

The Electron Avalanche Ionization of Air and a Simple Air Chemistry Model

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April 15, 1982

This report was sponsored by Defense Advanced Research Projects Agency (DoD),
DARPA Order No. 3718, monitored by NSWC under Contract No. N60921-81-WR-
W0190.



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THE ELECTRON AVALANCHE IONIZATION OF AIR AND SIMPLE AIR CHEMISTRY MODEL

1. Introduction

The avalanche ionization of air and other gaseous elements, caused by a static or an oscillating electric field (microwaves, lasers) is of considerable interest in gaseous breakdown studies. These studies provide an understanding of the breakdown mechanisms and facilitate the measurements of various electron transport coefficients. The understanding of gaseous breakdown and the ensuing plasma chemistry can be utilized fruitfully in many areas of applications, such as, high voltage switching, lasers, plasma maintenance and plasma heating.

Avalanche ionization occurs when a free electron gains sufficient energy, from the externally imposed electric field, to generate an ionization, and thus initiate the electron multiplication process. The initial free electron or electrons can be introduced into the gas by various means, such as a radiation source, an electron beam, etc.

To describe avalanche ionization in a gas, one requires the solution of the Boltzmann equation with an appropriate set of electron-atom or electron-molecule collision cross sections¹⁻³ where one obtains, in a self-consistent manner, the electron velocity distribution and the relevant transport coefficients. However, the knowledge of several quantities such as the electron drift velocity, the ionization coefficient, the electron temperature or the electron characteristic energy can also be utilized to describe avalanche ionization in a speedy and simple manner. These quantities, in general, depend on the electric field, E , and the gas pressure, P , and have been measured^{1,2,4,5} for various gaseous elements.

Manuscript submitted February 12, 1982.

On the other hand, the avalanche ionization can also be described by assuming a Maxwellian electron velocity distribution; for regions of $\frac{E}{P} > 35$ volts cm^{-1} Torr $^{-1}$ this method provides identical results compared⁶ to the solution of the Boltzmann equation.

In this report, we discuss a simple description of avalanche ionization in air, provide the ionization coefficient over a wide range of $\frac{E}{P}$ ($\frac{E}{P} = 50$ to 3000) and make comparison with previous results. The simple approach consists of a few equations which describe the ionization and the deionization in air, using appropriate coefficients developed in this report.

2. The Ionization Coefficient

The growth of a current beam as a function of distance, due to the avalanche ionization in a gaseous medium, can be described by

$$I = I_0 \text{Exp} (\alpha x) \quad (1)$$

where I_0 is the initial current at $x = 0$ and α is the ionization coefficient which is generally known⁷ as Townsends' first ionization coefficient. This coefficient, especially in the form of $\frac{\alpha}{P}$ has been measured as a function of $\frac{E}{P}$ for various gaseous elements results are quoted in Ref. 5, but in that reference reliable data for air and its constituents are limited to the region of E/P below 100 volt cm^{-1} Torr $^{-1}$. These units of $\frac{E}{P}$ are used throughout this report and henceforth implied throughout this report. The work of Rao and Raju⁸, however, extends the range to $\frac{E}{P} = 1000$ for dry air with no contribution from contaminants. Their data for air is given in Table 1 for $\frac{E}{P} = 54$ to $\frac{E}{P} = 1000$ and is also shown in Figure 1a. The data of Table 1 can be expressed reasonably well (within few percent) by the following expressions.⁸

$$\frac{\alpha}{P} = 8.34 \text{ Exp} \left(-\frac{273.8}{E/P} \right), \quad 120 > \frac{E}{P} > 54 \quad (2)$$

and

$$\frac{\alpha}{P} = 14.61 \text{ Exp} \left(\frac{-359}{E/P} \right), \quad 1000 > \frac{E}{P} > 120 \quad (3)$$

Table 1
The Air Ionization Coefficient $\left(\frac{\alpha}{P}\right)$ As a Function of (E/P)

<u>E/P</u>	<u>α / P</u>	<u>E/P</u>	<u>α/P</u>
54	5.24 (-2)	330	4.95
60	8.70 (-2)	360	5.47
66	1.32 (-1)	390	5.96
72	1.86 (-1)	420	6.41
80	2.72 (-1)	450	6.82
90	3.98 (-1)	480	7.21
100	5.40 (-1)	520	7.68
120	8.52 (-1)	540	7.9
130	9.93 (-1)	580	8.69
140	1.17	620	9.11
150	1.36	660	9.49
160	1.55	700	9.83
170	1.73	740	10.15
180	1.92	780	10.45
196	2.20	820	10.73
210	2.49	860	10.98
230	2.94	900	11.22
250	3.37	940	11.44
270	3.79	980	11.65
300	4.39		

The ionization coefficient for N_2 as measured by Folkard and Haydon⁹ for E/P from 60 to 1000, and that for O_2 as measured by Price, et al¹⁰ for $\frac{E}{P}$ from 30 to 60 are shown in Figure 1b. The extension of the ionization

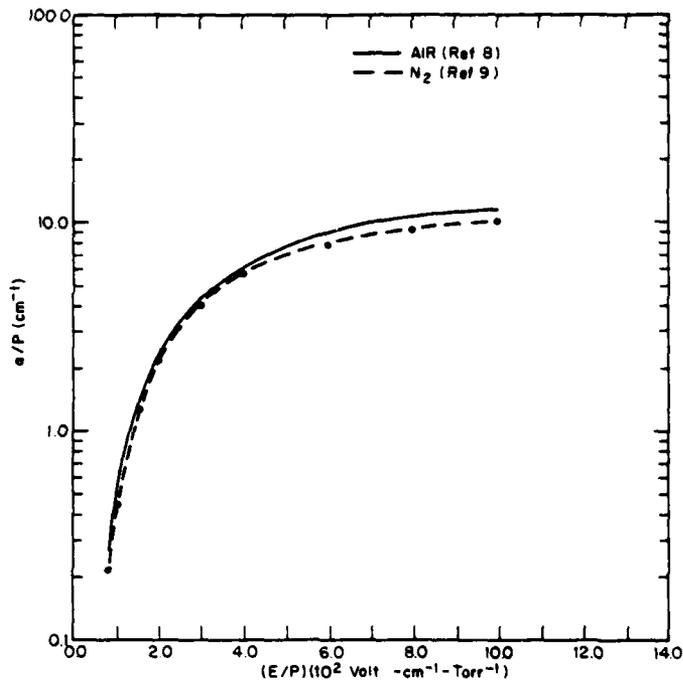


Fig. 1a - The ionization coefficient for Air and, N₂ as a function of $\frac{E}{P}$ (high E/P)

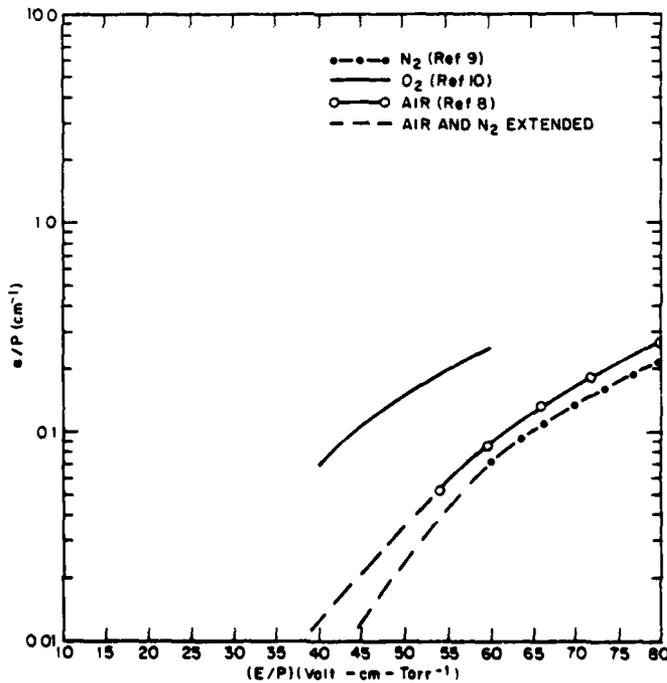


Fig. 1b - The ionization coefficient for Air, N₂ and O₂ as a function of E/P (low E/P)

coefficient for air and N_2 down to $E/P = 40$ is based on data from Ref.

5. However, Equation (2), if used below its lower limit will underestimate $\frac{\alpha}{P}$ by ~30%.

3. The Drift Velocity

The electron drift velocity in N_2 and O_2 has been measured by Schlumbohm¹¹ over a wide range of $\frac{E}{P}$. For N_2 the range of $\frac{E}{P}$ is from 100 to 3000, while for O_2 , the range is from 100 to 8000. Using these data¹¹, the drift velocity for N_2 and O_2 can be expressed¹¹, reasonably well, by the following relations

$$v_d = 3.3 \times 10^6 \left(\frac{E}{P}\right)^{1/2}, \quad 120 < \frac{E}{P} < 3000 \quad (4)$$

$$v_d = 3.75 \times 10^6 \left(\frac{E}{P}\right)^{1/2}, \quad 100 < \frac{E}{P} < 8000 \quad (5)$$

respectively, where the units of v_d are in cm sec^{-1} . The drift velocity in air can be obtained using the relation⁴ for the electron mobility, μ , in a gaseous mixture where

$$\mu = \left(\frac{f_1}{\mu_1} + \frac{f_2}{\mu_2}\right)^{-1} \quad (6)$$

Here, f_1 and f_2 are the fractions of N_2 and O_2 in air and μ_1 and μ_2 are the electron mobility in N_2 and O_2 , respectively. From Eqs.(4-6), we obtain the following expression for the electron drift velocity in air

$$v_d = 3.38 \times 10^6 \left(\frac{E}{P}\right)^{1/2}, \quad 100 < \frac{E}{P} < 3000 \quad (7)$$

For the region of $\frac{E}{P} < 100$ the electron drift velocity in N_2 and O_2 are shown in Fig. 2 based on the data of Wagner and Raether¹², and Jager and Otto¹³. The measurements of References 12 and 13 with Equation (6) predict the drift velocity in air which is in good agreement with the drift velocity measurements of Ryzko¹⁴, shown in Fig. 2, and is expressed as

$$v_d = 6.0 \times 10^6 + 2.5 \times 10^5 (E/P) \quad (8)$$

Felsenthal and Proud¹⁵ have proposed the following expression for the electron drift velocity in air

$$v_d = 7 \times 10^6 + 2 \times 10^5 \left(\frac{E}{P}\right) \quad (9)$$

based on measurements over a limited range of E/P ($\frac{E}{P} = 0.2-20$). They, however, extended Equation (9) to higher values of $\frac{E}{P}$ which clearly overestimates the drift velocity. The dependence of the drift velocity on $\frac{E}{P}$ is linear for $\frac{E}{P} < 100$, and varies as $\left(\frac{E}{P}\right)^{1/2}$ for $\frac{E}{P} > 100$ as shown by Equations (7) and (8). For example at $\frac{E}{P} = 1000$ Equation (9) predicts a drift velocity of 2.07×10^8 cm/sec compared to 1.06×10^8 cm/sec based on Eq. (7) which is obtained from the measurements¹¹ of the drift velocities in N_2 and O_2 .

4. The Ionization Frequency in Air

The ionization frequency ν_i is related to the ionization coefficient α by

$$\nu_i = \alpha v_d \quad (10)$$

or alternately

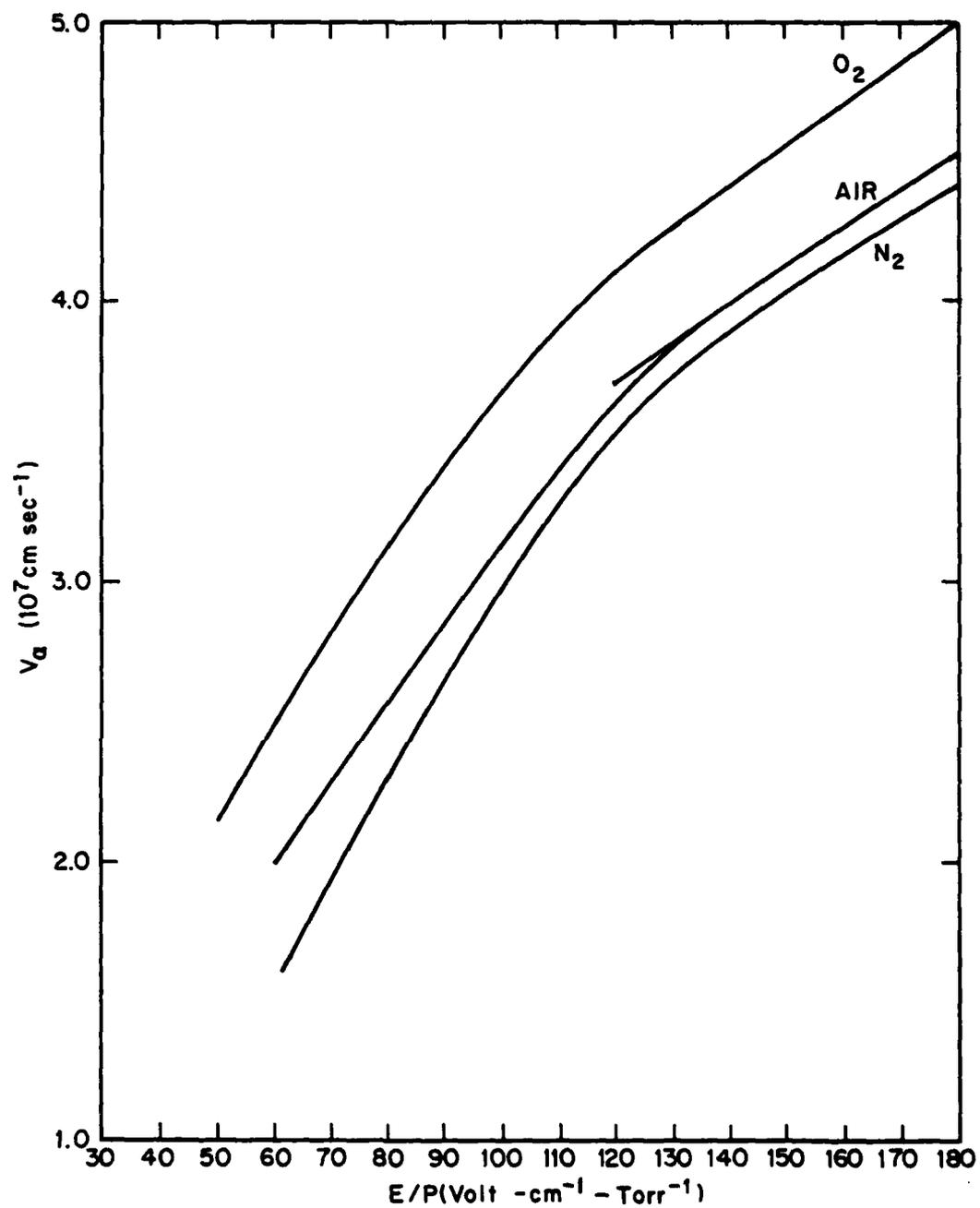


Fig. 2 - The electron drift velocity in N_2 , O_2 and Air

$$\frac{v_i}{p} = \frac{\alpha}{p} v_d \quad (11)$$

Thus, $\frac{v_i}{p}$ can be expressed as a function of $\frac{E}{p}$ through the dependence of both $\frac{\alpha}{p}$ and v_d on $\frac{E}{p}$. Using Equations (7) and (8) for the drift velocity and Equations (2) and (3) for $\frac{\alpha}{p}$ we obtain the following expressions for the ionization frequency in air.

$$\frac{v_i}{p} = 1.0 \times 10^7 [5 + 0.21 (E/P)] \text{Exp} \left(-\frac{273.8}{E/P} \right) \quad , 40 \leq \frac{E}{p} < 100 \quad (12)$$

and

$$\frac{v_i}{p} = 4.94 \times 10^7 \left(\frac{E}{p} \right)^{1/2} \text{Exp} \left(-\frac{359}{E/P} \right) \quad , 120 \leq \frac{E}{p} < 1000 \quad (13)$$

Figure 3 shows $\frac{v_i}{p}$ as a function of $\frac{E}{p}$ based on Equations (12) and (13).

However, the ionization frequency can also be obtained from the basic atomic processes if the electron velocity distribution is known. For a Maxwellian electron velocity distribution, the ionization rate coefficients for O_2 and N_2 have been calculated^{16, 17} using measured ionization cross sections. These rate coefficients can be used to obtain the corresponding ionization rate coefficient in air. The numerical values for the rate coefficients in N_2 and O_2 , shown in Figure 4, can be expressed¹¹ as

$$\langle \sigma v \rangle_{N_2} = \frac{10^{-9}}{\sqrt{T_e}} (-4.98 + 9.67 T_e + 0.49 T_e^2) \text{Exp} \left(-\frac{15.58}{T_e} \right) \quad (14)$$

$$\langle \sigma v \rangle_{O_2} = \frac{10^{-9}}{\sqrt{T_e}} (-2.02 + 3.39 T_e + 0.64 T_e^2) \text{Exp} \left(-\frac{12.06}{T_e} \right) \quad (15)$$

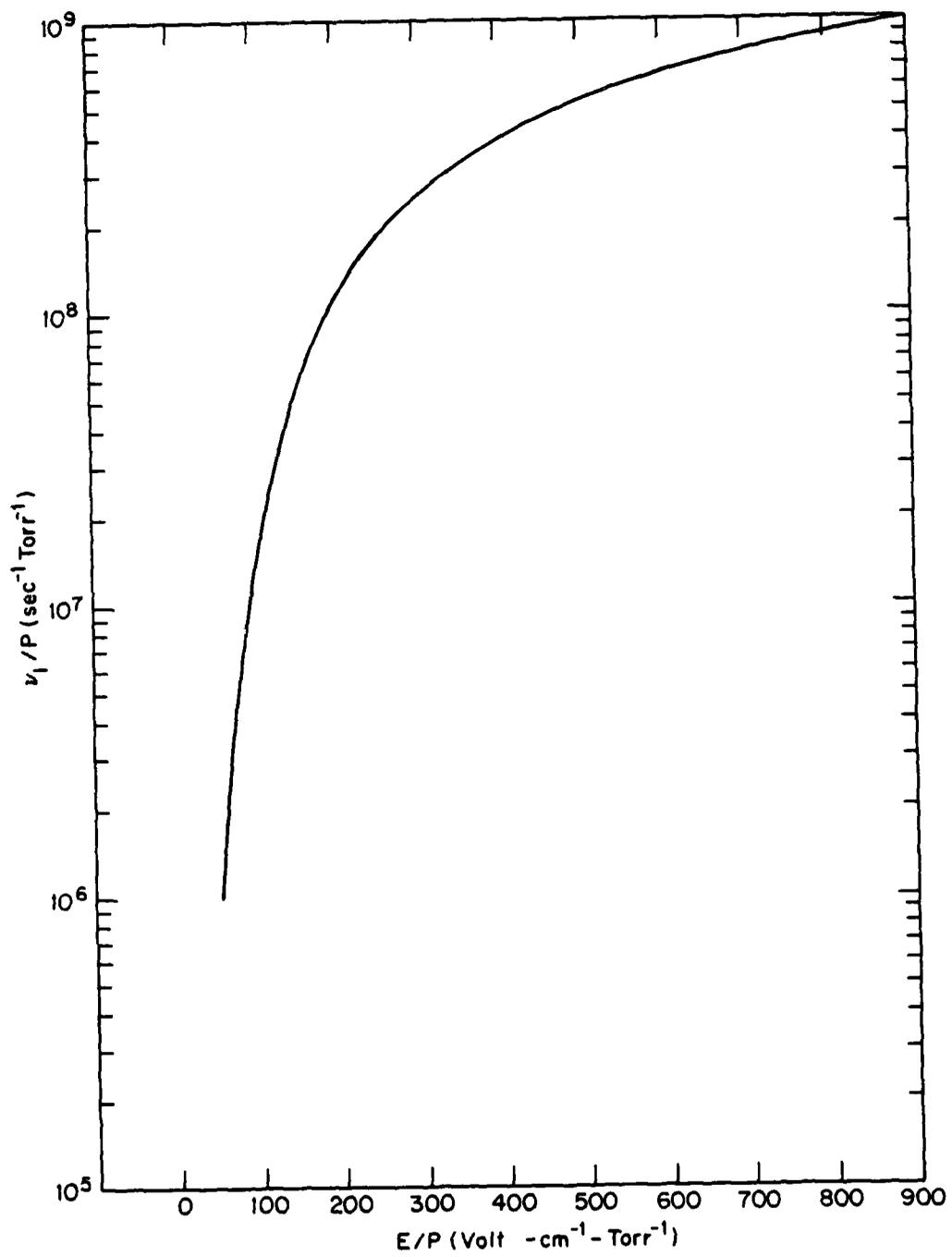


Fig. 3 - The ionization frequency in Air, $\frac{\nu_i}{P}$, as a function of E/P

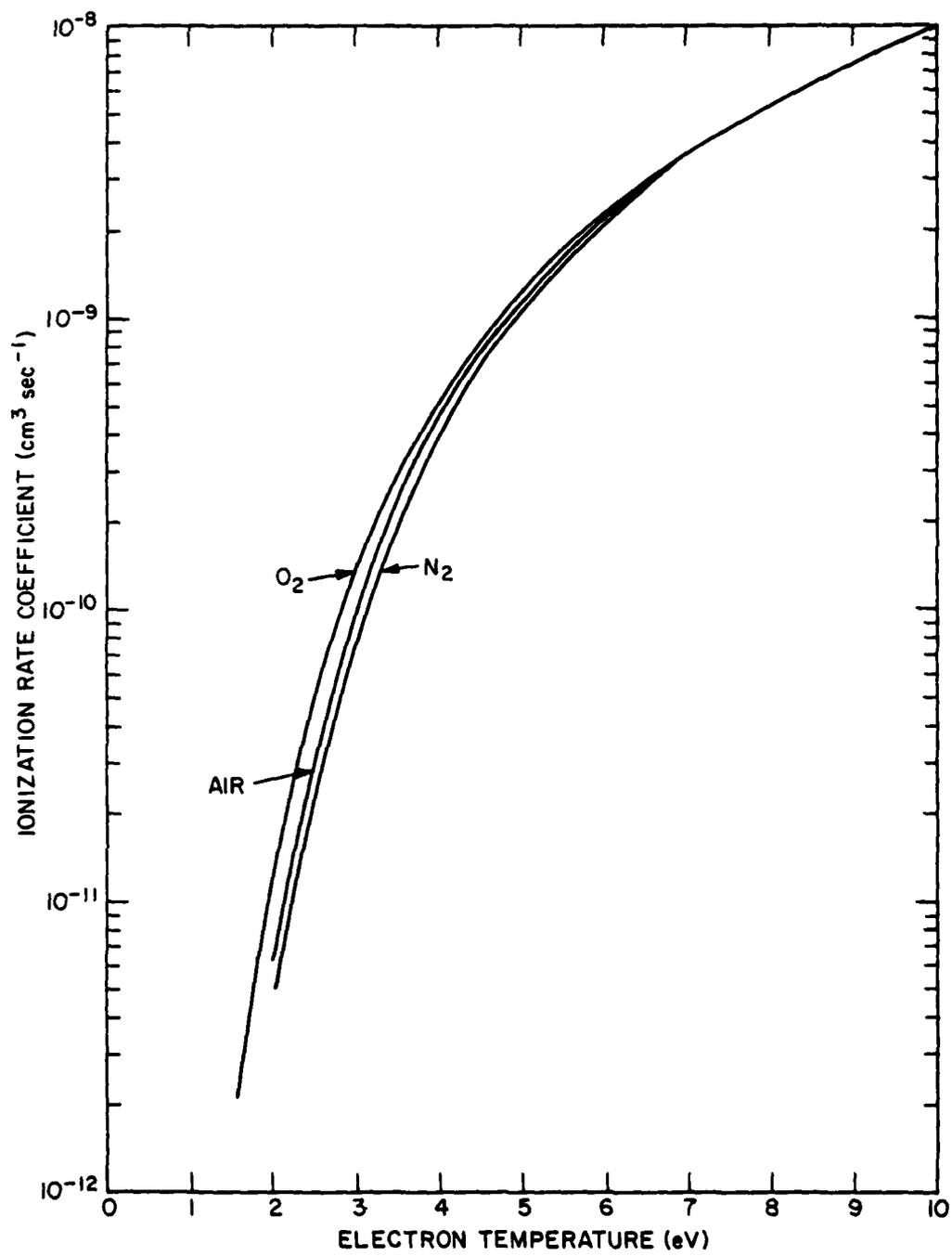


Fig. 4 - The Ionization Rate Coefficient of N_2 , O_2 and Air as a function the electron temperature

These expressions are valid for electron temperatures from 0.5 to 15 eV and deviate by less than 10% from the numerical values¹⁷. Using Equations (14) and (15) the ionization frequency in air can be expressed,

$$\frac{\nu_i}{P} = \frac{10^7}{\sqrt{T_e}} [14.093 + 27.366 T_e + 1.386 T_e^2] \text{Exp} \left(-\frac{15.58}{T_e} \right) + \frac{10^7}{\sqrt{T_e}} [1.430 + 2.470 T_e + 0.456 T_e^2] \text{Exp} \left(-\frac{12.06}{T_e} \right) \quad (16)$$

where T_e is in units of eV. The ionization frequency in air (Eq. 16) is shown in Figure 5 as a function of the electron temperature.

Lupan¹⁸ has developed an expression similar to Equation (16) based on a Maxwellian electron velocity distribution and assuming that the main ionization is from O_2 . His expression¹⁸ reads

$$\frac{\nu_i}{P} = 2.5 \times 10^7 [5.6 (\bar{E})^{1/2} + 0.6 (\bar{E})^{3/2}] \text{Exp} \left(-\frac{18.75}{\bar{E}} \right) \quad (17)$$

where $\bar{E} = 1.5 T_e$. Equation (17) predicts consistently higher values for the ionization frequency compared to Eq. (16). The discrepancy is a factor of 2 at $T_e = 2\text{eV}$ and 14% at $T_e = 10\text{eV}$, and is clearly due to the assumption by Lupan¹⁸ that ionization in air is mainly from O_2 . A glance at Figure 4 shows that the ionization rate coefficient in O_2 is always higher at lower T_e compared to that for air. At higher T_e the two converge to the same value, indicating that at higher temperatures the ionization rate coefficient for N_2 , O_2 and air are practically equal.

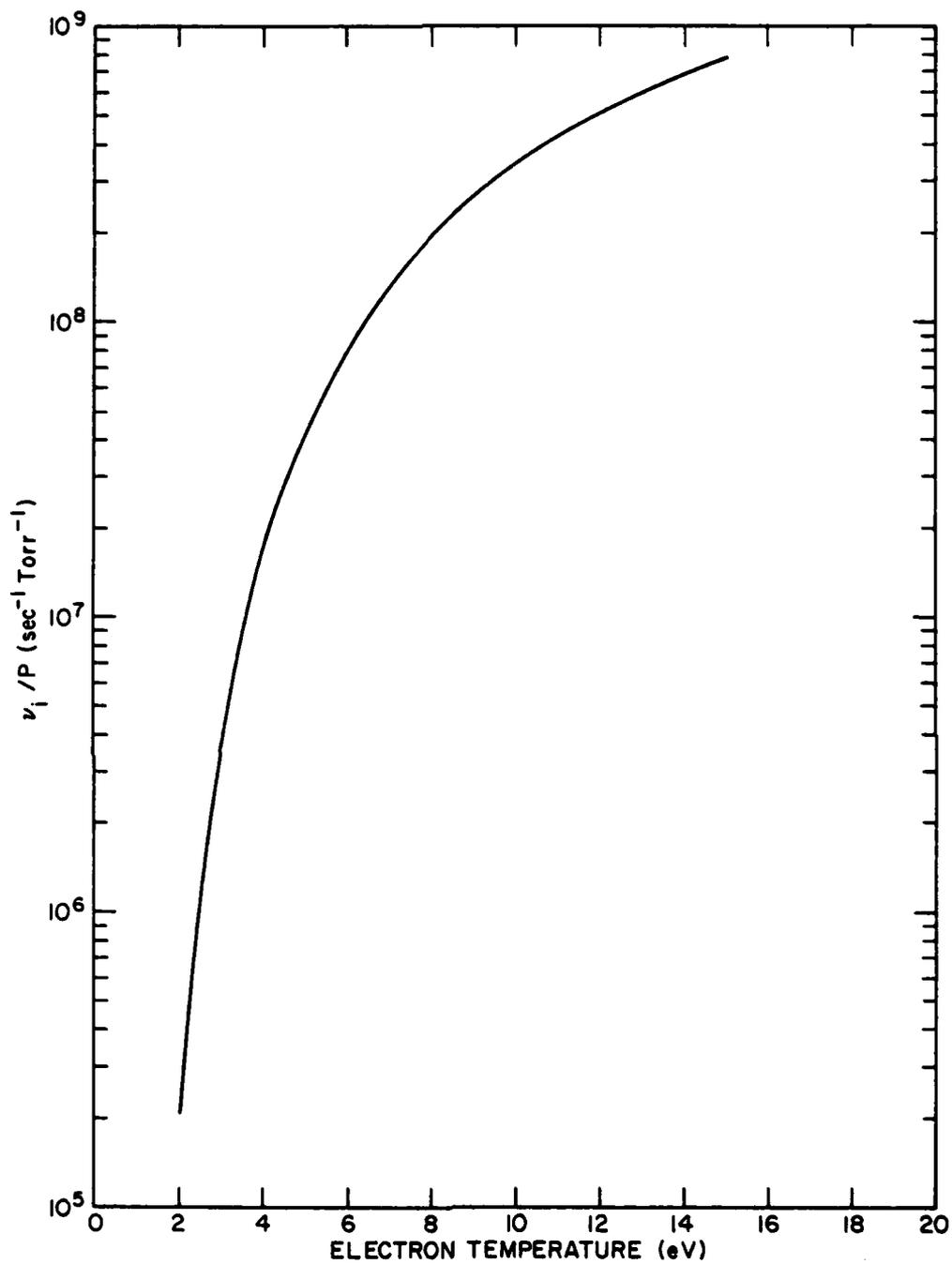


Fig. 5 - The ionization frequency in Air, $\frac{\nu_i}{P}$, as a function of the electron temperature

5. The Electron Temperature

The electron temperature, in an electric discharge, can be related to $\frac{E}{P}$. In general, however, one defines an electron characteristic energy^{1, 2}, ϵ_k , which for a Maxwellian electron distribution is equivalent to the average temperature, i.e., $\epsilon_k = T_e$.

In this work we would like to obtain the electron temperature in air as a function of E/P by utilizing the ionization frequency which was obtained, as a function of E/P and as a function of T_e (see Figures 3 and 5, respectively). From the results of Figures 3 and 5, one obtains a one to one correspondence between T_e and (E/P). This correspondence is expressed as

$$T_e = 0.1 \left(\frac{E}{P} \right)^{0.8} \quad (18)$$

where T_e is in eV. Eq. (18) gives a good correspondence to better than 15% for E/P from 60 to 500. At $\frac{E}{P} = 1000$, however, Equation (18) overestimates the temperature by 22%. Equation (18) is shown in Figure 6 and is compared with various results^{2,6,18,19}. There is generally a good agreement between Eq. (18) and the results of Reference 2 and 6 where the data is for N_2 and it is expected that the electron temperature is somewhat higher in N_2 than in air. Lupan's result¹⁸, valid for $T_e < 15\text{eV}$, is always higher than our calculation as given by Eq. (18). Therefore, the extension of Lupan's¹⁸ result to $\frac{E}{P} > 100$ will always overestimate the electron temperature.

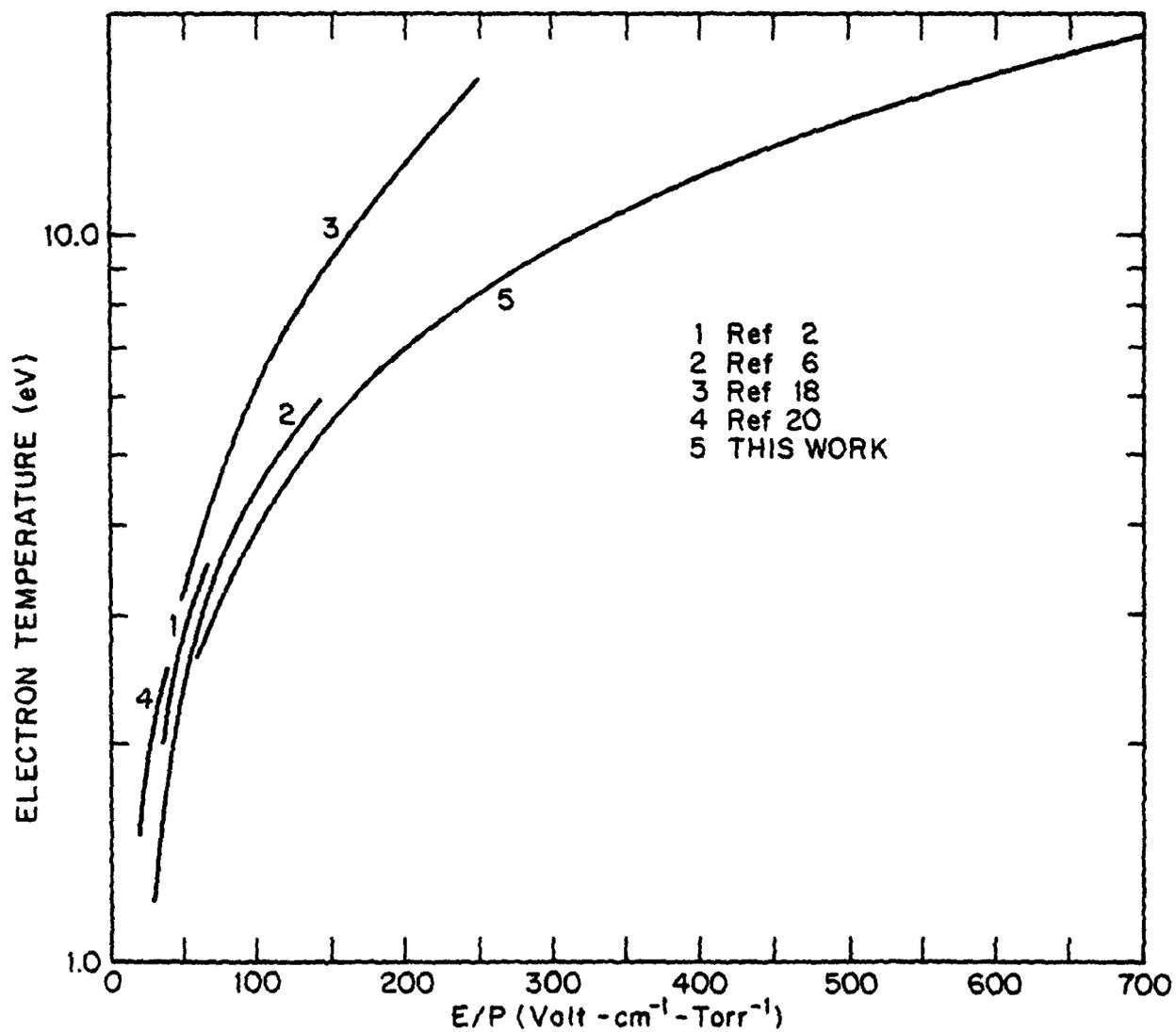


Fig. 6 - The electron temperature in air as a function of $\frac{E}{P}$

6. Avalanche Ionization in Air

To describe the ionization in air, a set of rate equations which gives the time histories of various ionic and air species is required. These rate equations must be solved simultaneously with an equation describing the electron energy or the electron temperature. However, for simplicity fewer rate equations can be utilized to generate a reasonable description for the avalanche generated ionization. In this section, we provide such a description with the appropriate parameters.

We consider the case of dry air, however, the ionization of air with impurities, e.g., H₂O will be discussed in a future report. The equations describing the avalanche ionization can be written as

$$\begin{aligned} \frac{3}{2} N_e \frac{dT_e}{dt} = & (\epsilon_s - \frac{3}{2} T_e) S + \gamma P^2 \frac{e^2 N_e}{m v_m} \left(\frac{E}{P} \right)^2 - N_e N_2 R(N_2) \\ & - N_e O_2 R(O_2) + N_e H_v \end{aligned} \quad (19)$$

$$\frac{dN_e}{dt} = S + N_e P \frac{v_1}{P} - \alpha_{ef} N_e^2 - \alpha_a N_e O_2 M - \alpha_{da} N_e O_2 \quad (20)$$

$$\frac{dN^-}{dt} = \alpha_a N_e O_2 M + \alpha_{da} N_e O_2 - \alpha_m N^-(N_e + \bar{N}) \quad (21)$$

$$\frac{dE_v}{dt} = N_e E_1 (1 - \text{Exp}(-E_1/T_v)) \sum_{v=1}^8 v X_v [1 - \text{Exp}(-\frac{v E_1 (T_v - T_e)}{T_v T_e})] \quad (22)$$

Here S is the volume production rate ($\text{cm}^{-3}\text{sec}^{-1}$) of electrons, due to any other source, ϵ_s is the average energy of these electrons. γ is a conversion factor, N_e is the plasma electron density, ν_m is the momentum transfer collision frequency (electron neutral plus electron ion), $R(N_2)$ is the rate of energy loss by the plasma electrons in N_2 and $R(O_2)$ is the corresponding rate in O_2 . α_{ef} is the effective recombination rate coefficient, α_a is the coefficient for electron attachment and α_{da} is the dissociative attachment rate coefficient. α_m is the coefficient for the mutual neutralization. N^- is the sum of the negative ions, and that the charge neutrality condition is assumed. E_v is the vibrational energy²² of N_2 , E_1 is the energy for the N_2 vibrational spacing (assumed a harmonic oscillator), T_v is the vibrational temperature, X_v is the excitation rate¹⁷ coefficient for the v th vibrational level and H_v is the vibrational heating rate of the electrons and corresponds to the sum of the negative terms in Eq. (22).

The rates of the energy loss by electrons in N_2 and O_2 as a function of the electron temperature are shown in Figures 7 and 8, respectively. These are obtained by using the relevant rate coefficients¹⁷ and the appropriate threshold energies²⁰. In these figures the energy loss to various processes are also indicated. These rates can be expressed as

$$R(N_2) = 3.87 \times 10^{-8} T_e \text{Exp}\left(-\frac{1.5}{T_e}\right) \quad , 0.2 \leq T_e \leq 1.0 \quad (23)$$

$$R(N_2) = 7.5 \times 10^{-9} [1 - 0.036T_e] + A \quad , 1 \leq T_e \leq 20 \quad (24)$$

where

$$A = 2.13 \times 10^{-7} \sqrt{T_e} [1 - 0.05 (T_e - 4)] \text{Exp} \left(-\frac{7.86}{T_e} \right) \quad (25)$$

and

$$R(O_2) = 1.0 \times 10^{-7} \sqrt{T_e} [1 + 0.05 (T_e - 4)] \text{Exp} \left(-\frac{7.86}{T_e} \right) \quad (26)$$

In addition to Equations (19-22), one must solve for the time variance of the electric field which enters into Equation (19). This can be accomplished by solving an appropriate electric circuit equation.

The effective recombination coefficient, α_{ef} , can be obtained, during the discharge, by appropriate steady state relations for the density of various ions. These relations must account for all source and depletion terms for each ion. For the case of the dry air with no air ion clusters, the effective recombination coefficient can be expressed as

$$\begin{aligned} N_e \alpha_{ef} = & \frac{D_1 Q(N_2^+)}{D_1 N_e + C_2 O_2 + \alpha_m N^-} + \frac{D_2 Q(O_2^+)}{D_2 N_e + \alpha_m N^-} \\ & + \frac{D_2 C_2 O_2 Q(N_2^+)}{(D_2 N_e + \alpha_m N^-) (D_1 N_e + \alpha_m N^- + C_2 O_2)} \\ & + \frac{D_2 C_1 O_2 Q(N^+)}{(D_2 N_e + \alpha_m N^-) (C_1 O_2 + \alpha_m N^-)} \end{aligned} \quad (27)$$

where $Q(i^+)$ is the volume production rate of the i^{th} ion due to the

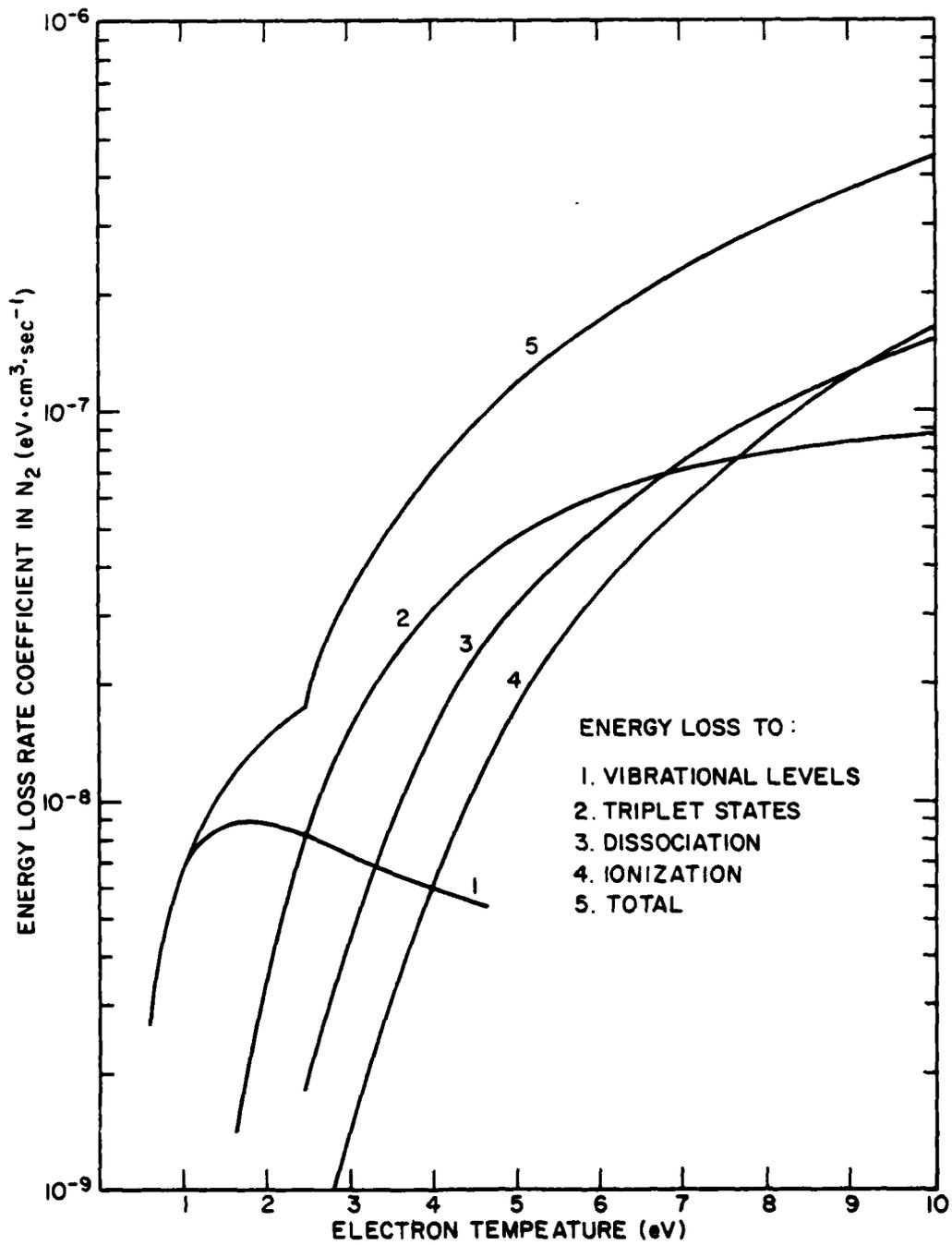


Fig. 7 - The Electron energy loss rate in N_2 as a function of T_e

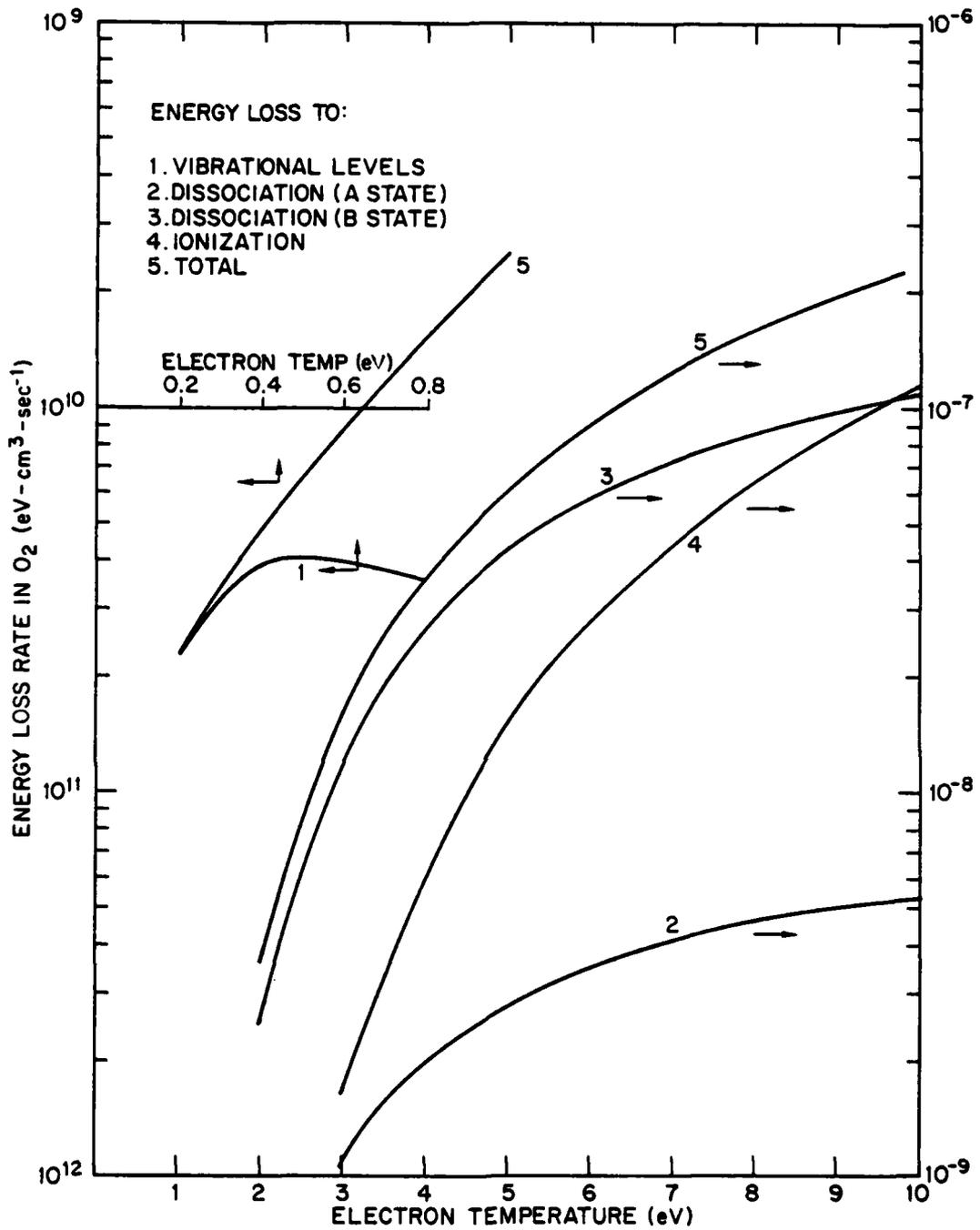


Fig. 8 - The electron energy loss rate in O₂ as a function of T_e

source term and the avalanche ionization. D_1 and D_2 are the dissociative recombination rate coefficients of N_2^+ and O_2^+ , respectively; and C_1 and C_2 are the charge exchange rate coefficients of N^+ and N_2^+ with O_2 , respectively. These coefficients can be found in Reference 21. However, if the steady state relations overestimate the positive ion densities especially at early times, one can use the following relation

$$\alpha_{ef} N_e = [K_1 D_1 + K_2 D_2 + \dots] [N_e + N^+] \quad (28)$$

where K_1 and K_2 indicate the fractions of the appropriate ions in the discharge.

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