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# Derivation of ionization equations for the simulation of auroral effects

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ABSTRACT. Equations are derived for calculating ionization rates for three basic types of electron energy spectrum distributions. These can be combined to model observed auroral electron energy distributions, in order to simulate auroral effects and effects due to electron precipitation. Calculated auroral 5577 Å/3914 Å intensity ratios, using the ionization rates obtained by means of the derived equations, at the altitudes of 120, 160 and 200 km, show good agreement with observations.

#### 1. Introduction

The main spectral emissions and general appearance of an aurora, as well as the height of maximum volume emission rate for a given radiation wavelength, depend principally upon the electron energy spectrum distribution of the electron flux penetrating the atmosphere. Electron impact excitation of the various states of the atmospheric species and indirect processes such as those caused by the ionization created by the electron flux are responsible for these emissions.

Some auroral electron spectrum distributions have been investigated by rocket and satellite studies and the results of a few of these studies are shown by Hones *et al.* (1971). Most of these reported distributions may be represented by combinations of the basic types of electron energy spectrum distributions such as :

- (a)  $J(E) = K_1 \cdot E \cdot \exp(-E/E_0)$
- (b)  $J(E) = K_2 \cdot \exp(-E/E_0)$
- (c)  $J(E) = K_3 \cdot E^{-\gamma}$

By means of analytical equations derived for the ionization created by the above basic types of electron energy distributions, it becomes possible to simulate the ionization caused by combinations of these basic types of distributions for electron fluxes penetrating the atmosphere, with the use of an assumed model atmosphere.

When the electron impact cross sections for the excited states of the atmospheric components are known, it is possible to simulate the major spectral emission and ionization features of auroras by determining the emissions due to impact excitation and those due to the indirect processes such as, for example, the dissociative recombination of  $O_2+$ . To illustrate the use of the derived equations, the 5577 Å/3914Å intensity ratio is calculated at a few altitudes using the model atmosphere employed by Walker and Rees (1968). The results show good agreement with previously reported observations of this ratio.

# 2. Approximations for number density, scale height and column density

Reasonable approximations for the number density and the column density of the atmosphere upto at least about 300 km are required for the calculations related to typical auroras. Some of this data can be obtained from model atmospheres such as the Cira 1965 model. The number density of an individual atmospheric component, as calculated by the Cira 1965 model atmosphere, is

$$n_i = n_{1i} \cdot (T_1/T) \cdot \exp[-(m_i/k) \cdot \int_{z_1}^z g \cdot dz/T] \quad (2 \cdot 1)$$

where  $n_i$ ,  $n_{1i}$  is the number density of the *i* component at altitude z,  $z_1$  (cm<sup>-3</sup>).

 $T, T_1$  is the temperature at altitude  $z, z_1$  (°K).

- $m_i$  is the molecular or atomic mass of the *i* component (gm).
- k is Boltzmann's constant.
- g is the acceleration due to gravity (cm/sec<sup>2</sup>).

The total number density of all atmospheric components may be approximated by the following expression (valid over a limited range of altitude);

$$n = n_1 \cdot \exp\left[-\left(z - z_1\right) / H_{\text{eff}}\right]$$
(2.2)  
here *n*, *n*, is the total number density of all at-

where n,  $n_1$  is the total number density of all atmospheric components, at altitude z,  $z_1$  (cm<sup>-3</sup>).

 $H_{\rm eff}$  is the effective scale height for the altitude range,  $z_1$  to z.  $H_{\rm eff}$  for the altitude range,  $z_1$  to z, is given by

$$H_{\rm eff} = (z - z_1) / \ln (n_1 / n)$$
 (2.3)

The column density increment between the altitudes  $z_1$  and z is approximated by integrating the number density expression, Eq. (2.2), thus

$$\therefore \bigtriangleup \eta = H_{\text{eff}} \cdot (n_1 - n) \tag{2.5}$$

The column density is obtained by summing the column density increments above the altitude for which it is required.

# 3. Derivation of the ionization rate equations

For obtaining some of the spectral emission properties of auroral phenomena, it is useful to know the total ionization at various altitudes caused by an electron flux having combinations of the various types of electron energy spectrum distributions mentioned in the introduction. That is, equations for the ionization rate established at each altitude under study should be derived from basic physical principles.

Assuming that the geomagnetic field lines are approximately vertical and that each high energy electron spirals about these lines at a given pitchangle as it approaches the denser atmosphere, it is possible to formulate a comparatively uncomplicated integral for the ionization rate. Since each precipitating high energy electron creates ion-pairs along its entire path, those electrons with sufficient energy to penetrate to a given altitude contribute to the ionization at that altitude. Hence the ionization rate at a given altitude, at each differential solid angle, 2.  $\pi \sin \theta \, d \, \theta$ . sterad., will be the sum of rate of energy loss per unit length by all of the electrons of the distribution (having energies over the minimum required to reach the altitude under consideration), divided by the average energy loss per ion-pair created,  $(\triangle E)_{av}$ . This total number of ion-pairs created per unit time is not altered by the fact that the primary electrons create secondary electron which, in turn, may have sufficient energy to create higher order electrons.

Therefore, if J(E) refers to the function for the assumed electron energy spectrum distribution of the precipitating electron flux, then the ionization rate at a given altitude is :

$$q = \int_{0}^{\theta_{m}} \int_{E_{1}(\theta)}^{E_{m}} \frac{1}{2 \cdot \pi \cdot \sin \theta \cdot d\theta \cdot (-dE/dy) \cdot J(E) \cdot dE/(\triangle E)_{av}}$$
(3.1)

where q is the ionization rate, (ion-pair/cm<sup>3</sup>/sec).

- $\theta$  is the angle with respect to the vertical direction. Since the geomagnetic field lines are assumed to be approximately vertical,  $\theta$  also corresponds to the pitch-angle of precipitating electrons, (at the differential solid angle located at  $\theta$ ).
- $\theta_m$  is the maximum possible pitch-angle, at a given altitude, for the electrons with the largest energy of the distribution.
- $E_1$  is the least value for the energy that an electron may have to penetrate to the given altitude at the assumed pitch angle,  $\theta$ .
- $E_m$  is the maximum electron energy for the electron energy spectrum distribution.

The steradian unit associated with the differential solid angle has been omitted in Eq. (3.1) for simplicity, but it cancels with the steradian  $^{-1}$  unit associated with the function, J(E).

The first equation will be derived for ionization at a given altitude created by electrons having a "Maxwellian" type of electron energy spectrum distribution of the types,  $J(E)=k_1$ .  $E.\exp(--E/E_0)$ , and assuming isotropy for the angular distribution of the precipitating electrons. By the latter assumption, for electrons with lower energies, deflections after collisions with air molecules will not affect the ion-pair production rate obtained by Eq. (3.1).

An equation which relates electron energy to the penetration and the pitch-angle of the electron (Citrynell 1974 a), is

$$E = E'. (\sec \theta)^p \tag{3.2}$$

where p=0.5785 and

$$E' = \left[\int N \cdot dy / (k_1 \cdot N_{\rm STP})\right]^p \tag{3.3}$$

 $k_1$  is 4.467.10<sup>-3</sup> cm. (kev)<sup>-1.7285</sup>, and  $N_{\rm S1P}$  is very closely twice the Loschmidt's number, 2.68719.10<sup>19</sup> cm<sup>-3</sup> (Weast 1970, p. F-84). A brief summary of the derivation of Eq. (3.2) is given in the appendix for the convenience of the reader. Differentiating Eq. (3.2) with respect to the altitude, y, yields

$$dE/dy = (\sec \theta)^{p} \cdot [\int N.dy/(k_{1} \cdot N_{\text{STP}})]^{p-1} \cdot (N/N_{\text{STP}}) \cdot p/k_{1}$$
(3.4)

since  $\theta$  may be assumed to be approximately constant without changing the value for the ioniza-

tion at a given altitude, significantly. N is the total atomic density at the altitude under consideration (units of atoms per cm<sup>3</sup>), and  $\int N.dy$  represents the total atomic column density at the given altitude, (units of atoms per cm<sup>2</sup>). Since it is the absolute value for the rate of energy loss per unit length that is requised for -dE/dy, Eq. (3.4) may be substituted for -dE/dy in Eq. (3.1). Hence, Eq. (3.1) may be written as

$$q = \xi_1 \cdot \int_0^{\theta_m} \sin \theta \cdot (\sec \theta)^p \cdot d\theta \cdot \int_{E_1(\theta)}^{E_m} E \cdot e^{-E/E_0} dE$$
(3.5)

where  $\xi_1 = 2.\pi. [\int N.dy/(k_1.N_{\text{STP}})]^{p-1}$ .  $(N/N_{STP}) \cdot p/k_1 \cdot k_1/(\triangle E)_{av}$  (3.6)

Integrating over the variable, E, and substituting the limits of integration,  $E_1(\theta) = E'$ . (see  $\theta$ )<sup>p</sup> and  $E_m$ , yields

$$q = \xi_1 \cdot E_0 \cdot \int_{0'}^{\theta_m} \sin \theta \cdot (\sec \theta)^p \cdot E' \cdot (\sec \theta)^p \cdot exp \left[ -(E'/E_0) (\sec \theta)^p \right] \cdot d\theta \\ + \xi_1 \cdot E_0^2 \cdot \int_{0}^{\theta_m} \sin \theta \cdot (\sec \theta)^p \cdot d\theta \\ - \xi_1 E_0^2 \cdot \exp \left[ -(E'/E_0) \cdot (\sec \theta)^p \right] \cdot d\theta \\ - \xi_1 E_0^2 \cdot \exp \left( -E_m/E_0 \right) \cdot (1 + E_m/E_0) \\ \cdot \int_{0}^{\theta_m} \sin \theta \cdot (\sec \theta)^p \cdot d\theta$$
(3.7)

By multiplying and dividing the integral in the last term of Eq. (3.7) by  $\sec^2\theta$ , this last term becomes

$$\xi_{1}E_{0}^{2} \cdot \exp(-E_{m}/E_{0}) \cdot (1+E_{m}/E_{0}) \cdot \int_{0}^{\theta_{m}} (\sec\theta)^{p-2} \\ \sec\theta \cdot \tan\theta \, d\theta \\ = \xi_{1} \cdot E_{0}^{2} \exp(-E_{m}/E_{0}) \cdot (1+E_{m}/E_{0}) \cdot [1-(\cos\theta_{m})^{1-p}]/(1-p))$$
(3.8)

By multiplying and dividing the integral in the second term of Eq. (3.7) by  $p.(E'/E)^{1+1/p}$ . sec  $\theta$ , the integral in the second term of Eq. (3.7) becomes

$$\begin{aligned} \text{Int}_{1} &= (1/p) \cdot (E_{0}/E')^{1-1/p} \cdot \int_{0}^{\theta_{m}} & \exp[-(E'/E_{0}) \cdot \\ & (\sec \theta)^{p}] \cdot [(E'/E_{0}) \cdot (\sec \theta)^{p}]^{-1/p} \cdot [(E'/E_{0}) \\ & \cdot p \cdot (\sec \theta)^{p-1} \cdot \sec \theta \tan \theta . d\theta] \end{aligned}$$

Substituting t for  $[(E'/E_0).(\sec \theta)^p]$  in Eq. (3.9) changes this integral to

$$\operatorname{Int}_{1} = (1/p) \cdot (E_{0}/E') \cdot {}^{1-1/p} \cdot \int_{t_{0}}^{t_{\theta m}} e^{-t} \cdot t^{-1/p} \cdot dt$$
(3.10)

where  $t_0$  and  $t\theta_m$  are the new integration limits which correspond to 0 and  $\theta_m$ , respectively.

By setting  $\varphi$ -1 equal to -1/p and by the use of two integrals which are equivalent to the integral in Eq. (3.10), Int<sub>1</sub> is transformed to

$$\operatorname{Int}_{1} = (1/p) \cdot (E'/E_{0})^{-\mathfrak{P}} \left( \int_{t_{0}}^{\infty} e^{-t.t^{-1}.dt} - \int_{t\theta_{m}}^{\infty} e^{-t.t^{\mathfrak{P}^{-1}}dt} \right)$$
(3.11)

hence

$$\operatorname{Int}_{1} = (1/p) \cdot (E'/E_{0})^{-\varphi} \cdot [\Gamma(\varphi, t_{0}) - \Gamma(\varphi, t_{\theta m})]$$
(3.12)

where  $\Gamma(\varphi, t_0)$  is an incomplete gamma function  $t_0 = E'/E_0$ 

$$t_{\theta m} = (E'/E_0) \cdot (\sec \theta_m)^p = E_m/E_0$$

Substituting Eq. (3.12) for the integral in the second term of Eq. (3.7), this second term becomes

$$\xi_1 \cdot E_0^{\ 2} \cdot \operatorname{Int}_1 = (\xi_1 \cdot E_0^{\ 2}/p) \cdot (E'/E_0)^{-\varphi} \cdot [\Gamma(\varphi, t_0) \\ -\Gamma(\varphi, t_{\theta_m})]$$
(3.13)

By multiplying and dividing the intergral in the first term of Eq. (3.7) by  $(E_0/p) \cdot (E_o/E')^{1-1/p}$ , changes this intergral to

$$\begin{aligned} \text{Int}_2 &= (E_0/p) \cdot (E_0/E')^{1-1/p} \cdot \int_0^{\theta_m} \exp\left[-(E'/E_0)\right] \\ (\sec \theta)^p \left[ \cdot [(E'/E_0) \cdot (\sec \theta)^p]^{1-1/p} \cdot (E'/E_0) \cdot p \right] \end{aligned}$$

 $(\sec \theta)^{p-1} \cdot \sec \theta \cdot \tan \theta \cdot d\theta \qquad (3.14)$ 

Here, again, t may be substituted for  $\Gamma(E'/E)$  (see  $\theta)^p$ ) so that

$$I_{1}(E_{0}/E_{0}) = (E_{0}/p) \cdot (E_{0}/E') \stackrel{\varphi}{\to} \int_{-\infty}^{t_{\theta}} e^{-t} \cdot t \, \omega^{-1} \cdot dt \ (3.1)$$

Int<sub>2</sub> = 
$$(E_0/p).(E_0/E') \stackrel{\varphi}{\longrightarrow} \int_{t_0} e^{-t} t \, \omega^{-1} dt \, (3.15)$$

where  $\omega = 2 - 1/p$  and  $\varphi = 1 - 1/p$ 

By using two integral in place of the integral is Eq. (3.15), as was done for the similar situation in Eq. Eq. (3.11), the first term in Eq. (3.7) changes to

$$\xi_1 \cdot \underline{E}_0^2 \cdot \operatorname{Int}_2 = (\xi_1 \cdot \underline{E}_0^2/p) \cdot (\underline{E}'/\underline{E}_0)^{-\varphi} \cdot \lfloor \Gamma(\omega, t_0)$$

$$-\Gamma(\omega, t_{\theta m})] \qquad (3.16)$$

Therefore, the ionization rate, q, at a given altitude caused by an electron flux penetrating the atmosphere and having a 'Maxwellian' type of electron energy spectrum distribution,  $J(E) = k_1$ . E. exp  $(-E/E_0)$ , is found by combining the results, Eq. (3.8), Eq. (3.13), and Eq. (3.16), to yield

$$q = (\xi_1 \cdot E_0^{2}/p) \cdot (E'/E_0)^{-\varphi} \cdot [\{\Gamma(\omega, t_{\theta}) - \Gamma(\omega, t_{\theta_m})\}] \\ + \{\Gamma(\varphi, t_o) - \Gamma(\varphi, t_{\theta_m})\}] \\ - \xi_1 \cdot E_o^{2} \cdot \exp((-E_m/E_o) \cdot (1 + E_m/E_o) \cdot$$

where 
$$\xi_1 = 2 \cdot \pi \cdot [\int N \cdot dy / (k_1 \cdot N_{S1P})]^{p-1} \cdot (N/N_{STP}) \cdot (p/k_1) \cdot k_1 / (\Delta E)_{av}$$
  
 $\omega = 2 - 1/p = 2 - 1.7285 = 0.2715$   
 $\varphi = 1 - 1/p = 1 - 1.7285 = -0.7285$   
 $E' = [\int N \cdot dy / (k_1 \cdot N_{STP})]^p$   
 $t_o = E'/E_o$   
 $t_{\theta m} = E_m/E_o$   
 $\Gamma(u,v) \equiv \int_v^{\infty} e^{-t} \cdot t^{u-1} \cdot dt$ 

 $E_m$  is the maximum electron energy of energy spectrum distribution.

- N is the atomic number density at the given altitude, (cm<sup>-3</sup>).
- $\int N.dy$  is the total atomic column density at the given altitude, (cm<sup>-2</sup>).

When the electron energy spectrum distribution is of the type,  $J(E) = k_2 \exp(-E/E_0)$ , the derivation follows a pattern similar to the derivation of equation (3.17)). Hence, only the resulting equaation for the ionization rate, q, is given here; this equation is

$$q = (\boldsymbol{\xi}_2 \cdot \boldsymbol{E}_o | \boldsymbol{p}) \cdot (\boldsymbol{E}' | \boldsymbol{E}_o)^{-\boldsymbol{\varphi}} \cdot [\boldsymbol{\Gamma}(\boldsymbol{\varphi}, t_o) - \boldsymbol{\Gamma}(\boldsymbol{\varphi}, t_{\theta m})] - \boldsymbol{\xi}_2 \cdot \boldsymbol{E}_o \cdot \exp(-\boldsymbol{E}_m | \boldsymbol{E}_o) \cdot$$

 $[1-(E'/E_m)-\Phi]/(1-p)$  (3.18) where the meaning of the symbols are given with the derivation of Eq. (3.17).

The ionization rate caused by the atmospheric penetration of an electron flux having the third type of electron energy spectrum distribution listed in the introduction,  $J(E) = k_3 \cdot E^{-\gamma}$ , will now be derived. Beginning with Eq. (3.1) and again substituting Eq. (3.4) for -dE/dy results in the following equation :

$$q = \xi_3 \cdot \int_0^{\theta_m} \sin \theta \cdot (\sec \theta)^{p \cdot d\theta} \cdot \int_{E_1(\theta)}^{E_m} E^{-\gamma} dE$$
(3.19)

The meaning of the symbols used in Eq. (3.19) are given with the derivation of Eq. (3.17). Integrating over the variable, E, and substituting the limits of integration,  $E_1(\theta) = E'$ . (see  $\theta$ )<sup>p</sup> and  $E_m$ , yields

$$q = - \left[\xi_{3} \cdot E'^{1-\gamma}/(1-\gamma)\right] \cdot \int_{0}^{\theta m} (\sec \theta) p \cdot (2-\gamma) \cdot \sin \theta \cdot d\theta$$
$$+ \left[\xi_{3} \cdot E_{m}^{1-\gamma}/(1-\gamma)\right] \cdot \int_{0}^{\theta m} (\sec \theta)^{p} \cdot \sin \theta \cdot d\theta$$
$$(3.20)$$

Multiplying and dividing both integrands in the

right-hand member of Eq. (3.20) by  $(\sec \theta)^2$  changes the form of the equation to

$$q = - [\xi_3 \cdot E'^{1-\gamma}/(1-\gamma)].$$

$$\cdot \int_{-\infty}^{\theta_m} (\sec \theta) p \cdot (2-\gamma)^{-2} \cdot \sec \theta \cdot \tan \theta \cdot d\theta$$

$$+ [\xi_3 \cdot E_m^{1-\gamma}/(1-\gamma)]. \int_{-\infty}^{\theta_m} (\sec \theta)^{p-2} \cdot \sec \theta \cdot \tan \theta \cdot d\theta \qquad (3.21)$$

The integration of Eq. (3.21) and the substitution of equivalent expressions results in the ionization rate equation for an electron energy spectrum distribution of the type,  $J(E)=k_3.E-\gamma$ , which is

$$q = [\xi_3 \cdot E'^{1-\gamma}/(1-\gamma)] \cdot [1 - (E_m/E')^{\lfloor p \cdot (2-\gamma)-1 \rfloor/p}] / [p \cdot (2-\gamma) - 1] + [\xi_3 \cdot E_m^{1-\gamma}/(1-\gamma)] \cdot [1 - (E'/E_m)^{-\phi}] / (1-p)$$
(3.22)

where the meaning of the symbols are given with Eq. (3.17). The conditions,  $\gamma \neq 1$  and  $\gamma \neq 2-1/p$ , apply to Eq. (3.22).

For the case where  $\gamma = 1$ , the integration proceeds in a different manner. Substituting  $\gamma = 1$  into Eq. (3.19) and integrating over the variable *E*, yields

$$q = -\xi_{3} \cdot p \cdot \int_{0}^{\theta_{m}} (\sec \theta)^{p} \cdot \sin \theta \cdot \ln (\sec \theta) \cdot d\theta$$
$$+ \xi_{3} \cdot \ln(E_{m}/E') \cdot \int_{0}^{\theta_{m}} (\sec \theta)^{p} \cdot \sin \theta \cdot d\theta$$
(3.23)

Multiplying and dividing both integrands in the right-hand member of Eq. (3.23) by  $(\sec \theta)^2$ , changes the forms of the expressions so that they may be directly integrated, yielding the following equation after the substitution of the limits of integration :

$$q = -[\xi_3 \cdot p/(p-1)^2] \cdot [(\sec\theta_m)^{(p-1)} \{ \ln (\sec\theta_m)^{p-1} - 1\} + 1] + [\xi_3 \cdot \ln (E_m/E')/(p-1)]$$

$$[(\sec\theta_m)^{p-1} - 1] \qquad (3.24)$$

Thus, by using the expressions  $\varphi = 1 - 1/p$  and  $E_m = E'$ . (sec.  $\theta_m$ )<sup>p</sup>, Eq. (3.24) may be simplified to yield the ionization rate equation for the particular case when  $\gamma = 1$ , which is

$$q = [\xi_3/\varphi \cdot (1 - p)] \cdot [1 + \ln (E_m/E')\varphi - (E_m/E')\varphi]$$

$$(3.25)$$

For the case where  $\gamma = 2 - 1/p$ , a different form of ionization rate equation will result if this substitution is made in Eq. (3.19). Here, one of the integral will become  $\int \tan \theta \, d\theta$ , which will result in

$$\begin{array}{l} & (=\xi_3 \cdot E_m - \frac{\varphi}{\varphi} \cdot (p-1)] \cdot [1 - (\sec \theta_m)^{p-1}] \\ & + [\xi_3 \cdot E'^{-\varphi} / [\varphi \cdot (p-1)] \cdot \ln (\sec \theta_m)^{p-1} \end{array}$$

$$(3.26)$$

Therefore, by the use of the expressions  $\varphi = 1 - 1/p$  and  $E = E' (\sec \theta_m)^p \operatorname{Eq.}(3.26)$  may be simplified to yield the ionization rate equation for the particular case when  $\gamma = 2 - 1/p$ , which is  $q = [\xi_3 E'^{-\varphi} / \{\varphi \cdot (1-p)\}] \cdot [1-\ln(E_m/E')\varphi]$  $-(E_m/E')^-\varphi$ (3.27)

## 4. Calculation of the 5577Å /3914Å intensity ratio

The 5577 A/3914 A intensity ratio of an aurora or of an electron precipitation event provides a good method for checking the validity the derived of analytical equations for calculating ionization rates since this ratio may be checked against known observed values; these values are about 2.1., upto an altitude of 140 km (Dalgarno and Khare 1967).

The 5577 A radiation wavelength is emitted durng a transition of an atomic oxygen atom in the excited Is state to the lower energy level excited Ip state. The intensity of this radiation emission depends upon the generation rate of atomic oxygen atoms in the Is states, the Einstein coefficient for the transition, and the rate of quenching by  $O_2$ , O, and  $N_2$ . The two major processes that are responsible for the creation of Is states during auroral and electron precipitation events are direct electron impact excitation and dissociative recombination of  $O_2^+$ . The latter process may be represented by  $O_2^+ + e \rightarrow 0^* + 0$  where about 5 per cent of the excited states generated are assumed to be the Is states.

The 3914 A radiation wavelength is emitted during a transition of an  $N_2^+$  ion from the excited  $B^2\Sigma_u$  + state at an energy level of 18.75 ev to a lower energy level. Direct electron impact excition is the only process assumed to take place which generates this excited state.

To work with a specific case, a flux of electrons with an electron energy spectrum distribution of the type  $J(E) = k_3 \cdot E^{-\gamma}$  is assumed to penetrate the model atmosphere (given Table 2, p. 461, Walker and Rees 1968], (plus the Ar values of the Cira, 1965 model atmosphere)  $k_3$  is assumed to be  $1.0.10^8$  cm<sup>-2</sup>. sec<sup>-1</sup>.sterad<sup>-1</sup>.kev<sup>-1</sup>, with  $\gamma = 2$ . The maximum and minimum energy values are assumed to be 100. key and 1. key, respectively. The resulting total ionization rate, calculated by employing Eq. (3.22), is Altitude (km) 80 120 160 200 q (ion-pair/cm<sup>3</sup>/sec) × 10<sup>3</sup> 1.09 8.20 3.08 1.69

with the above values for the total ionization rate' q, the individual atmospheric component's ioniza tion rates at the given altitudes may be obtained ' A brief review of equations which may be used for this part of the calculations is also given in the appendix.

The production rate of a given excited state may be calculated by means of the following equation (Citrynell 1974):

$$\begin{array}{l} q (X_{rk}) = \left[\sigma_{rk \text{ eff}} \cdot W_{rk} / (\Sigma \sigma_{rk, \text{eff}} \cdot W_{rk})\right] \cdot q(X_{r}^{+}) \cdot w_{r} / W_{rk} \\ \text{where,} \end{array}$$

- $q(X_{rk})$ represents the production rate of the excited state, X,k, (cm<sup>-3</sup>.sec<sup>-1</sup>)
- $q(X_r^+)$ represents the individual atmospheric component's,  $(X_{*})$ , ionization rate, (ionpair.cm-3.sec-1.).
- is the ratio of the total energy loss, (to Wr the  $X_r$  species) per ion-pair produced, (ev/ion-pair).
- Write is the energy level of the excited state, X,k, (ev).
- is the effective electron impact cross ork;eff section for the entire electron energy spectrum distribution, for the k excited state of the r species, (cm<sup>2</sup>).

Based upon the results of previous work by the author and upon the results of work by Green and Barth (1965) and Stolarski and Green (1967), the ratio  $[\sigma_{rk}, eff. W_{rk}/(\Sigma \sigma_{rk}, eff. W_{rk})]$  is assumed to be

0.0232 for the O(I<sub>S</sub>) state and 0.0410 for the  $N_2^+(B^2 \Sigma_0^+)$  state, with  $w_r=35$ . ev/ion-pair associated with  $q(O^+)$  and with  $w_r = 36.2 \text{ ev/ion-pair asso-}$ ciated with  $q(N_2^+)$ .

By means of the production rate of the excited state obtained, the volume emission rate may be calculated using

$$\eta(\lambda) = \underbrace{A_{rk1} \cdot [q(X_{rk}) + q'(X_{rk}) + \Sigma k_i \cdot (Y_i) \cdot Z_i)]}_{[A_{rk2} + \Sigma k_j \cdot (Y_j)]} + \underbrace{i}_{i} \underbrace{i}_{i}$$

where,

 $\eta(\lambda)$  is the volume emission rate of the radiation wavelength,  $\lambda$  (photon.cm<sup>-3</sup>.sec<sup>-1</sup>).

 $A_{rk1}$  is the Einstein coefficient for the radiation wavelength,  $\lambda$  representing the emission of a photon due to a transition from the state,  $X_{rk}$ , to a particular lower energy level, (sec<sup>-1</sup>).

 $q'(X_{rk})$  represents the production rate of the excited state,  $X_{rk}$ , due to cascading processes in which transitions from states at higher energy levels to the energy level of the given state take place, (cm<sup>-3</sup>. sec<sup>-1</sup>).

 $k_i$  and  $k_j$  are reaction rate coefficients (cm<sup>3</sup>/sec)

 $(Y_i)$  and  $(Z_i)$  are the number densities of atmospheric components which react chemically to produce the excited state,  $X_{rk}$  (cm<sup>-3</sup>).

 $(Y_i)$  is the number density of an atmospheric component which reacts chemically to reduce the the number of atoms, molecules or ions at the given excited state,  $X_{rk}$ , or which otherwise act to deactivate the state, (quenching agents) (cm<sup>-3</sup>).

#### TABLE 4.1

Principal reactions used for obtaining volume emission rates

	Reaction	Rate coefficient	Reference
1	$N_2^++O_2 \rightarrow O_2^++N_2$	4•7(-11) <sup>a</sup>	Dunkin et al. (1968)
2	$N_2^++0 \rightarrow N0^++N$	1•4(-10)	Fehsenfeld <i>et al.</i> (1970)
3	$N_2$ ++0 $\rightarrow$ 0++ $N_2$	<1.0(-11)	Hunt (1973)
4	$N_2$ ++N0 $\rightarrow$ NO++ $N_2$	3.3(-10)	Fehsenfeld et al. (1970)
5	$0_2$ ++N0 $\rightarrow$ N0++ $0_2$	6+3(-10)	Fehsenfeld et al. (1970)
6	$0++N_2 \rightarrow NO++N$	$1 \cdot 0(-12)$	Dunkin et al. (1968)
7	$0++0_{2} \rightarrow 0+_{2}+0$	2.0(-11)	Schmeltekopf et al. (1967)
8	$N^++0_2 \rightarrow N0^++0$	3.0(-10)	Hunt (1973)
9	$\mathrm{N_2}{}^+{}+\mathrm{O_2}{}\rightarrow\mathrm{O_2}{}^+{}+\mathrm{N}$	3.0(-10)	Fehsenfeld et al. (1970)
10	$N_2$ ++e $\rightarrow$ N+N	$2 \cdot 9(-7) \ (300/T_e)^{1/3}$	Walker and Rees (1968)
11	$0_2$ ++e $\rightarrow$ 0*+0	$2 \cdot 2(-7) \cdot (300/T_{e})$	Rees et al. (1969)
12	$0++e \rightarrow 0$	$1 \cdot 0(-6)$	b
13	$N^{+}+e \rightarrow N$	$1 \cdot 0(-6)$	b
14	N0++e $\rightarrow$ N+0	$4 \cdot 6(-7) \cdot (300/T_e)$	Biondi (1968)
15	$O(Is) + O_2 \rightarrow O + O_2$	4•3(-12)• exp(-1700 / <i>RT</i> )	Slanger and Black (1973)
16	$0(Is)+0 \rightarrow 0+0$	1•2(-11) exp(-450/ <i>RT</i> )	Slanger and Black (1973)
17	$\rm O(Is) \! + \! N_2 \! \rightarrow O \! + \! N_2$	<1.0(-17)	Zipf (1968)

a- units cm<sup>3</sup>/sec- (-x)=10<sup>-X</sup> b- assumed rate of coefficient

 $A_{rk_2}$  represents the sum of all the Einstein coefficients for radiation which are transitions from the state  $X_{rk}$  to lower states (sec<sup>-1</sup>).

In this way, the velues of  $\eta$  (5577.Å) and  $\eta$  (3914.Å) are calculated. For convenience and for understanding the relative importance of the major excited state generating processes, the calculation for the  $\eta$  (5577.Å) is divided into a part due to direct electron impact excitation and a part due to the dissociative recombination of the molecular oxygen ion. Table 4.1 lists the principal reactions used for obtaining the volume emission rate due to the dissociative recombination of  $0_2^+$ . Table 4.2 gives the results of the volume emission rate calculations. Table 4.3 lists the resulting 5577Å/3914Å intensity ratios for the altitudes that were checked.

In addition to the neutral atmospheric constituents already mentioned, the assumed nitric oxide concentrations given in Table 4.1A were also used to calculate the equilibrium concentrations of the major ions formed.

TABLE 4.1A Assumed Nitric Oxide concentrations

					the second se	
A	60	70	80	90	100	110
С	3.0×10 <sup>8</sup>	$1.0 \times 10^{8}$	$2.0  imes 10^7$	$1.3  imes 10^7$	$8.0 \times 10^{7}$	$1.0 \times 10^{8}$
A	120	130	140	150	160	200
С	$9.0  imes 10^7$	$7 \cdot 0 \times 10^7$	$8.0  imes 10^{6}$	1.0×106	$6 \cdot 0 \times 10^5$	$1.0  imes 10^4$
					N	

A=Altitude (km) C=Concentration (cm<sup>-3</sup>)

 TABLE 4.2

 Volume emission rates (ph./cm³/sec)

Altitude	η(3914 Å)	η(5577 Å)	$\eta(5577 \stackrel{\mathrm{o}}{\mathrm{A}})$
(km)		E.I.E.	D.R.
120	387	142	41.1
160	139	108	35.7
200	69.8	86-2	11.6

E.I.E. refers to electron impact excitation.

D.R. refers to dissociative recombination, (reaction No. 11).

TABLE 4·3 5577Å/3914 Å intensity ratio

E.I.E.	D.R.	COMB
Ratio	Ratio	Ratio
0-367	0.106	0.473
0.778	0.229	1.01
1.24	0.166	1.41
	E.I.E. Ratio 0.367 0.778 1.24	E.I.E. D.R. Ratio Ratio 0.367 0.106 0.778 0.229 1.24 0.166

E.I.E. Ratio is the ratio due to electron impact excitation D.R. Ratio is r.tio due to dissociative recombination (reaction No. 11).

COMB Ratio is the combined ratio, (*i.e.* the ratio due to the effect of electron impact excitation combined with the effect due to dissociative recombination).

#### 5. Discussion

For work with the third type of electron energy distribution listed in the introduction, calculation require the use of Eq. (3.22). If  $E' < E_{\min}$  (the minimum energy of the distribution), it is necessary to first calculate  $q=q(E_{m,1})$  with  $E_m=E_{m,1}=E_{\max}$  (the maximum energy, of the distribution); next,  $q=q(E_{m,2})$  is calculated with  $E_m=E_{m,2}=E_{\min}$ . The ionization for this case will be

$$q = q(E_{m,1}) - q(E_{m,2})$$
 (5.1)

If, however,  $E > E_{\min}$ , the ionizatio rate q, is simply that given by Eq. (3.22) with  $E_m = E_{\max}$ . [*i.e.*,  $q = q(E_{m,1})$ ].

The analytical expressions for the ionization rate, equations that have been derived in section 3, of this paper together with the other methods discussed in sections 2, 4 and the appendix achieve a significant simplification of the work that would otherwise be required to model the effects of an electron precipitation event or an aurora. REFERENCES

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However, the electron temperature,  $T_e$ , which was required for the rate coefficients of reactions 3 and 5 of Table 4.1, necessitated the use of values which were approximated from the results of the work by Walker and Rees (1968).

In conclusion, it may be noted that the results for the 5577 Å/3914 Å intensity ratios listed in Table 4.3, which were obtained by the use of one of the derived analytical equations for ionization

Bethe, H. A. and Ashkin, J.

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Zipf, E.C.

rate and by the use of the other methods discussed, show good agreement with observations. Observed values are about  $2.\pm1$  (Dalgarno and Khare 1967).

The low combined ratio at 120 km, in Table 4.3, is due to the low, dissociative recombination, 5577. Å emission caused by a lower concentration of  $0_2$ +resulting from charge transfer to NO, (No. 5, Table 4.1).

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- APPENDIX A.1

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#### Brief summary of the derivation of Eq. (3.2) : (Citrynell 1974)

By negleting relatively small terms and by using substitutions of good approximations for certain terms, the basic equation given by Bethe and Ashkin 1953 (Eq. 52, p. 254), for the electron energy loss per unit path length, may be simplified to the following form

$$-dE/dx = (a \cdot N \cdot Z/E) \cdot \ln(b \cdot E^2)$$
(A1.1)

where,

- $\vec{E}$  is the kinetic energy of the incident electron.
- x is the distance along the path through the material.
- N is the number of atoms of the material per unit volume.
- Z is the nuclear charge of an atom of the material.

$$a = \Pi \cdot e^4 / (1 - \beta^2)^{1/2}$$

$$b = 1/(C' \cdot I^2 \cdot (1 - \beta^2)^{1/2})$$

The Collisional Deactivation of Metastable Atoms

Laboratory Measurements of Aeronomic Interest,

University, Toronto, Canada, Sep., 3-4, 1968.

Molecules in the Upper Atmosphere, Symposium

e is the magnitude of the charge of an electron C' is a constant.

*I* is the average excitation potential over all electrons of an atom.

 $\beta = v/c$ 

v is the velocity of the incident electron.

c is the velocity of light.

Over the limited extent of electron energies applicable to the auroral region and the D-region of the atmosphere, the expression,  $(1 - \beta^2)^{1/2}$ does not vary sufficiently to change the values of *a* and *b* to an appreciable degree. Hence, *a* and *b*  may be regarded as constants. The distance through which a high energy particle penetrates a given material before being stopped is known as the range of the particle for that material. This may be determined for high energy electrons penetrating air at given values of temperature and pressure. For this case, N and Z in Eq. (A1.1) are constant; hence, by multiplying both members of Eq. (A1.1) by  $-(2.b, E, dx)/\ln(b.E^2)$  and then integrating the range of high energy electrons in air is obtained as  $R=[1/(2\cdot a \cdot b \cdot Z \cdot N)] \cdot E_i[2\cdot \ln(b^{1/2} \cdot E)]$  (A1.2) where  $E_i$  is the exponential integral function.

If the geomagnetic field lines are assumed to be approximately vertical in high-latitude regions and if y is the vertical component of the actual distance traversed along the helical type of path, the energy-loss equation for electrons precipitating in the auroral and D-region of the atmosphere may be obtained directly from Eq. (A1.1) as

$$-dE/dy = (a \cdot N \cdot Z/E). \quad \ln(b \cdot E^2) \cdot \sec \theta \quad (A1.3)$$

where the pitch angle,  $\theta$ , is the angle between the geomagnetic field lines and the helical type of path of the precipitating electron. By multiplying both members of Eq. (A1.3) by-(2.b.E.dy)/ ln (bE<sup>2</sup>) and then integrating the penetration equation of a high energy electron precipitating in the atmosphere may be approximately

$$\int Z \cdot N \cdot \sec \theta \cdot dy = [1/(2 \cdot a \cdot b)] \cdot E_{1}[2 \cdot \ln(b^{1/2} \cdot E)] (A1.4)$$

If the penetration equation, (A1.4), is divided by the range equation, (A1.2), this yields

$$\frac{[\{Z \cdot N \cdot \sec\theta \cdot dy\}/R = [\{1/(2 \cdot a \cdot b)\} \cdot E_i \{2 \cdot \ln(b^{1/2} \cdot E)\}]}{[\{1/(2 \cdot a \cdot b \cdot Z \cdot N_{\text{STP}})\} \cdot E_i \{2 \cdot \ln(b^{1/2} \cdot E)\}] }$$
(A1.5)

Since a, b and E are the same in the numerator and the denominator of the right-hand member, and since Z and  $\theta$  may be assumed to be approximately constant (without significantly changing the result for most of region of the atmosphere concerned, Eq. (A1.5) can be smplified to

$$\int N \cdot dy = N_{\rm STP} \cdot R \cdot \cos \theta \tag{A1.6}$$

A good approximation for the range of an energetic electron in air at STP, for electron energies that are used in the ionization of this region of the atmosphere, is given by

$$R = 4.467 \cdot 10^{-3}$$
. cm<sup>•</sup>(kev)<sup>-1.7285</sup>.  $E^{1.7258}$  (A1.7)

where the kinetic energy, E, is expressed in kev units. Since  $N_{\text{STP}}$  is very closely twice the Loschmidt's number, if the range, R, as given in Eq. (A1.7), is substituted into Eq. (A1.6) and the resulting equation is solved for E, this will yield

$$E = \begin{bmatrix} \int N \cdot dy / (2.40.10^{17} \text{ cm}^{-2}) ]^{0.5785} \text{ kev.} \\ (\text{Al}.8) \end{bmatrix}$$

Eq. (A1.8) may be written in the symbolic form given in Eq. (3.2) as E=E'. (sec  $\theta$ )<sup>p</sup> (A1.9)

#### APPENDIX A-2

#### Brief review of equations for the ionizations rates of atmospheric components

When high energy electrons penetrate the atmosphere, the ionization rate is approximately given by

$$q(N_{2}^{+} + N^{+}) = [(N_{2}) / (M)] \cdot (\partial E / \partial') / (36.2 \text{ ev/ion-pair})$$
(A2.1)

- where  $(qN_2^+ + N^+)$  is the ionization rate for molecular nitrogen, (ion-pair. cm<sup>-3</sup>. sec<sup>-1</sup>).
  - (X) refers to the number density of the gas, X, (cm<sup>-3</sup>).
  - (M) refers to the total number density of all species, (cm<sup>-3</sup>).
  - $(\partial E / \partial t)$  is the total energy transfer rate to all species, per unit volume, (ev.cm<sup>-3</sup>. sec<sup>-1</sup>).

The production rate of most of the ions may be calculated using the method developed by Walker and Rees (1968), where

$$q(N^+) = 0.25.q(N_2^+)$$
 (A2.2)

$$q(N_2^+ + N^+) = q(N_2^+) + q(N^+)$$
 (A2.3)

Therefore

$$q(N_2^+) = q(N_2^+ + N^+) / 1.25$$
 (A2.4)

For molecular oxygen ions

$$q(\mathbf{O}_2^+) = 0.8 \cdot q(\mathbf{N}_2^+ + \mathbf{N}^+) \cdot (\mathbf{O}_2) / (\mathbf{N}_2)$$
(A2.5)  
and for atomic oxygen ions

$$\begin{array}{l} q\,(\mathrm{O^{+}}) = \ 0.5 \cdot q \ (\mathrm{O_{2^{+}}}) + \ 0 \cdot 5 \cdot q(\mathrm{N_{2^{+}}} \\ + \mathrm{N^{+}}) \cdot (\mathrm{O}) / (\mathrm{N_{2}}) \end{array} \tag{A2.6}$$

Besides the ion-pair production rates suggested by Walker and Rees, the following ionization rate equations are useful :

$$q(\operatorname{Ar}^+) = [(\operatorname{Ar}) / (M)] \cdot (\partial E / \partial t) / (24 \cdot 3 \text{ ev/ion-pair})$$
(A2.7)

 $q(\text{He}^+) = [(\text{He}) / (M)] \cdot (\gamma E/\partial t) / (30.2 \text{ ev/ion-pair})$ (A2.8)

The total ionization rate is equal to

 $q = q(N_2^+ + N^+) + q(O_2^+) + q(O^+) + q(Ar^+) + q(He^+)$ (A2.9)