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ABSTRACT

NRL has developed two computer codes to describe the ionization and deionization phenomena of the upper atmosphere. The detailed physics and the chemistry of these codes, called the Simple and the Master Codes, describe the disturbed *E* and *F* regions of the ionosphere. The Simple Code carries less species (atoms, molecules, and ions) than the Master Code, but both codes are used to calculate three temperatures—electron, N_2 vibrational, and heavy particle. Both codes agree with each other in electron density calculations to better than 20%.

PROBLEM STATUS

This is an interim report on a continuing problem.

AUTHORIZATION

NRL Problem H02-27
DNA Subtask HC 04001

Manuscript submitted March 16, 1973.

THE PHYSICS AND CHEMISTRY OF TWO NRL CODES FOR THE DISTURBED *E* AND *F* REGIONS

INTRODUCTION

This report discusses, in detail, the physics and chemistry of two NRL codes for the disturbed *E* and *F* regions of the ionosphere. These codes, named the Master Code and the Simple Code, were developed to calculate the electron density and the visible and infrared emissions in the disturbed regions.

The Master Code was put into a computer language, at one time or another, by Joan Pierre, A.D. Anderson, and Joan Lewis of NRL. As for the Simple Code, A.D. Anderson (CDC version) and T.R. Young (IBM version) are responsible for the computer language and the integration schemes. The version of the Simple Code by T. Young has been utilized in conjunction with MHD calculations for a disturbed atmosphere. In addition to its use for a disturbed atmosphere, it has also been used in the modeling (1) of the ionosphere where the ionization source is the radiation from the sun. A compact and complete line-by-line deposition of the sun's radiation and the appropriate cross sections for the Simple Code appear elsewhere (2).

The Master Code was first developed (3, 4) for the *F* region as a deionization code, and later evolved into a full deposition and late-time deionization code (5). The Simple Code, an offspring of the Master Code, was designed so that it could be incorporated into large-scale flow codes. In a deionization calculation, the Simple Code, with some adjustments for the initial conditions which are discussed later, gives electron densities within better than 20% of the Master Code (5).

BASIC RATE EQUATIONS FOR THE MASTER CODE

The following equations describe the time histories of the species included in the Master Code. Here N_e is the electron density, and the rest of the species have their usual spectroscopic meaning designating the atom, molecule, or their ions. Whenever the state of the species is undefined, its ground state is implied. For example, N is the ground state of nitrogen atom. The coefficients, on the other hand, are discussed in the next section.

$$\begin{aligned} \frac{dN_e}{dt} = & -N_e \{ D_1 N_2^+ + D_2 NO^+ + D_3 [O_2^+(x) + O_2^+(a^4\pi)] \} \\ & - N_e [\alpha_1 O^+ + \alpha_2 N^+ + \alpha_2 N^+(^1D)] + Q(e). \end{aligned} \quad (1)$$

$$\begin{aligned}
\frac{dN_2}{dt} = & C_1 N_2^+ O + C_2 N_2^+ O_2 + C_3 N_2^+ N + C_2 N_2^+ [O_2(a^1\Delta) + O_2(b^1\Sigma)] \\
& + C_{16} N NO + N_e N_2(A) Y_{12} + C_{16} N(^2D) NO \\
& + A_1 N_2(A) - C_5 O^+(^2p) N_2 + C_3 N_2^+ N(^2D) \\
& - Q(N_2) - C_5 O^+(^2D) N_2 - C_{15} O N_2 - N_e (X_{11} + X_{11a} + X_{12}) N_2 \\
& - K_{TV} O^+ N_2 - C_{15a} O(^1D) N_2 + C_{20} N_2(A) O. \tag{2}
\end{aligned}$$

$$\begin{aligned}
\frac{dN_2(A)}{dt} = & + C_4 N_2^+ NO + N_e N_2 (X_{11} + X_{11a} + X_{12}) \\
& - Q[N_2(A)] - A_1 N_2(A) - N_e N_2(A) Y_{12} - C_{20} N_2(A) O. \tag{3}
\end{aligned}$$

$$\begin{aligned}
\frac{dN_2^+}{dt} = & Q(N_2^+) + C_5 [O^+(^2D) + O^+(^2p)] N_2 \\
& - D_1 N_e N_2^+ - C_1 N_2^+ O - C_2 N_2^+ O_2 - C_3 N_2^+ [N + N(^2D)] - C_2 N_2^+ [O_2(a^1\Delta) + O_2(b^1\Sigma)] \\
& - C_4 N_2^+ NO - C_6 N_2^+ O. \tag{4}
\end{aligned}$$

$$\begin{aligned}
\frac{dN}{dt} = & D_1 N_e N_2^+ + C_6 N_2^+ O + C_7 N^+ [O + O(^1D)] - N_e N (X_{13} + X_{14}) \\
& + C_8 N^+ O_2 + \frac{1}{2} C_9 N^+ NO + C_{18} O NO + C_8 N^+ [O_2(a^1\Delta) + O_2(b^1\Sigma)] \\
& + Y_{13} N_e N(^2D) + Y_{14} N_e N(^2p) + K_{TV} O^+ N_2 + C_{18a} O(^1D) NO + C_7 N^+(^1D) O \\
& + \alpha_2 N_e N^+ + C_{15} O N_2 + C_8 N^+(^1D) O_2 \\
& - Q(N) - C_3 N_2^+ N + C_{21} N(^2D) N_2 + C_{23} N(^2D) NO \\
& - C_{10} N O_2^+ - C_{16} N NO - C_{17} N O_2 + C_{15a} O(^1D) N_2 \\
& - C_{17} N [O_2(a^1\Delta) + O_2(b^1\Sigma)]. \tag{5}
\end{aligned}$$

$$\begin{aligned}
\frac{dN(^2D)}{dt} = & X_{13} N_e N + Y_{15} N_e N(^2p) + D_1 N_e N_2^+ - C_{10} N(^2D) O_2^+ \\
& + D_2 N_e NO^+ + A_2 N(^2p) + \frac{2}{3} \alpha_2 N_e N^+(^1D) \\
& - Q(N^2D) - Y_{13} N_e N(^2D) - X_{15} N_e N(^2D) - C_{16} N(^2D) NO \\
& - C_{14} N(^2D) O_2 - C_3 N_2^+ N(^2D) + \frac{1}{2} C_9 N^+ NO + C_9 N^+(^1D) NO \tag{6}
\end{aligned}$$

$$\begin{aligned}
& -C_{14}N(^2D)[O_2(a^1\Delta) + O_2(b^1\Sigma)] + C_8N^+(^1D)[O_2(a^1\Delta) + O_2(b^1\Sigma)] \\
& -C_{21}N(^2D)N_2 - C_{22}N(^2D)NO.
\end{aligned} \tag{6}$$

(Continued)

$$\begin{aligned}
\frac{dN(^2p)}{dt} &= X_{14}N_eN + X_{15}N_eN(^2D) \\
& - Y_{14}N_eN(^2p) - Y_{15}N_eN(^2p) - A_2N(^2p) \\
& - Q(N^2p) + \frac{1}{3}\alpha_2N_eN^+(^1D).
\end{aligned} \tag{7}$$

$$\begin{aligned}
\frac{dN^+}{dt} &= Q(N^+) + C_3N_2^+N + Y_{16}N_eN^+(^1D) + Y_{17}N_eN^+(^1S) \\
& - C_{11}N^+O_2(a^1\Delta) + A_3N^+(^1D) - N_eN^+(X_{16} + X_{17}) - C_7N^+O(^1D) \\
& - C_7N^+O - C_9N^+NO - (C_8 + C_{11} + C_{12})N^+O_2 \\
& - C_{11}N^+O_2(b^1\Sigma) - \alpha_2N_eN^+ - C_8N^+[O_2(a^1\Delta) + O_2(b^1\Sigma)].
\end{aligned} \tag{8}$$

$$\begin{aligned}
\frac{dN^+(^1D)}{dt} &= Q[N^+(^1D)] + X_{16}N_eN^+ + Y_{18}N_eN^+(^1S) + C_3N_2^+N(^2D) \\
& + A_4N^+(^1S) - X_{18}N_eN^+(^1D) - Y_{16}N_eN^+(^1D) \\
& - A_3N^+(^1D) - C_8N^+(^1D)[O_2(a^1\Delta) + O_2(b^1\Sigma)] \\
& - C_7N^+(^1D)O - C_9N^+(^1D)NO - (C_8 + C_{11} + C_{12})N^+(^1D)O_2 \\
& - \alpha_2N_eN^+(^1D).
\end{aligned} \tag{9}$$

$$\begin{aligned}
\frac{dN^+(^1S)}{dt} &= Q[N^+(^1S)] + X_{17}N_eN^+ + X_{18}N_eN^+(^1D) \\
& - Y_{17}N_eN^+(^1S) - Y_{18}N_eN^+(^1S) \\
& - A_4N^+(^1S).
\end{aligned} \tag{10}$$

$$\begin{aligned}
\frac{dO}{dt} &= D_2N_eNO^+ + \beta_1D_3N_e[O_2^+ + O_2^+(a^4\pi)] \\
& + q_1O(^1D)N_2 + Y_{19}N_eO(^1D) - N_eO X_{19} \\
& + Y_{20}N_eO(^1S) + A_5O(^1D) + C_5O^+(^2D)N_2 - N_eO X_{20} \\
& + \alpha_1N_eO^+ + C_{13}O^+[O_2(a^1\Delta) + O_2(b^1\Sigma)] + C_5O^+(^2p)N_2
\end{aligned} \tag{11}$$

$$\begin{aligned}
& + C_{10}NO_2^+ + C_{11}[N^+ + N^+(^1D)]O_2 + C_{10}N(^2D)O_2^+ + C_{11}N^+[O_2(a^1\Delta) + O_2(b^1\Sigma)] \\
& + C_{13}O^+O_2 + C_5O^+(^2D)O_2 + C_{14}N(^2D)O_2 + C_5O^+(^2D)[O_2(a^1\Delta) + O_2(b^1\Sigma)] \\
& + C_{17}N[O_2(a^1\Delta) + O_2(b^1\Sigma)] + C_{16}NNO + \frac{1}{2}C_{16}N(^2D)NO + C_{17}NO_2 \\
& + \eta_1D(\lambda)O_2 - Q(O) - (C_1 + C_6)N_2^+O \\
& + q_2O(^1S)(O + O_2) - C_7N^+O - C_{15}ON_2 - C_{18}ONNO \\
& + C_5O^+(^2p)[O_2 + O_2a(^1D) + O_2(b^1\Sigma)] + C_{14}N(^2D)[O_2(a^1\Delta) + O_2(b^1\Sigma)] \\
& + C_7N^+(^1D)O + C_{13b}O^+NO - C_{20}N_2(A)O - 3C_{23}OOO.
\end{aligned} \tag{11}$$

(Continued)

$$\begin{aligned}
\frac{dO(^1D)}{dt} & = \beta_2D_3N_e[O_2^+ + O_2^+(a^4\pi)] + X_{19}N_eO - C_7N^+O(^1D) \\
& + Y_{21}N_eO(^1S) + A_6O(^1S) + \eta_2D(\lambda)O_2 - X_{21}N_eO(^1D) \\
& - q_1O(^1D)N_2 - Y_{19}N_eO(^1D) - A_5O(^1D) + \frac{1}{2}C_{16}N(^2D)NO \\
& - Q(O^1D) - C_{15a}O(^1D)N_2 - C_{18a}O(^1D)NO.
\end{aligned} \tag{12}$$

$$\begin{aligned}
\frac{dO(^1S)}{dt} & = X_{20}N_eO + X_{21}N_eO(^1D) + \beta_3D_3N_e[O_2^+ + O_2^+(a^4\pi)] \\
& - Y_{20}N_eO(^1S) - Y_{21}N_eO(^1S) - A_6O(^1S) - q_2O(^1S)(O + O_2) \\
& - Q(O^1S) + C_{20}N_2(A)O + C_{23}OOO.
\end{aligned} \tag{13}$$

$$\begin{aligned}
\frac{dO^+}{dt} & = Q(O^+) + Y_{22}N_eO^+(^2D) \\
& + Y_{23}N_eO^+(^2p) + C_1N_2^+O + C_7N^+(^1D)O \\
& + C_7N^+[O + O(^1D)] + C_{12}N^+O_2 + C_{12}N^+(^1D)O_2 \\
& - K_{TV}O^+N_2 - X_{22}N_eO^+ - X_{23}N_eO^+ \\
& - \alpha_1N_eO^+ - C_{13}O^+[O_2 + O_2a(^1D) + O_2b(^1\Sigma)] - C_{13b}O^+NO.
\end{aligned} \tag{14}$$

$$\begin{aligned}
\frac{dO^+(^2D)}{dt} & = Q(O^+^2D) + X_{22}N_eO^+ \\
& + Y_{24}N_eO^+(^2p) + A_7O^+(^2p) \\
& - X_{24}N_eO^+(^2D) - Y_{22}N_eO^+(^2D) \\
& - C_5O^+(^2D)[N_2 + O_2 + O_2(a^1\Delta) + O_2(b^1\Sigma)].
\end{aligned} \tag{15}$$

$$\begin{aligned}
\frac{dO^+(^2p)}{dt} = & Q[O^{+2}(p)] + X_{23}N_e O^+ + X_{24}N_e O^+(^2D) \\
& - Y_{23}N_e O^+(^2p) - Y_{24}N_e O^+(^2p) \\
& - A_7 O^+(^2p) - C_5 O^+(^2p)[N_2 + O_2 + O_2 a(^1\Delta) + O_2(b^1\Sigma)]. \quad (16)
\end{aligned}$$

$$\begin{aligned}
\frac{dNO^+}{dt} = & Q(NO^+) + K_{TV} O^+ N_2 + C_{11} N^+ [O_2 + O_2(a^1\Delta) + O_2(b^1\Sigma)] \\
& + C_4 N_2^+ NO + C_6 N_2^+ O + C_9 N^+ NO + C_{10} NO_2^+ + C_{19} O_2^+ NO \\
& - D_2 N_e NO^+ + C_{10} N(^2D) O_2^+ + C_9 N^+(^1D) NO \\
& + C_{11} N^+(^1D) O_2 + C_{13b} O^+ NO. \quad (17)
\end{aligned}$$

$$\begin{aligned}
\frac{dNO}{dt} = & C_{12} N^+ O_2 + C_{14} N(^2D) O_2 - C_9 N^+(^1D) NO + C_{12} N^+(^1D) O_2 \\
& + C_{15} O N_2 + C_{17} N O_2 + C_{15a} O(^1D) N_2 + C_{14} N(^2D) [O_2(a^1\Delta) + O_2(b^1\Sigma)] \\
& - Q(NO) - C_4 N_2^+ NO - C_9 N^+ NO - C_{16} N(^2D) NO \\
& - C_{16} N NO - C_{18} O NO - C_{19} O_2^+ NO - C_{18a} O(^1D) NO \\
& + C_{17} N [O_2(a^1\Delta)] + O_2(b^1\Sigma) - C_{13b} O^+ NO. \quad (18)
\end{aligned}$$

$$\begin{aligned}
\frac{dO_2}{dt} = & Y_{25} N_e O_2(a^1\Delta) + Y_{26} N_e O_2(b^1\Sigma) \\
& + A_8 O_2(b^1\Sigma) + A_9 O_2(a^1\Delta) + C_{18} O NO + C_{18} O(^1D) NO \\
& + C_{19} O_2^+ NO - (X_{25} + X_{26}) N_e O_2 - C_8 N^+(^1D) O_2 \\
& - Q(O_2) - D(\lambda) O_2 - C_2 N_2^+ O_2 - C_5 [O^+(^2D) + O^+(^2p)] O_2 \\
& - C_8 N^+ O_2 - C_{11} N^+ O_2 - C_{12} N^+ O_2 - C_{13} O^+ O_2 \\
& - C_{14} N(^2D) O_2 - C_{17} N O_2 - C_{12} N^+(^1D) O_2 \\
& - C_{11} N^+(^1D) O_2 + C_{23} OOO + C_{24} O_2(a^1\Delta) O_2 \\
& + C_{25} O_2(b^1\Sigma) N_2 + C_{26} O_2(a^1\Delta) O. \quad (19)
\end{aligned}$$

$$\begin{aligned}
\frac{dO_2(a^1\Delta)}{dt} = & X_{25} N_e O_2 - C_2 N_2^+ O_2(a^1\Delta) - C_8 N^+(^1D) O_2(a^1\Delta) \\
& - A_9 O_2(a^1\Delta) - Y_{25} N_e O_2(a^1\Delta) - C_{11} N^+ O_2(a^1\Delta) \\
& - C_{13} O^+ O_2(a^1\Delta) - Q[O_2(a^1\Delta)] - C_5 [O^+(^2D) + O^+(^2p)] O_2(a^1\Delta) \quad (20)
\end{aligned}$$

$$\begin{aligned}
& -D(\lambda) O_2(a^1\Delta) - C_8 N^+ O_2(a^1\Delta) - C_{14} N(^2D) O_2(a^1\Delta) - C_{17} N O_2(a^1\Delta) \\
& - C_{24} O_2(a^1\Delta) O_2 - C_{26} O_2(a^1\Delta) O. \tag{20}
\end{aligned}$$

(Continued)

$$\begin{aligned}
\frac{dO_2(b^1\Sigma)}{dt} = & X_{26} N_e O_2 - C_2 N_2^+ O_2(b^1\Sigma) - C_{11} N^+ O_2(b^1\Sigma) \\
& - Y_{26} N_e O_2(b^1\Sigma) - C_{13} O^+ O_2(b^1\Sigma) - C_8 N^+(^1D) O_2(b^1\Sigma) \\
& - A_8 O_2(b^1\Sigma) - Q[O_2(b^1\Sigma)] - C_5 O^+(^2D) O_2(b^1\Sigma) \\
& - D(\lambda) O_2(b^1\Sigma) - C_8 N^+ O_2(b^1\Sigma) - C_5 O^+(^2p) O_2(b^1\Sigma) \\
& - C_{14} N(^2D) O_2(b^1\Sigma) - C_{17} N O_2(b^1\Sigma) - C_{25} O_2(b^1\Sigma) N_2. \tag{21}
\end{aligned}$$

$$\begin{aligned}
\frac{dO_2^+}{dt} = & C_2 N_2^+ O_2 + C_8 N^+ [O_2 + O_2(a^1\Delta) + O_2(b^1\Sigma)] + Q(O_2^+) + C_8 N^+(^1D) O_2 \\
& + C_{13} O^+ [O_2 + O_2(a^1\Delta) + O_2(b^1\Sigma)] + \frac{1}{2} C_5 O^+(^2D) [O_2 + 2O_2(a^1\Delta) + 2O_2(b^1\Sigma)] \\
& - D_3 N_e O_2^+ - C_{10} N O_2^+ - C_{19} O_2^+ NO + C_2 N_2^+ [O_2(a^1\Delta) + O_2(b^1\Sigma)] \\
& - C_{10} N(^2D) O_2^+ + C_8 N^+(^1D) [O_2(a^1\Delta) + O_2(b^1\Sigma)]. \tag{22}
\end{aligned}$$

$$\begin{aligned}
\frac{dO_2^+(a)}{dt} = & Q[O_2^+(a)] - D_3 N_e O_2^+(a) + \frac{1}{2} C_5 O^+(^2D) O_2 \\
& + C_5 O^+(^2p) [O_2 + O_2(a^1\Delta) + O_2(b^1\Sigma)]. \tag{23}
\end{aligned}$$

REACTIONS AND RATE COEFFICIENTS

In this section the rate coefficients and other symbols which appeared in the previous section are identified and discussed.

Dissociative Recombination Rate Coefficients

The quantities D_1 , D_2 , and D_3 are the dissociative recombination rate coefficients of N_2^+ , NO^+ , and O_2^+ , respectively. These coefficients depend on the electron temperature (6), as well as on the vibrational temperature (7, 8) of the molecular ion.

The temperature dependence of these coefficients according to O'Malley (7) is

$$D \propto T_e^{-1/2} (1 - e^{-h\nu/kT_v})$$

which has, for small and large T_v , a $T_e^{-1/2}$ and a $T_e^{-1/2} T_v^{-1}$ dependence, respectively.

These temperature dependencies are borne out experimentally for Ar_2^+ ; Mehr and Biondi (9) ($T_v = 300K$) and shock tube experiments (7) ($T_v = T_e$) show $T_e^{-0.67}$ and $T_e^{-3/2}$ dependences, respectively (see Fig. 1).

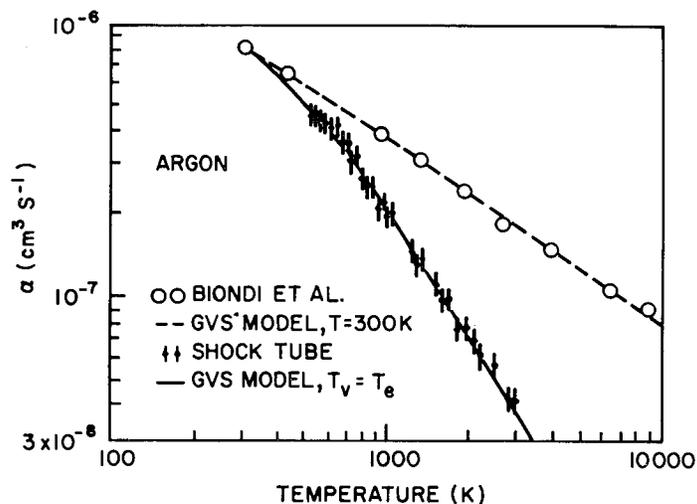


Fig. 1—The T_e dependence of the experimental recombination rate for Ar_2^+ for (a) $T_v = 300K$ (Mehr and Biondi, Ref. 9) and (b) $T_v = T_e$ (shock tube experiments, Ref. 7).

The tabulation below shows expressions fitted to experimental data for D_1 , D_2 , and D_3 . The expression for D_2 , perhaps, is more realistic since all temperatures were varied over a large range (6, 10) of interest. For D_1 , D_2 , and D_3 the fits are basically made to data from Biondi (6).

$$D_1 = 4.33 \times 10^{-8} \left(\frac{1}{T_e} \right)^{0.39}$$

$$D_2 = 6.23 \times 10^{-9} \left(\frac{1}{T_e} \right)^{1.2}$$

$$D_3 = \begin{cases} 1.51 \times 10^{-8} \left(\frac{1}{T_e} \right)^{0.7}, & T_e \leq 0.1 \text{ eV} \\ 2.1 \times 10^{-8} \left(\frac{1}{T_e} \right)^{0.5}, & T_e > 0.1 \text{ eV}. \end{cases}$$

The states of the products of the dissociative recombinations are of considerable importance both for deionization and radiation emission calculations. A simple deionization calculation shows the effects of these products, as shown in Fig. 2. However, the products of the dissociative recombinations are not really well known, except for N_2^+ where a recent ab initio calculation by Michels et al. (11) indicates that the products are 50% $N(^2D)$ and 50% $N(^4S)$. For O_2^+ , on the other hand, the often-quoted values of Zipf (12) are $\beta_1 = 1.0$, $\beta_2 = 0.9$, and $\beta_3 = 0.1$, which correspond to the productions of $O(^3p)$, $O(^1D)$, and $O(^1S)$, respectively. These results, however, have yet to be published

as a paper. As for NO^+ , no data is available; the products may be 100% $N(^2D)$ and 100% $O(^3p)$.

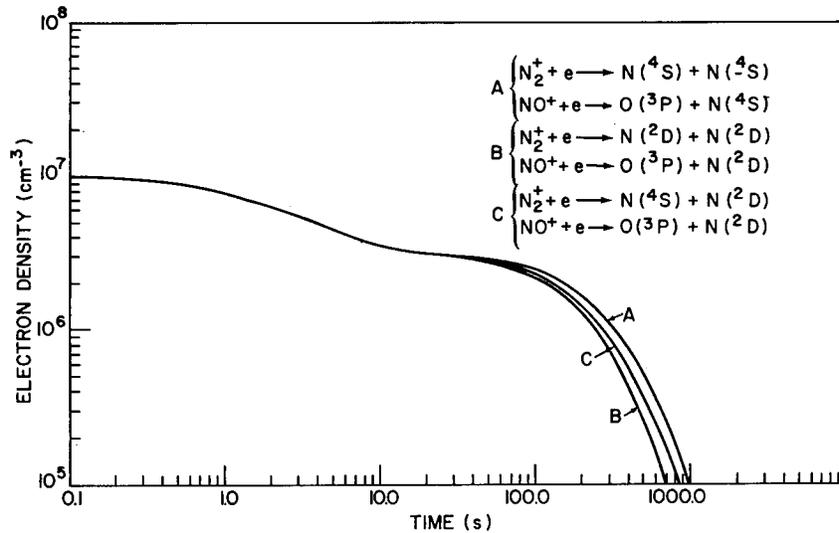


Fig. 2—Deionization calculation showing the effects of recombination products on the electron density.

Electron Impact Excitation and Deexcitation Rate Coefficients

In the basic rate equations developed for the Master Code, the X_{ij} 's are electron impact excitation rate coefficients, and the Y_{ij} 's are the corresponding deexcitation rate coefficients. These coefficients are identified in Table 1 below with the physical process. The reference for the cross section of the given process is also given. These cross sections are utilized to obtain (13) the appropriate rate coefficients. In the absence of cross sections, the reference indicates the source for the collision strength.

Table 2 gives electron impact excitation cross sections for low-lying metastable states of O , N , O_2 , and the triplet states of N_2 .

Table 3, on the other hand, gives expression for the excitation cross sections of the low-lying metastable states of O^+ and N^+ where threshold collision strength values are utilized.

Charge Exchange, Ion/Molecule Rearrangement, Neutral Particle Reactions, and Quenching Reactions

Table 4 summarizes some of the important reactions and their rate coefficients. Among these reactions are: Charge exchange, ion-molecule rearrangement, neutral particle reactions, and quenching reactions.

Table 1
 Electron Impact Excitation Rate (X_{ij}) and Deexcitation Rate (Y_{ij})
 Coefficients Used in the Basic Rate Equations for the Master Code

Rate Coefficient	Process	Ref.*
$X_{11} + X_{11a}$	$e + N_2 \rightarrow N_2(C^3\pi) + N_2(B^3\pi) + e$	14
X_{12}	$e + N_2 \rightarrow N_2(A^3\Sigma) + e$	14
Y_{12}	←	
X_{13}	$e + N \rightarrow N(^2D) + e$	15
Y_{13}	←	
X_{14}	$e + N \rightarrow N(^2p) + e$	15
Y_{14}	←	
X_{15}	$e + N(^2D) \rightarrow N(^2p) + e$	15
Y_{15}	←	
X_{16}	$e + N^+ \rightarrow N^+(^1D) + e$	17
Y_{16}	←	
X_{17}	$e + N^+ \rightarrow N^+(^1S) + e$	17
Y_{17}	←	
X_{18}	$e + N^+(^1D) \rightarrow N^+(^1S) + e$	17
Y_{18}	←	
X_{19}	$e + O \rightarrow O(^1D) + e$	15
Y_{19}	←	
X_{20}	$e + O \rightarrow O(^1S) + e$	15
Y_{20}	←	
X_{21}	$e + O(^1D) \rightarrow O(^1S) + e$	15
Y_{21}	←	
X_{22}	$e + O^+ \rightarrow O^+(^2D) + e$	18
Y_{22}	←	

Table 1—(Continued)

Rate Coefficient	Process	Ref.*
X_{23}	$e + O^+ \rightarrow O^+(^2p) + e$	18
Y_{23}	←	
X_{24}	$e + O^+(^2D) \rightarrow O^+(^2p) + e$	18
Y_{24}	←	
X_{25}	$e + O_2 \rightarrow O_2(a^1\Delta) + e$	16
Y_{25}	←	
X_{26}	$e + O_2 \rightarrow O_2(b^1\Sigma) + e$	16
Y_{26}	←	

*Refers to references at end of report.

Other Reactions

The quantities q_1 and q_2 are quenching rate coefficients of $O(^1D)$ by N_2 , and of $O(^1S)$ by O and O_2 , respectively. The corresponding values are 5×10^{-11} cm³/sec (28) and $\sim 10^{-13}$ cm³/sec (20), respectively. α_1 and α_2 are collisional radiative recombination rates for O^+ and N^+ , respectively.

A rough estimate (20) for these recombination rates is

$$\alpha_1 = \alpha_2 = 10^{-19} \left(\frac{0.025}{T_e} \right)^{4.5} N_e \text{ for } T_e < 0.2 \text{ eV.}$$

The radiative recombination, on the other hand, is

$$5.2 \times 10^{-14} \sqrt{\frac{14}{T_e}} \left(0.43 + \frac{1}{2} \log \frac{14}{T_e} \right),$$

where hydrogenic rates (29) are utilized.

The radiative lifetimes of the metastable states are given in Table 5.

Finally, the Q terms appear as either $Q(A^+)$ or $Q(A)$. $Q(A^+)$ implies the ion source due to photoionization and partial electron impact ionization of species A. On the other hand, $Q(A)$ implies the depletion of species A by the above processes.

IMPORTANT REACTIONS

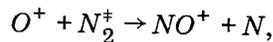
In this section certain important reactions presented in the earlier section titled Basic Rate Equations for the Master Code are pointed out.

Deposition Phase

When the *E* and the *F* regions of the ionosphere are irradiated by a disturbing ionizing radiation, then one must know the absorption and the ionization cross sections of the constituents of the two regions. Furthermore, in order to calculate the electron temperature and the prompt radiation from the disturbed regions, one must also know the partial photoionization cross sections of the species. For example, a 20-eV photon would ionize N_2 with N_2^+ being in $X^2\Sigma$, $A^2\pi$ or $B^2\Sigma$ states. The last two ionic states radiate the well-known 3914A line and the Mienel bands, respectively. For *O*, on the other hand, 4S , 2D , and 2p states are created, resulting in two metastable states of O^+ . The metastable $O^+(^2D)$ plays an important role in the deionization process where it charge exchanges resonantly with N_2 and O_2 , thus creating N_2^+ and O_2^+ . As a result, an atomic ion is converted into a molecular ion, which is removed faster by dissociative recombination.

Deionization Phase

The most important deionization processes are, of course, the dissociative recombinations of N_2^+ , O_2^+ , and NO^+ . These processes are prompt, especially for O_2^+ and N_2^+ which are created directly by the photoionization process. On the other hand, NO^+ is formed via another important process,



where the N_2 is vibrationally excited. Thus, the vibrational temperature of N_2 must be calculated since, in a highly disturbed atmosphere with $N_e \geq 10^6$, the vibrational excitation of N_2 is due to electron excitation. The metastable states must also be known since these metastable states act as a heating source for the electron via superelastic collisions which, in turn, would keep up the vibrational temperature of N_2 .

The ion/molecule charge exchanges are the next important processes since they convert an atomic ion into a molecular ion. Among these, $O^+(^2D)$, perhaps, plays an important role since it resonantly charge exchanges with N_2 (31) and O_2 (21). This ion/molecule reaction may result (32) in two new laser systems, one in the infrared and the other in the visible.

For electron density calculations, one could eliminate many of the metastable states discussed in the earlier section on Basic Rate Equations for the Master Code, thus simplifying and reducing the number of rate equations (see next section). However, if one is interested in radiation emission calculations, the time histories of the metastable states, especially those aeronomically important species, must be calculated.

Table 2
 Electron Impact Excitation Cross Sections for Low-Lying Metastable
 States of O , N , O_2 , and the Triplet States of N_2

TE	$\Omega(3p-1s)$	$\Omega(10-1s)$	$\Omega(3p-3s)$	$\Omega(4s-2d)$	$N(4s-2p)$	$N(20-2p)$	$N(4s-4p)$	$N(10mz)$
0.1	1.73E-18	1.79E-29	6.19E-49	1.10E-67	3.44E-19	3.80E-25	2.57E-14	2.37E-50
0.2	5.58E-14	1.96E-19	8.17E-29	3.14E-38	6.29E-14	3.37E-17	1.18E-11	2.63E-29
0.3	2.01E-12	7.13E-15	4.60E-22	3.09E-24	3.92E-12	1.67E-14	9.39E-11	3.01E-22
0.4	1.28E-11	6.04E-14	1.15E-18	1.71E-23	3.19E-11	3.90E-13	2.67E-10	1.07E-18
0.5	6.00E-11	2.55E-13	1.30E-16	1.59E-20	1.13E-10	2.63E-12	5.04E-10	1.50E-16
0.6	8.66E-11	7.25E-13	3.53E-11	1.46E-18	2.64E-10	9.46E-12	7.79E-10	4.12E-15
0.7	1.52E-10	1.60E-12	9.40E-11	3.81E-17	4.84E-10	2.37E-11	1.05E-09	4.48E-14
0.8	3.24E-10	2.99E-12	1.30E-10	4.43E-16	7.61E-10	1.33E-09	2.71E-13	2.88E-17
0.9	4.24E-10	4.93E-12	1.60E-10	3.01E-15	1.08E-09	8.10E-11	1.60E-09	1.11E-12
1.0	5.30E-10	7.48E-12	2.09E-10	1.40E-14	1.43E-09	1.29E-10	1.85E-09	3.48E-12
1.1	6.38E-10	1.05E-11	4.77E-12	4.95E-14	1.73E-09	1.77E-10	2.09E-09	8.89E-12
1.2	7.47E-10	1.43E-11	2.49E-10	1.49E-13	2.16E-09	2.37E-10	2.32E-09	1.95E-11
1.3	8.56E-10	1.85E-11	2.90E-10	3.50E-13	2.53E-09	3.04E-10	2.53E-09	3.83E-11
1.4	9.63E-10	2.32E-11	3.68E-10	7.58E-13	2.89E-09	3.75E-10	2.73E-09	6.83E-11
1.5	1.07E-09	2.82E-11	4.05E-10	1.49E-12	3.24E-09	4.50E-10	3.09E-09	1.14E-10
1.6	1.17E-09	3.37E-11	4.41E-10	2.69E-12	3.58E-09	5.28E-10	3.40E-09	1.78E-10
1.7	1.27E-09	3.94E-11	4.76E-10	4.54E-12	3.91E-09	6.07E-10	3.25E-09	2.64E-10
1.8	1.36E-09	4.53E-11	5.09E-10	6.27E-11	4.23E-09	6.87E-10	3.40E-09	3.77E-10
1.9	1.46E-09	5.15E-11	5.41E-10	8.25E-11	4.53E-09	7.68E-10	3.54E-09	4.18E-10
2.0	1.54E-09	5.78E-11	5.72E-10	1.11E-11	4.73E-09	8.47E-10	3.67E-09	4.62E-10
2.1	1.63E-09	6.42E-11	6.01E-10	1.62E-11	4.82E-09	9.27E-10	3.79E-09	5.01E-10
2.2	1.71E-09	7.07E-11	6.30E-10	2.29E-11	5.09E-09	1.01E-09	3.91E-09	5.43E-10
2.3	1.79E-09	7.72E-11	6.57E-10	3.14E-11	5.35E-09	1.08E-09	4.01E-09	5.83E-10
2.4	1.87E-09	8.37E-11	6.82E-10	4.20E-11	5.59E-09	1.08E-09	4.11E-09	6.22E-10
2.5	1.94E-09	9.02E-11	7.07E-10	5.49E-11	5.83E-09	1.16E-09	4.21E-09	6.64E-10
2.6	2.01E-09	9.67E-11	7.31E-10	7.03E-11	6.05E-09	1.23E-09	4.29E-09	7.05E-10
2.7	2.07E-09	1.03E-10	7.53E-10	8.44E-11	6.25E-09	1.30E-09	4.38E-09	7.46E-10
2.8	2.13E-09	1.10E-10	7.75E-10	1.09E-10	6.46E-09	1.44E-09	4.45E-09	7.87E-10
2.9	2.20E-09	1.16E-10	7.96E-10	1.34E-10	6.65E-09	1.50E-09	4.53E-09	8.28E-10
3.0	2.25E-09	1.22E-10	8.16E-10	1.61E-10	6.83E-09	1.57E-09	4.60E-09	8.69E-10
3.1	2.31E-09	1.28E-10	8.35E-10	1.92E-10	7.00E-09	1.63E-09	4.66E-09	9.09E-10
3.2	2.36E-09	1.34E-10	8.53E-10	2.26E-10	7.16E-09	1.69E-09	4.72E-09	9.49E-10
3.3	2.41E-09	1.40E-10	8.71E-10	2.64E-10	7.31E-09	1.75E-09	4.78E-09	9.89E-10
3.4	2.46E-09	1.45E-10	8.88E-10	3.05E-10	7.45E-09	1.80E-09	4.83E-09	1.02E-09
3.5	2.51E-09	1.51E-10	9.04E-10	3.51E-10	7.59E-09	1.86E-09	4.88E-09	1.06E-09
3.6	2.55E-09	1.56E-10	9.20E-10	4.00E-10	7.72E-09	1.88E-09	4.88E-09	1.10E-09
3.7	2.60E-09	1.63E-10	9.35E-10	4.53E-10	7.84E-09	1.91E-09	4.93E-09	1.14E-09
3.8	2.64E-09	1.69E-10	9.49E-10	5.09E-10	7.96E-09	1.96E-09	4.97E-09	1.18E-09
3.9	2.68E-09	1.74E-10	9.63E-10	5.70E-10	8.07E-09	1.96E-09	5.01E-09	1.22E-09
4.0	2.71E-09	1.79E-10	9.76E-10	6.34E-10	8.18E-09	2.01E-09	5.05E-09	1.26E-09
4.1	2.75E-09	1.84E-10	9.89E-10	7.03E-10	8.29E-09	2.10E-09	5.09E-09	1.30E-09
4.2	2.78E-09	1.89E-10	1.00E-09	7.75E-10	8.37E-09	2.14E-09	5.12E-09	1.34E-09
4.3	2.82E-09	1.94E-10	1.01E-09	8.46E-10	8.46E-09	2.18E-09	5.15E-09	1.38E-09
4.4	2.85E-09	1.99E-10	1.03E-09	9.10E-10	8.55E-09	2.22E-09	5.18E-09	1.42E-09
4.5	2.88E-09	2.04E-10	1.04E-09	9.70E-10	8.63E-09	2.26E-09	5.21E-09	1.46E-09
4.6	2.91E-09	2.09E-10	1.05E-09	1.01E-09	8.71E-09	2.30E-09	5.24E-09	1.50E-09
4.7	2.94E-09	2.13E-10	1.06E-09	1.06E-09	8.79E-09	2.33E-09	5.26E-09	1.54E-09
4.8	2.96E-09	2.17E-10	1.07E-09	1.11E-09	8.87E-09	2.37E-09	5.29E-09	1.58E-09
4.9	2.99E-09	2.21E-10	1.08E-09	1.16E-09	8.95E-09	2.40E-09	5.31E-09	1.62E-09
5.0	3.02E-09	2.25E-10	1.09E-09	1.21E-09	9.04E-09	2.43E-09	5.33E-09	1.66E-09

Table 2--(Cont.)

TF	A3 SIGMA	A3 PI	C3 PI	D3 SIGMA	E3 SIGMA	N2 IONIZ	N2+IX-B)	O2 A DEL	O2 B SIG	O2 IONIZ
0.1	7.49E-38	3.90E-41	2.43E-57	5.09E-65	1.19E-60	7.79E-78	0.0	3.42E-14	1.27E-17	1.37E-15
0.2	5.29E-23	4.19E-25	9.45E-33	3.50E-37	1.43E-34	1.92E-43	6.94E-50	1.81E-12	2.76E-14	1.99E-12
0.3	5.23E-13	1.02E-19	1.59E-24	7.10E-28	7.55E-26	6.14E-37	2.16E-36	8.20E-12	4.15E-13	2.62E-11
0.4	1.73E-15	5.27E-17	2.11E-20	3.24E-23	1.76E-21	3.65E-26	1.18E-29	1.94E-11	1.74E-12	1.04E-10
0.5	5.80E-14	2.30E-15	6.31E-18	2.04E-19	7.35E-19	1.09E-22	1.29E-25	3.45E-11	4.31E-12	2.51E-10
0.6	6.12E-13	2.92E-14	2.92E-16	1.49E-18	4.09E-17	2.32E-20	6.30E-23	5.31E-11	8.10E-12	4.69E-10
0.7	3.33E-12	1.81E-13	4.26E-15	3.21E-17	7.19E-16	1.09E-19	5.23E-21	7.46E-11	1.30E-11	7.56E-10
0.8	1.19E-11	7.21E-13	3.26E-14	3.20E-16	6.13E-15	1.96E-17	1.44E-19	9.85E-11	1.86E-11	1.10E-09
0.9	3.23E-11	2.13E-12	1.58E-13	1.91E-15	3.24E-14	1.83E-16	1.89E-18	1.24E-10	2.50E-11	1.51E-09
1.0	7.18E-11	5.09E-12	5.60E-13	7.98E-15	1.22E-13	1.15E-15	1.49E-17	1.52E-10	3.17E-11	1.96E-09
1.1	1.38E-10	1.04E-11	1.57E-12	2.57E-14	3.60E-13	5.13E-15	8.04E-17	1.80E-10	3.88E-11	2.46E-09
1.2	2.39E-10	1.91E-11	3.71E-12	6.78E-14	8.86E-13	1.79E-14	3.28E-16	2.09E-10	4.60E-11	2.99E-09
1.3	3.79E-10	3.19E-11	7.67E-12	1.54E-13	1.80E-12	5.17E-14	1.08E-15	2.39E-10	6.32E-11	3.56E-09
1.4	5.63E-10	4.96E-11	1.43E-11	3.12E-13	3.61E-12	1.29E-13	3.01E-15	2.68E-10	5.03E-11	4.15E-09
1.5	7.94E-10	7.30E-11	2.44E-11	5.72E-13	6.31E-12	2.86E-13	7.30E-15	3.98E-10	6.76E-11	4.77E-09
1.6	1.07E-09	1.03E-10	3.89E-11	9.74E-13	1.03E-11	5.75E-13	1.59E-14	3.27E-10	7.46E-11	5.40E-09
1.7	1.39E-09	1.39E-10	5.88E-11	1.55E-12	1.57E-11	1.07E-12	3.16E-14	3.55E-10	8.15E-11	6.06E-09
1.8	1.76E-09	1.91E-10	8.47E-11	2.35E-12	2.30E-11	1.86E-12	5.82E-14	3.83E-10	8.82E-11	6.72E-09
1.9	2.17E-09	2.31E-10	1.17E-10	3.41E-12	3.21E-11	3.07E-12	1.01E-13	4.10E-10	5.46E-11	7.40E-09
2.0	2.62E-09	2.87E-10	1.57E-10	4.75E-12	4.35E-11	4.81E-12	1.65E-13	4.35E-10	1.01E-10	8.09E-09
2.1	3.10E-09	3.50E-10	2.05E-10	6.44E-12	5.70E-11	7.25E-12	2.59E-13	4.62E-10	1.07E-10	8.78E-09
2.2	3.61E-09	4.20E-10	2.60E-10	8.43E-12	7.28E-12	7.28E-12	3.90E-13	4.86E-10	1.13E-10	9.48E-09
2.3	4.15E-09	4.95E-10	3.23E-10	1.08E-11	9.10E-11	1.05E-11	5.67E-13	5.09E-10	1.18E-10	1.02E-08
2.4	4.71E-09	5.77E-10	3.94E-10	1.35E-11	1.49E-11	1.49E-11	7.99E-13	5.32E-10	1.24E-10	1.09E-08
2.5	5.29E-09	6.64E-10	4.73E-10	1.67E-11	1.12E-10	2.04E-11	1.10E-12	5.53E-10	1.29E-10	1.16E-08
2.6	5.89E-09	7.55E-10	5.59E-10	2.02E-11	1.59E-10	3.59E-11	1.47E-12	5.73E-10	1.34E-10	1.23E-08
2.7	6.49E-09	8.52E-10	6.52E-10	2.41E-11	1.86E-10	4.62E-11	1.93E-12	5.93E-10	1.39E-10	1.30E-08
2.8	7.11E-09	9.53E-10	7.53E-10	2.83E-11	2.15E-10	5.86E-11	2.49E-12	6.11E-10	1.43E-10	1.37E-08
2.9	7.73E-09	1.06E-09	8.59E-10	3.30E-11	2.46E-10	7.30E-11	3.16E-12	6.29E-10	1.47E-10	1.44E-08
3.0	8.35E-09	1.17E-09	9.71E-10	3.80E-11	2.79E-10	8.99E-11	3.95E-12	6.45E-10	1.51E-10	1.51E-08
3.1	8.98E-09	1.29E-09	1.09E-09	4.33E-11	3.13E-10	1.09E-10	4.87E-12	6.62E-10	1.55E-10	1.58E-08
3.2	9.60E-09	1.39E-09	1.21E-09	4.90E-11	3.48E-10	1.31E-10	5.92E-12	6.77E-10	1.59E-10	1.65E-08
3.3	1.02E-08	1.51E-09	1.34E-09	5.49E-11	3.85E-10	1.55E-10	7.12E-12	6.92E-10	1.62E-10	1.72E-08
3.4	1.08E-08	1.62E-09	1.47E-09	6.12E-11	4.23E-10	1.84E-10	8.48E-12	7.06E-10	1.65E-10	1.79E-08
3.5	1.14E-08	1.74E-09	1.61E-09	6.77E-11	4.61E-10	2.15E-10	1.00E-11	7.19E-10	1.69E-10	1.85E-08
3.6	1.20E-08	1.86E-09	1.74E-09	7.45E-11	5.01E-10	2.49E-10	1.17E-11	7.31E-10	1.72E-10	1.92E-08
3.7	1.26E-08	1.99E-09	1.88E-09	8.14E-11	5.41E-10	2.87E-10	1.36E-11	7.43E-10	1.75E-10	1.99E-08
3.8	1.32E-08	2.11E-09	2.03E-09	8.86E-11	5.82E-10	3.28E-10	1.57E-11	7.54E-10	1.77E-10	2.06E-08
3.9	1.38E-08	2.23E-09	2.17E-09	9.60E-11	6.23E-10	3.73E-10	1.79E-11	7.64E-10	1.80E-10	2.12E-08
4.0	1.43E-08	2.36E-09	2.32E-09	1.04E-10	6.64E-10	4.21E-10	2.04E-11	7.74E-10	1.82E-10	2.19E-08
4.1	1.49E-08	2.48E-09	2.47E-09	1.11E-10	7.06E-10	4.73E-10	2.30E-11	7.84E-10	1.85E-10	2.25E-08
4.2	1.54E-08	2.60E-09	2.61E-09	1.19E-10	7.48E-10	5.29E-10	2.59E-11	7.92E-10	1.87E-10	2.32E-08
4.3	1.60E-08	2.73E-09	2.76E-09	1.27E-10	7.89E-10	5.89E-10	2.90E-11	8.01E-10	1.89E-10	2.38E-08
4.4	1.55E-08	2.85E-09	2.91E-09	1.35E-10	8.31E-10	6.53E-10	3.23E-11	8.09E-10	1.91E-10	2.44E-08
4.5	1.70E-08	2.97E-09	3.06E-09	1.43E-10	8.72E-10	7.21E-10	3.58E-11	8.16E-10	1.93E-10	2.51E-08
4.6	1.74E-08	3.09E-09	3.21E-09	1.51E-10	9.14E-10	7.93E-10	3.95E-11	8.23E-10	1.95E-10	2.57E-08
4.7	1.79E-08	3.21E-09	3.36E-09	1.59E-10	9.54E-10	8.69E-10	4.34E-11	8.30E-10	1.97E-10	2.63E-08
4.8	1.84E-08	3.33E-09	3.50E-09	1.67E-10	9.95E-10	9.49E-10	4.76E-11	8.36E-10	1.98E-10	2.69E-08
4.9	1.88E-08	3.45E-09	3.65E-09	1.76E-10	1.03E-09	1.03E-09	5.20E-11	8.42E-10	2.00E-10	2.75E-08
5.0	1.92E-08	3.56E-09	3.79E-09	1.84E-10	1.07E-09	1.12E-09	5.66E-11	8.48E-10	2.01E-10	2.81E-08

Table 3
Electron Impact Excitation Rate Coefficients for Low-Lying
Metastable States of O^+ and N^+

Excitation Rate Coefficient	Deexcitation Rate Coefficient
$X_{16} = \frac{2.72 \times 10^{-8}}{\sqrt{T_e}} \exp\left(-\frac{1.88}{T_e}\right)$	$Y_{16} = \frac{4.88 \times 10^{-8}}{\sqrt{T_e}}$
$X_{17} = \frac{3.04 \times 10^{-9}}{\sqrt{T_e}} \exp\left(-\frac{4.03}{T_e}\right)$	$Y_{17} = \frac{2.74 \times 10^{-8}}{\sqrt{T_e}}$
$X_{18} = \frac{6 \times 10^{-9}}{\sqrt{T_e}} \exp\left(-\frac{2.15}{T_e}\right)$	$Y_{18} = \frac{3 \times 10^{-8}}{\sqrt{T_e}}$
$X_{22} = \frac{7.15 \times 10^{-8}}{\sqrt{T_e}} \exp\left(-\frac{3.31}{T_e}\right)$	$Y_{22} = \frac{2.86 \times 10^{-8}}{\sqrt{T_e}}$
$X_{23} = \frac{8.8 \times 10^{-9}}{\sqrt{T_e}} \exp\left(-\frac{5.0}{T_e}\right)$	$Y_{23} = \frac{5.87 \times 10^{-9}}{\sqrt{T_e}}$
$X_{24} = \frac{1.35 \times 10^{-8}}{\sqrt{T_e}} \exp\left(-\frac{1.69}{T_e}\right)$	$Y_{24} = \frac{2.26 \times 10^{-8}}{\sqrt{T_e}}$

Table 4
Charge Exchange Rate Coefficients, Ion/Molecule Rearrangement,
and Neutral Particle Reactions

Rate Coefficient	Process	Magnitude (cm^3/s)*	Ref. †
C_1	$O \rightarrow N_2 + O^+$	1×10^{-12}	19
C_2	$N_2^+ + O_2 \rightarrow N_2 + O_2^+$	$7.9 \times 10^{-12} \times T^{-1/2}$	19, 20
C_3	$N_2^+ + N \rightarrow N_2 + N^+$	1×10^{-12}	19, 20
C_4	$NO \rightarrow N_2(A) + NO^+$	5×10^{-10}	19
C_5	$O^+(^2D) + N_2 \rightarrow N_2^+(A) + O$	1.3×10^{-9}	21
C_6	$N_2^+ + O \rightarrow NO^+ + N$		22

Table 4—(Continued)

Rate Coefficient	Process	Magnitude (cm ³ /s)*	Ref.†
C_7	$O \rightarrow N + O^+$	1×10^{-12}	20 (estimated)
C_8	$N^+ + O_2 \rightarrow O_2^+ + N$	3.0×10^{-10}	19
C_9	$NO \rightarrow N + NO^+$	8.0×10^{-10}	19
C_{10}	$N + O_2^+ \rightarrow NO^+ + O$	1.8×10^{-10}	20
C_{11}	$N^+ + O_2 \rightarrow NO^+ + O$	3×10^{-10}	19
C_{12}	$N^+ + O_2 \rightarrow NO + O^+$	1.0×10^{-12}	20
C_{13}	$O^+ + O_2 \rightarrow O + O_2^+$	2×10^{-11}	19
C_{14}	$N(^2D) + O_2 \rightarrow NO + N$	6×10^{-12}	20
C_{15}	$O + N_2 \rightarrow NO + N$	$1 \times 10^{-10} e^{-\frac{3.26}{T}}$	20
C_{16}	$N + NO \rightarrow N_2 + O$	2.2×10^{-11}	20
C_{17}	$N + O_2 \rightarrow NO + O$	$2.4 \times 10^{-11} e^{-\frac{0.3}{T}}$	20
C_{18}	$O + NO \rightarrow O_2 + N$	$5.3 \times 10^{-12} e^{-\frac{1.7}{T}}$	20
C_{19}	$NO + O_2^+ \rightarrow O_2 + NO^+$	6×10^{-10}	19
K_{TV}	$O^+ + N_2 \rightarrow NO^+ + N$	1.2×10^{-12} (except when N_2 is vibrationally excited; see appendix)	22
C_{20}	$N_2(A) + O \rightarrow O(^1S) + N_2$	3×10^{-12}	23
C_{21}	$N(^2D) + N_2 \rightarrow N + N_2$	1.6×10^{-14}	24
C_{22}	$N(^2D) + NO \rightarrow NO + N$	7×10^{-11}	24
C_{23}	$O + O + O \rightarrow O(^1S) + O_2$	1.5×10^{-34}	25
C_{24}	$O_2(a^1D) + O_2 \rightarrow O_2 + O_2$	2.3×10^{-18}	26
C_{25}	$O_2(b^1\Sigma) + N_2 \rightarrow O_2 + N_2$	2.5×10^{-15}	27
C_{26}	$O_2(a^1\Delta) + O \rightarrow O_2 + O$	$< 1.0 \times 10^{-15}$	27

*Room temperature except when temperature dependence is given.

†Refers to References at end of report.

Table 5
Radiative Lifetimes of Metastable States

Rate (s ⁻¹)	State	Lifetime (s)	Ref.
A ₁	N ₂ (A ³ Σ)	1	20
A ₂	N(² p)	13	30
A ₃	N ⁺ (¹ D)	250	30
A ₄	N ⁺ (¹ S)	0.92	30
A ₅	O(¹ D)	140	30
A ₆	O(¹ S)	0.7	30
A ₇	O ⁺ (² p)	6	30
A ₈	O ₂ (b ¹ Σ)	12	20
A ₉	O ₂ (a ¹ Δ)	2.7 × 10 ³	20

BASIC RATE EQUATIONS FOR THE SIMPLE CODE

The Simple Code was developed to calculate the electron density for a flow system where a large multispecies code cannot be utilized. Two metastable states, O(¹D) and N(²D), were carried for obvious reasons. O(¹D) emits the 6300A line. Furthermore, O(¹D) is quenched by N₂ at a fast rate (28), where it was suggested that it may excite (33) N₂ at the seventh vibrational level. However, it appears (34) now that a very small amount of the energy ends up in the vibrational mode of N₂. N(²D) was included since it is largely responsible for the NO formation in the disturbed atmosphere. Therefore, one could calculate the fundamental and the overtone emission from NO. This Simple Code calculates emissions from metastable states, which are not included, by using steady-state relations.

Since this code does not calculate N₂⁺ and O⁺(²D), certain initial adjustments have to be made from the Master Code to the Simple Code. For example, O⁺(²D) is partitioned into charge exchange with N₂, resulting in N₂⁺, and an electron deexcitation process. Furthermore, the resultant N₂⁺ is immediately removed and partitioned as N, N(²D), and other possible processes.

The relevant Simple Code rate equations are:

$$\frac{dN_2}{dt} = -K_{TV}N_2 O^+ + C_{16}NO[N + N(^2D)] - C_{15}N_2[O + O(^1D)].$$

$$\begin{aligned} \frac{dN}{dt} = & -N_e N X_{13} + N_e N(^2D) Y_{13} - C_{10} N O_2^+ + \alpha N^+ N_e \\ & + C_7 [O(^1D) + O] N^+ + C_8 N^+ O_2 + \frac{1}{2} C_9 N^+ NO + K_{TV} N_2 O^+ \\ & + C_{18} [O(^1D) + O] NO + C_{15} N_2 [O + O(^1D)] - C_{16} N NO - C_{17} N O_2. \end{aligned}$$

$$\begin{aligned} \frac{dN(^2D)}{dt} = & -N_e N(^2D) Y_{13} + N_e N X_{13} + D_2 N_e N O^+ - C_{10} N(^2D) O_2^+ \\ & - C_{14} N(^2D) O_2 - C_{16} N(^2D) NO + \frac{1}{2} C_9 N^+ NO. \end{aligned}$$

$$\begin{aligned} \frac{dN^+}{dt} = & -N^+ O_2 (C_8 + C_{11} + C_{12}) - C_7 N^+ O - \alpha_2 N^+ N_e \\ & - C_9 N^+ NO - C_7 N^+ O(^1D). \end{aligned}$$

$$\begin{aligned} \frac{dO}{dt} = & D_2 N_e N O^+ - N_e O X_{19} + N_e O(^1D) Y_{19} + C_{10} N O_2^+ \\ & + C_{10} N(^2D) O_2^+ + O(^1D) A_5 + C_{13} O^+ O_2 - C_7 N^+ O + \alpha_1 O^+ N_e \\ & + q_1 O(^1D) N_2 + C_{11} N^+ O_2 + \beta_1 D_3 N_e O_2^+ + C_{14} N(^2D) O_2 + C_{17} N O_2 \\ & + C_{16} N NO + \frac{1}{2} C_{16} N(^2D) NO - C_{15} O N_2 - C_{18} O NO + C_{13b} O^+ NO. \end{aligned}$$

$$\begin{aligned} \frac{dO(^1D)}{dt} = & N_e O X_{19} - N_e O(^1D) Y_{19} - O(^1D) A_5 - q_1 O(^1D) N_2 \\ & + \beta_2 D_3 N_e O_2^+ + \frac{1}{2} C_{16} N(^2D) NO - C_{15} O(^1D) N_2 \\ & - C_{18} O(^1D) NO - C_7 N^+ O(^1D). \end{aligned}$$

$$\begin{aligned} \frac{dO^+}{dt} = & -K_{TV} N_2 O^+ + C_7 N^+ O - C_{13} O^+ O_2 + C_7 N^+ O(^1D) \\ & + C_{12} N^+ O_2 - \alpha O^+ N_e - C_{13b} O^+ NO. \end{aligned}$$

$$\begin{aligned} \frac{dNO^+}{dt} = & K_{TV} O^+ N_2 - D_2 N_e N O^+ + C_{11} N^+ O_2 + C_{19} O_2^+ NO \\ & + C_{10} N O_2^+ + C_9 N^+ NO + C_{10} N(^2D) O_2^+ + C_{13b} O^+ NO. \end{aligned}$$

$$\begin{aligned} \frac{dNO}{dt} = & C_{12} N^+ O_2 + C_{14} N(^2D) O_2 - C_9 N^+ NO - C_{19} O_2^+ NO \\ & + C_{15} O N_2 + C_{17} N O_2 + C_{15} O(^1D) N_2 - C_{16} NO [N + N(^2D)] \\ & + C_{18} NO [O + O(^1D)] - C_{13b} O^+ NO. \end{aligned}$$

$$\begin{aligned} \frac{dO_2}{dt} &= -C_{13}O^+O_2 - C_8N^+O_2 - C_{11}N^+O_2 + C_{19}O_2^+NO \\ &\quad + C_{18}NO[O + O(^1D)] - C_{17}NO_2 \\ &\quad - C_{12}N^+O_2 - C_{14}N(^2D)O_2. \\ \frac{dO_2^+}{dt} &= C_8N^+O_2 + C_{13}O^+O_2 - D_3N_eO_2^+ - C_{10}NO_2^+ \\ &\quad - C_{19}O_2^+NO - C_{10}N(^2D)O_2^+. \end{aligned}$$

THE ELECTRON, THE HEAVY PARTICLE, AND THE N_2 VIBRATIONAL TEMPERATURES

The electrons, the heavy particles, and other modes of freedom, such as the vibrational excitation of N_2 , gain energy directly or indirectly from the disturbing radiation field. The ejected photoelectrons, for example, gain their kinetic energies directly by acquiring the excess energy of the ionizing photon. The heavy particles, on the other hand, gain energy directly by sharing the excess energy of the dissociating photon. Indirectly, however, the heavy particles share the exothermic energies of charge exchange and re-arrangement reactions. The vibrational mode is excited by collisions with electrons and other particles and, hence, falls into the indirect category.

Electron Temperature

The electrons gain energy during the irradiation phase from the energetic photoelectrons. They lose energy through all elastic and inelastic collisions with the appropriate species. The inelastic collisions include the metastable electronic states of atoms, atomic ions, molecules and molecular ions, and the vibrational states of N_2 . These states, in turn, may act as a heating source for cool electrons through superelastic collisions. The electronic states which are excited by electron impact, and subsequently radiate and thus act as a cooling mechanism, are the optically allowed transitions in atoms and atomic ions, the triplet states of N_2 , and the Mienel and 3914Å band of N_2^+ .

For optically allowed transitions in atoms and their ions, one could use an excitation rate coefficient based on a Seaton (35) cross section averaged with the velocity over an Maxwellian electron velocity distribution. Such a rate with the appropriate (36) Gaunt factors $\langle g \rangle$, and the temperature in electrovolts, is given by

$$\langle \sigma V \rangle = \frac{1.6 \times 10^{-5} f_{ij} \langle g \rangle}{E_{ij} \sqrt{T_e}} \exp \left(- \frac{E_{ij}}{T_e} \right)$$

where f_{ij} is the oscillator strength for a transition whose excitation energy is E_{ij} .

The energy loss rate by electrons to atmospheric ions in electron-ion collisions can be expressed as

$$\frac{dT_e}{dt} = -3 \times 10^{-9} N_e \left(\frac{T_e - T_a}{T_e^{3/2}} \right)$$

where T_a is the heavy particle temperature (ions, atoms, molecules are prescribed by one temperature). Here, the equation time given by Spitzer (37) is utilized.

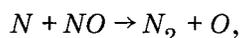
Heavy Particle Temperature

The heavy particles include any charged or neutral particle, except the electron. Their translational energy arises mainly from the dissociation of the molecules, the dissociative recombinations of the molecular ions, and the charge exchange and rearrangement collisions. Table 6 is a list of the exothermic energies which act as a heating source for the heavy particles.

The heavy particles gain energy from the electrons by elastic collisions. The interchange between the vibrational and the translational modes results in raising or lowering the heavy particle temperature.

Vibrational Temperature

It was pointed out earlier that the vibrational excitation of N_2 plays an important role in the deionization process of a disturbed atmosphere. This is due to the fact that an atomic ion is converted to a molecular ion at a faster rate when N_2 is vibrationally excited. In the appendix, the vibrational temperature due to electron impacts alone is developed in detail. However, when the electron density is low enough, other competing rates such as



results in the vibrational excitation (38, 39) of N_2 , which is capable in dissociating ozone. The above reaction, with N being in the 2D state, may excite N_2 to higher vibrational states. These and other reactions must also be included in the calculation of the vibrational temperature of N_2 .

Table 6
Exothermic Energies Associated with Heavy Particle Reactions

Reactions Identified by Their Coefficients	Exothermic Energy (eV)
D_1	3.45*
D_2	0.39*
D_3	4.78*

Table 6—(Continued)

Reactions Identified by Their Coefficients	Exothermic Energy (eV)
C_1	1.96
C_2	3.52
C_3	1.04
C_4	0.0†
C_5	0.0‡
C_6	3.06¶
C_7	0.92
C_8	2.48
C_9	5.27
C_{10}	4.20¶
C_{11}	6.67¶
C_{12}	2.32¶
C_{13}	1.56
C_{13b}	4.3
C_{14}	2.77¶
C_{15}	-3.25
C_{16}	3.25
C_{17}	1.4¶
C_{18}	-1.40
C_{19}	2.79
K_{TV}	1.10¶
C_{21}	2.37
C_{22}	2.37

Table 6—(Continued)

Reactions Identified by Their Coefficients	Exothermic Energy (eV)
C_{24}	1.0
C_{25}	1.6
C_{26}	1.0
q_1	1.96
q_2	4.16

*This exothermic energy arises as a result of the assumed states of the products of the dissociative recombination.

†Resonance, resulting in $N_2(A)$.

‡Resonance, resulting in $N_2^+(A, v = 1)$. $O^+(2D)$ also charge exchanges resonantly with O_2 .

¶Part or all of the exothermic energy may end up in the vibrational states of the end product.

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APPENDIX
The Vibrational Temperature of N_2

In the disturbed ionosphere, especially in the E and the F layers, the removal of the electrons is mainly due to their dissociative recombinations with the molecular ions. This is true as long as $A^+ \leq 10^4 M^+$, where A^+ and M^+ are the atomic and the molecular ions, respectively. Part of the electron removal is due to NO^+ , which can be formed in the ionosphere according to



and has a reaction rate coefficient (A1) of 1.3×10^{-12} cm³/s when the reactants are at room temperature. However, the above reaction depends heavily (A1) on the vibrational excitation of N_2 . The reaction rate in Eq. (A1) may go up (A1) by a factor of 40 with increasing vibrational temperature of N_2 . Therefore, a knowledge of this vibrational temperature is essential for the deionization calculations of the disturbed ionosphere. One of the processes to excite N_2 vibrationally in the disturbed ionosphere is the inelastic collisions with low-energy electrons. The cross sections for the electron impact excitations of eight ground state vibrational levels of N_2 have been measured by Schulz (A2). These cross sections are averaged with the electron velocity over an Maxwellian electron velocity distribution to obtain the corresponding excitation rate coefficients (A3) and are shown in Fig. A1. These rates are also given in Table A1 as a function of the electron temperature.

In this report we use the electron impact excitation rates to develop an expression for the rate of the vibrational energy of N_2 . From the vibrational energy one may obtain the vibrational temperature. We shall assume the nitrogen molecule to be a harmonic oscillator with equal energy spacings of 0.3 eV between the vibrational states. Let N_2 denote the total number of nitrogen molecules, E_1 the energy of the first vibrational state, and $N_2(v)$ the concentration of the v th vibrational level. The total vibrational energy is

$$E_{vib}^T = \frac{E_1}{\exp\left(\frac{E_1}{T_v}\right) - 1} N_2 \quad (A2)$$

where $E_1 / \exp(E_1 / T_v) - 1$ is the average energy of a harmonic oscillator with a vibrational temperature T_v . Here we are using T_v to denote kT_v . Thus for nitrogen,

$$E_{vib}^T = \frac{0.3 N_2}{\left(\frac{0.3}{T_v}\right) - 1} \quad (A3)$$

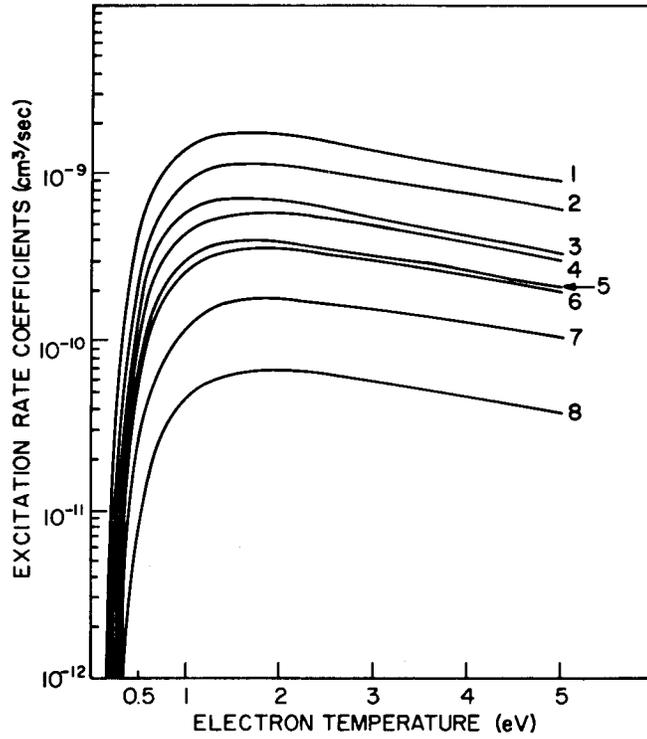


Fig. A1—Excitation rate coefficients as a function of electron temperature for eight ground-state vibrational levels of N_2 .

The rate equation for any vibrational state can be written as

$$\frac{dN_2(v)}{dt} = N_e N_2(0) X_v - N_e N_2(v) Y_v \quad (\text{A4})$$

where X_v is the excitation of the v th vibrational level by electron impact through collisions with nitrogen in the zeroth vibrational level. These rates are electron-temperature dependent and are shown in Fig. A1. Y_v is the corresponding deexcitation rate and can be obtained via detailed balancing. The rate of energy stored in the v th vibrational level is

$$vE_1 \frac{dN_2(v)}{dt} = N_e N_2(0) X_v vE_1 - N_e N_2(v) Y_v vE_1. \quad (\text{A5})$$

Therefore, the total vibrational energy rate is

$$\frac{dE_{vib}^T}{dt} = N_e N_2(0) E_1 \sum_{v=1}^8 X_v v - N_e E_1 \sum_{v=1}^8 N_2(v) Y_v v \quad (\text{A6})$$

where the summation should, in principle, be to ∞ . However, the higher the electron temperature, the lower the impact excitation cross section for higher states. Equation (A6) can be written as

Table A1
 N_2 Vibrational Excitation Rate Coefficients

Rate Coefficients								
T_e/X_v	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8
0.1	1.98(-14)*	1.49(-16)	6.28(-17)	1.57(-17)	5.58(-18)	1.37(-18)	2.27(-19)	2.51(-20)
0.2	4.01(-12)	1.48(-12)	8.81(-13)	4.16(-13)	2.16(-13)	1.14(-13)	3.28(-14)	7.81(-15)
0.3	5.63(-11)	2.82(-11)	1.83(-11)	1.05(-11)	6.20(-12)	4.13(-12)	1.45(-12)	4.31(-13)
0.4	2.08(-10)	1.14(-10)	7.59(-11)	4.76(-11)	3.02(-11)	2.24(-11)	8.71(-12)	2.85(-12)
0.5	4.38(-10)	2.52	1.68(-10)	1.11(-10)	7.33(-11)	5.77(-11)	2.39(-11)	8.26(-12)
0.6	6.96(-10)	4.11	2.74	1.88	1.27(-10)	1.04(-10)	4.47	1.60(-11)
0.7	9.43(-10)	5.66	3.77	2.65	1.82	1.52	6.76	2.47
0.8	1.16(-9)	7.04	4.67	3.35	2.32	1.98	9.00(-11)	3.33
0.9	1.34	8.20	5.41	3.96	2.75	2.38	1.10(-10)	4.12
1.0	1.48	9.12	5.99	4.45	3.11	2.72	1.27	4.80
1.1	1.58	9.84(-10)	6.43	4.85	3.38	2.99	1.42	5.37
1.2	1.66	1.04(-9)	6.75	5.15	3.60	3.20	1.53	5.83
1.3	1.71	1.08	6.96	5.39	3.75	3.37	1.62	6.19
1.4	1.74	1.10	7.09	5.56	3.86	3.48	1.69	6.46
1.5	1.76	1.12	7.16	5.67	3.93	3.57	1.74	6.65
1.6	1.77	1.12	7.17	5.75	3.96	3.62	1.77	6.78
1.7	1.76	1.12	7.15	5.79	3.97	3.65	1.79	6.86
1.8	1.75	1.12	7.09	5.81	3.96	3.66	1.80	6.89
1.9	1.73	1.11	7.00	5.80	3.94	3.65	1.80	6.89
2.5	1.56	1.02(-9)	6.26	5.51	3.61	3.45	1.71	6.46
3.0	1.39	9.21(-10)	5.57	5.15	3.36	3.20	1.58	5.88
3.5	1.24	8.29	4.93	4.77	2.93	2.95	1.44	5.29
4.0	1.11(-9)	7.47	4.38	4.43	2.64	2.73	1.32	4.74
4.5	9.95(-10)	6.74	3.90	4.12	2.38	2.55	1.21	4.24
5.0	8.96(-10)	6.11(-10)	3.49(-10)	3.84(-10)	2.16(-10)	2.39(-10)	1.12(-10)	3.80(-11)

*Numbers in parenthesis indicate powers of 10 by which the entries are to be multiplied. Where no parenthesis are given the entries are multiplied by the power of 10 for the preceding entries.

$$\frac{dE_{vib}^T}{dt} = N_e N_2(O) E_1 \sum_{v=1}^8 v X_v \left[1 - \exp\left(\frac{vE_1(T_v - T_e)}{T_e T_v}\right) \right] \quad (A7)$$

or

$$\frac{dE_{vib}^T}{dt} = N_e E_1 \frac{N_2}{Q(T_v)} \sum_{v=1}^8 v X_v \left[1 - \exp\left(\frac{vE_1(T_v - T_e)}{T_e T_v}\right) \right] \quad (A8)$$

where we have used Boltzman relations and detailed balancing for Y_v and $N_2(v)$.

Finally, the vibrational energy rate per molecule is

$$\frac{dE_{vib}}{dt} = N_e E_1 \sum_{v=1}^8 v X_v \left[1 - \exp\left(\frac{vE_1(T_v - T_e)}{T_e T_v}\right) \right] \left(1 - e^{-E_1/T_e} \right). \quad (A9)$$

To calculate Eq. (A9) we have obtained approximate expressions for X_v which fit the tabulated values (see Table A1) within less than 20%. These rate coefficients are:

$$\left. \begin{aligned} X_1 &= 10^{-8} \exp(-1.6/T_e) (1.73 - 1.124\sqrt{T_e} + 0.1074T_e) \\ X_2 &= 10^{-8} \exp(-1.72/T_e) (1.245 - 0.814\sqrt{T_e} + 0.0695T_e) \\ X_3 &= 10^{-9} \exp(-1.71/T_e) (7.863 - 5.091\sqrt{T_e} + 0.488T_e) \\ X_4 &= 10^{-9} \exp(-1.83/T_e) (5.789 - 2.595\sqrt{T_e} - 0.46T_e) \\ X_5 &= \frac{10^{-9}}{\sqrt{T_e}} \exp(-1.7/T_e) (-2.428 + 8.34\sqrt{T_e} - 4.17T_e) \\ X_6 &= \frac{10^{-9}}{\sqrt{T_e}} \exp(-1.82/T_e) (-2.428 + 8.34\sqrt{T_e} - 4.17T_e) \\ X_7 &= \frac{10^{-9}}{\sqrt{T_e}} \exp(-1.92/T_e) (-1.214 + 4.17\sqrt{T_e} - 2.085T_e) \\ X_8 &= \frac{10^{-9}}{\sqrt{T_e}} \exp(-2.02/T_e) (-0.49 + 1.685\sqrt{T_e} - 0.842T_e) \end{aligned} \right\} 0.2 \leq T_e \leq 1.6 \text{ (eV)}$$

and

$$\left. \begin{aligned} X_1 &= 10^{-9} (2.140 - 0.234T_e) \\ X_2 &= 10^{-9} (1.355 - 0.15T_e) \\ X_3 &= 10^{-10} (9.034 - 0.915T_e) \\ X_4 &= 10^{-10} (6.569 - 0.58T_e) \\ X_5 &= 10^{-10} (4.832 - 0.545T_e) \\ X_6 &= 10^{-10} (4.266 - 0.37T_e) \\ X_7 &= 10^{-10} (2.040 - 0.19T_e) \\ X_8 &= 10^{-11} (7.982 - 0.876T_e) \end{aligned} \right\} 1.6 \leq T_e \leq 5 \text{ (eV)}$$

where T_e is the electron temperature.

These excitation rates and their corresponding deexcitation rates can also be used (A4) in the deionization calculations by following the time histories of eight vibrational levels.

Finally, the reaction rate for Eq. (A1) can be expressed as

$$\begin{aligned} K_{TV} &= 10^{-12} (1 - e^{-0.3/T_v} \\ &\quad \times 1 \cdot 2 + 1 \cdot 2 e^{-0.3/T_v} + 50 e^{-0.6/T_v} \\ &\quad + 120 e^{-0.9/T_v} + 260 e^{-1.2/T_v} + 400 e^{-1.5/T_v} \\ &\quad + 500 e^{-1.8/T_v} + 500 e^{-2.1/T_v} + 500 e^{-2.4/T_v}) . \end{aligned}$$

Here, the reaction rate coefficients for each vibrational level (A1) was utilized and the level distribution was considered in vibrational equilibrium.

References

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