirical cross sections (SECS).

3. Energy Degradation Calculations

For the purposes of energy loss studies we may separate out three types of loss functions. The loss due to excitation of a state W_j which is given by

$$L_j(E) = W_j \sigma_j(E) \quad (5)$$

The loss due to the creation of an ion which is given by

$$L_i(E) = I_i \sigma_i(E) \quad (6)$$

Finally, we can assign a loss to the corresponding secondary electrons

$$L_{si} = \int_0^{E_m} E_s S(E, E_s + I) dE_s \quad (7)$$

Adding all such loss functions together, we obtain the total loss function

$$\begin{aligned} -\frac{1}{n} \frac{dE}{dx} &= L(E) \\ &= \sum_j L_j(E) + \sum_i [L_i(E) + L_{si}(E)] \end{aligned} \quad (8)$$

which governs the rate of change of the electron energy in gases having n target molecules per unit volume. The fact that this total loss function involves all the excitation and ionization processes is the reason energy degradation calculations are so tedious and why atomic physicists have avoided them at low energies where certain convenient sum rules break down. Nevertheless, suppose we have all these cross sections, we can then compute energy transfer functions defined by

$$E_j(E_p) = W_j \int_{W_j}^{E_p} dE \frac{\sigma_j(E)}{L(E)} \quad (9)$$

This represents the portion of energy which goes to the particular excited state when the energy of the primary degrades from E_p to zero. In a similar way we can calculate the corresponding quantities which appears as ionization energy, and which is invested in the kinetic energy of secondary electrons from the neutral molecules. Because of the complex form of $L(E)$ these energy transfer functions could normally not be represented in analytic form. However, for many purposes it is possible to use the approximate form

$$E'_j(E) = [\sum_k (E/E_k)^{K_k} + R_L] / \pi a_0^2 (2R_L) \quad (10)$$

where E_k and K_k are a set of adjusted constants and where R_L is a fluctuating but small residual. To the extent that R_L can be ignored, then the energy transfer functions are analytically integrable and dependent simply upon the parameters of the cross section and the loss function.

$S(E,W)$ and $L(E)$, now can be used to infer the secondary electron energy distribution which is obtained when a primary electron degrades to zero energy. From such a distribution we can then take every energy interval and recycle it through the calculations in such a way as to find the deposition of energy deposited by the secondary electrons. We can then again recycle the calculation to get the tertiary electron distributions, etc. Very fortunately, the processes are rapidly converging and very few quaternaries appear in typical calculations even if one starts with very

high energy primaries. So much for the general nature of energy loss calculations. Let us next consider some results of the application of such calculations to atmospheric process in the 100 to 500 kilometer region.

4. Auroral and Airglow Calculations

In Table 1 we give the results of our second generation calculation of auroral intensities for an IBC III aurora. The results are based upon assumed incident 10 keV, 1 keV, and 100 eV primary electrons in a 45% N₂, 45% O and 10% O₂ mixture. It is rather interesting to note that these calculations give 32, 32 and 41 eV per ion pair which is the most reasonable result yet, one which has not previously been derived from basic cross sections.

Intensity of Lines in IBC III Aurora

Line Å	10 keV	1 keV	0.1 keV	Exper.
O 989	172	152	303	
O 1218	12	13	47	
O 1304	182	176	360	
O 1356	92	93	240	
O 5577	94	97	200	100
N ₂ LBH	1300	1380	2670	450-1850
N ₂ 1st P.	1260	1250	2560	2000
N ₂ VK	320	320	630	30-150
N ₂ 1 Neg.	165	165	165	165
O ₂ 2 Neg.	191	183	137	

The relative intensity of these representative lines are also quite reasonable. They suggest that these spectral line intensities are not very sensitive to the initial electron flux. For the most part the results are in accord with the available observations. However, definitive observations, particularly in the ultraviolet region, will have to be determined from future space vehicles flying in the 100-500 kilometer region.

It will only be possible to sketch briefly the nature of our calculations of altitude profiles of dayglow emissions. Here we first start from the Hinterregger, Hall, Schmitke solar ultraviolet spectrum. This is shown in Fig. 9. The bar graphs represent the groups which are the most important in producing photoelectrons. We assumed

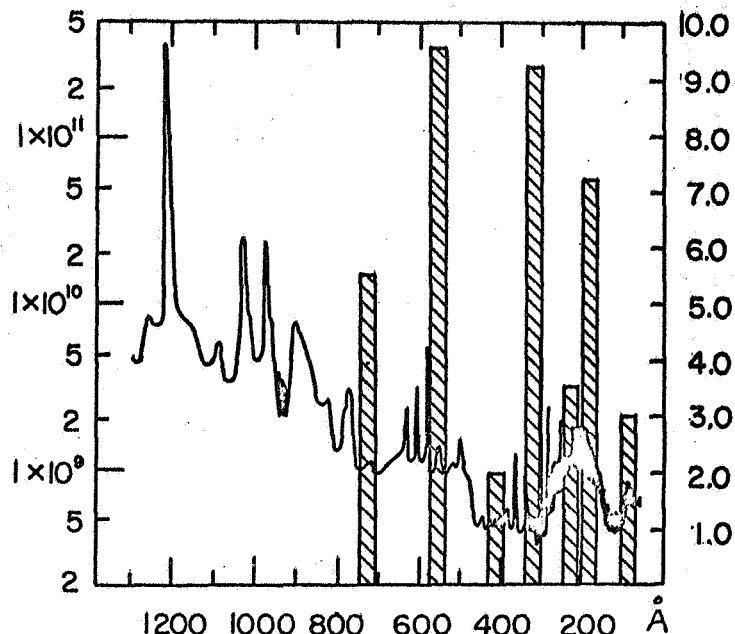


Fig. (9) Solar EUV spectrum, left scale unit: photons/cm² sec Å, right scale unit: 10⁹ photons/cm² sec

that these photoelectrons originate at the various levels of the ionosphere as calculated by HHS. Assuming next that photoelectrons having the energies

$$E_{pil} = (hc/\lambda_p) - I_{il} \quad (11)$$

where I_{il} is the ionization energy of the state active in the conversion of the incident photon to a photoelectron. In our calculation we essentially treated these photoelectrons as if they were auroral electrons. We also allowed for the varying concentrations of N₂, O and O₂ in the 100-300 kilometer regime. Fig. 10 gives a representative result showing the profile of several N₂ lines. To the extent of the available data these results seem quite reasonable. However it remains for future experiments to apply the acid test.

5. Discussion and Conclusions

In conclusion it must be emphasized that our results are no better than the semi-empirical cross sections for N₂, O and O₂ which we have extracted from our phenomenological studies. However, we must remember that we have placed these semi-empirical cross sections in a simple parametric form for application to degradation calculations and have proceeded in a straight forward fashion from our analytic representations of basic molecular properties to their aeronautical

consequences. Indeed, the calculations are basically a matter of bookkeeping in which one keeps track of all the energy deposited in the atmosphere in the form of incident electrons in the case of the aurora calculations or in the form of ultraviolet light in the case of the airglow calculations. In view of this we might look to a comparison of our results in relation to the results of future experiment which will be performed in the space laboratories which you design to provide a basis for obtaining a better set of semi-empirical cross sections. Thus, in an indirect way the space experiment will provide a measurement of a fundamental molecular cross section which has been so difficult to obtain from laboratory experiments or theoretical analyses.

Thus it appears that SECS will be very beneficial to the marriage of atomic and space physics and that it will lead in a natural way to offsprings in the form of better cross sections and improved knowledge and understanding of both disciplines.

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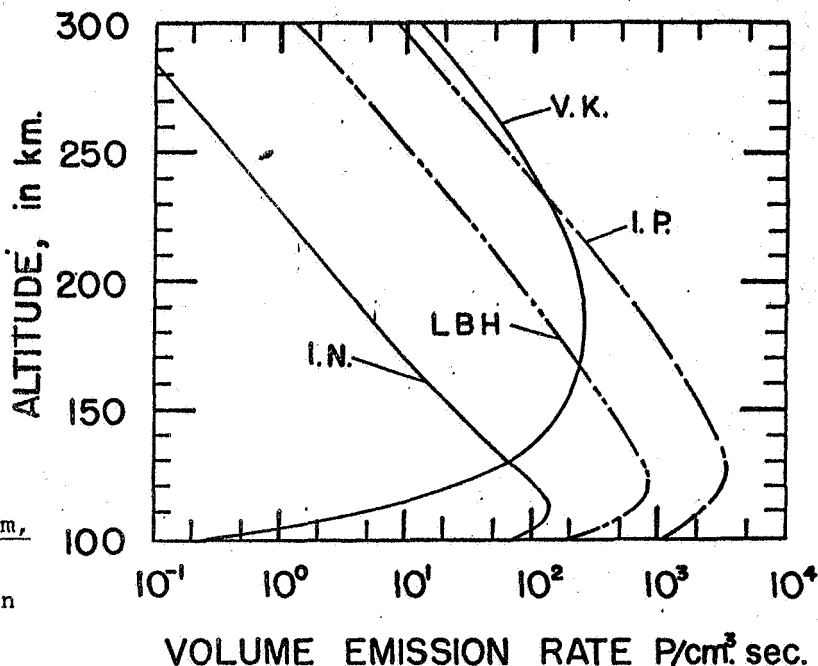


Fig. (10) Volume emission rate for representative dayglow lines (photons/cm³ sec).