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SOLUTIONS OF REACTION RATE EQUATIONS PERTAINING TO ELECTRON IRRADIATION OF 4:1 MIXTURES OF N_2 AND O_2

by

Franklin E. Niles
Edna L. Lortie

September 1967

U. S. ARMY MATERIEL COMMAND
BALLISTIC RESEARCH LABORATORIES
ABERDEEN PROVING GROUND, MARYLAND

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REPORT NO. 1372

SEPTEMBER 1967

SOLUTIONS OF REACTION RATE EQUATIONS PERTAINING TO ELECTRON IRRADIATION OF 4:1 MIXTURES OF N_2 AND O_2

Franklin E. Niles
Edna L. Lortie

Ballistic Measurements Laboratory

RDT&E Project No. 1V014501B53A

A B E R D E E N   P R O V I N G   G R O U N D,   M A R Y L A N D

B A L L I S T I C   R E S E A R C H   L A B O R A T O R I E S

REPORT NO. 1372

FENiles/ELLortie/sn/ilm
Aberdeen Proving Ground, Md.
September 1967

SOLUTIONS OF REACTION RATE EQUATIONS PERTAINING TO ELECTRON IRRADIATION OF 4:1 MIXTURES OF N_2 AND O_2

ABSTRACT

One of the Keneshea computer codes has been adapted for use on the Ballistic Research Laboratories Electronic Scientific Computer (BRLESC) at Aberdeen Proving Ground. Using this modified code, reaction rate equations have been solved for the following 15 species: e, NO_2^-, O^-, O_2^-, O_3^-, N_2^+, NO^+, O^+, O_2^+, N, NO, N_2O, NO_2, O, and O_3. The calculations were made for a 4:1 mixture of N_2 and O_2 at 1 torr total pressure and 300°K. Rate constants as given by Keneshea and Fowler (Research Report AFCRL-66-741, October 1966) were used. Initial electron production rates of 1.61×10^6, 1.61×10^7, 1.61×10^8, and 1.61×10^9 cm^{-3} sec^{-1} were used, where a rate of 1.61×10^9 cm^{-3} sec^{-1} corresponds to an irradiating electron beam current density of 100 microampere per square meter impinging on the cavity of the G. C. Dewey experimental system (Technical Report ECOM-01354-F, September 1966). The solutions are presented as number densities versus time after the start of the irradiating electron beam. A description of the modified code is presented.

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I. INTRODUCTION

The number densities of electrons, positive ions, negative ions, and neutral species in the ionosphere are constantly changing. These changes are primarily due to a changing ionization source and to the chemical reactions which the various species undergo. The time rate of change of the number density of a particular species is given by the reaction rate equation for that species. Since a reaction rate equation can be written for each species, the number densities of the various species can be determined by the simultaneous solution of all the reaction rate equations. Computer programs for solving these reaction rate equations have been prepared by Keneshea.[1,2,3*] His 1963 code has been modified to adapt it for use on the BRLESC computer at the Ballistic Research Laboratories (BRL).

The Keneshea computer codes are designed to solve the reaction rate equations that pertain to the atmosphere below 150 km in that the codes do not include any transport phenomena. The modified code, described in this report, considers that the number densities of O_2 and N_2 are maintained in a constant reservoir and solves for the number densities of the following 15 species: e, NO_2^-, O^-, O_2^-, O_3^-, N_2^+, NO^+, O^+, O_2^+, N, NO, N_2O, NO_2, O, and O_3. For this work 166 reactions involving these 17 species were considered, although some were in effect eliminated by setting the rate constant[**] to zero.

This code does not consider excited state species nor some of the ions known to exist in the atmosphere. These species could be included by adding additional reaction rate equations.

Superscript numbers denote references which may be found on page 38.

***The reaction rate is the product of the rate constant and the number densities of the species involved in the reaction. A true reaction rate constant for any given reaction is a function of temperature only. For this work all the species are assumed to be in thermal equlibrium at $300^\circ K$.*

The customary approach to understanding the changing ionosphere has been to lump the species into electrons, negative ions, positive ions, and neutrals. This approach utilizes effective rate constants and gives an overall picture of what is taking place. However, the role of the individual species is hidden. Since the number densities of the species are changing, the relative importance of the reaction rates must be changing. This requires that the effective rate constants must change when the lumped-species approach is used.

On the other hand, the Keneshea computer codes consider the role of the individual species. This allows one to compare the solutions of the reaction rate equations with experimentally observed number densities. Keneshea[4] has made this comparison for a diurnal variation at Fort Churchill, Canada, and for the July 1963 solar eclipse. Keneshea and Fowler[5] have computed profiles for the November 1966 solar eclipse. This eclipse was the subject of an intensive experimental program, which, when the data are reduced, will provide number densities for comparison with the computed profiles.

Comparisons of calculated number densities with *in situ* measurements in the ionosphere are fine and should be made. However, because of the many unknowns, agreement or disagreement does not confirm or invalidate the computer solutions. As with all computer solutions, the solutions are only as good as the input information. In the Keneshea codes a model atmosphere must be assumed. The initial number densities of all the species and the temperature for a particular altitude must be read into the computer. Also, the rate of ionization and changes in the rate of ionization must be read into the computer. Determining the proper rate of ionization is particularly troublesome for the November 1966 solar eclipse because of the presence of the nearby South Atlantic anomaly. Reaction rate constants must be given to every reaction which is considered. Many of the rate constants presently used are no more than educated guesses.

Unfortunately the D and E-region of the ionosphere (60-150 km) is not accessible to balloon or satellite observation which could continuously monitor the change in number densities of the species. Instead, one must rely on rocket or gun probes which give data only for a specific time. Species identification is normally limited to electrons and positive ions, with the absolute number densities subject to considerable uncertainty. Other experiments give some information on neutral species and negative ions, but the number densities of these are either unknown or questionable.

In light of the uncertainties involved in comparing the solution of the Keneshea computer program with *in situ* measurements, a comparison with an experiment in which the initial number densities and rate of ionization can be controlled is deemed desirable. The work at the G. C. Dewey Corporation reported by Hirsh et al[6] seems to be the best available for a comparison study. While an actual comparison will no be made in this report, the computations have been made for conditions which are obtainable with the G. C. Dewey experimental system.

II. DESCRIPTION OF THE G. C. DEWEY EXPERIMENT

The experimental system at the G. C. Dewey Corporation[6] was designed to study ionization and deionization processes in the upper atmosphere arising from prolonged irradiation by beta particles from trapped fission debris subsequent to the detonation of a nuclear device at high altitudes. The upper atmosphere differs from all laboratory experiments in that it is not confined by walls. Thus, the upper atmosphere is characterized solely by volume processes, whereas in all laboratory experiments, collisions of the various species with the walls and other wall effects must be considered. Futhermore, all laboratory experiments are never completely free from system-induced impurities which may affect the results. The G. C. Dewey experiment minimizes these differences in the following manner. First, it utilizes a reaction chamber which is 4 feet in diameter and 2 feet long, thus providing a large volume and reducing wall effects. Second, ultrahigh vacuum techniques are employed. Third, gases of known purity are used.

A schematic diagram of the experimental system is shown in Figure 1. A divergent beam of 1.5 MeV electrons from a Van de Graaff accelerator tranverses a thin foil window which serves as one end of a cylindrical ultrahigh frequency cavity containing the gas to be studied. The geometry of the beam divergence is chosen to provide a flux of electrons which is nearly uniform throughout the volume of the cavity, so that the gas contained in the cavity is ionized by a spatially uniform source.

Three diagnostic techniques are available for studying the irradiated gas. First, densities of free secondary electrons can be deduced by resonant cavity methods. Second, a mass spectrometer is available to measure ion currents for selected positive and negative ions which diffuse to the container wall. Third, an optical spectrometer is available to examine the light emitted by the flourescing gas. It is possible to apply all three techniques simultaneously in order to provide detailed information on the instantaneous state of the irradiated gas.

Two methods of ionization can be employed. The electron beam can irradiate the gas continuously or in pulses. Time-resolved measurements can be made during the irradiation period and during the period without irradiation. Electron density, ion densities, and optical emission intensities can be measured as functions of pressure, chemical composition of the gas, and irradiating electron beam current density.

Hirsh et al[6] have made measurements using research grade O_2, N_2, and air* over the pressure range 0.005 to 10 torrs. The Van de Graaff accelerator can produce 1.5 MeV electrons at current densities up to 1.7 microamperes per square meter. These primary electrons ionize N_2 and O_2 producing N_2^+, O_2^+, secondary electrons, excited state species, and other

---

*LIF-O-GEN research grade air has been used. The minimum purity is quoted as 99.999 percent with a typical purity of 99.9995 percent. The O_2 percentage is held constant at 20.930 percent. The maximum allowable impurities in parts per million are as follows: Ar - 15, CO_2 - 0.5, CO - 1, He - 5, H_2 - 1, H_2O - <2, CH_4 - 1, N_2O - 0.1, C_2H_2 - 0.05, and total hydrocarbon - 1.

ionic species. The latter two types of species have negligible number densities. Thus, the initial species considered to be undergoing reactions after the irradiation of the research grade air are N_2^+, O_2^+, e, N_2, and O_2. Other species are quickly created, however, as a result of the various reactions.

Charge particles produced in the cavity proceed by ambipolar diffusion to the wall. Since the Keneshea codes do not include depopulation by diffusion, a proper comparison between experimental measurements and computer code solutions can only be made if the depopulation by diffusion is much less than other depopulating processes. The depopulating frequency by diffusion is approximately given by

$$\nu_{diff} = D_{eff} \frac{p}{\Lambda^2 p} \quad (1)$$

where for a right circular cylindrical container of radius R and height h

$$\frac{1}{\Lambda^2} = \left(\frac{2.405}{R}\right)^2 + \left(\frac{\pi}{h}\right)^2 . \quad (2)$$

For the G. C. Dewey cavity $\Lambda^2 = 230\ cm^2$. Hirsh et al[6] have measured $D_{eff}p = (160 \pm 15)\ cm^2$ torr/sec for ambipolar diffusion of electrons and ions in research grade air. For a total pressure of 1 torr, ν_{diff} = 0.7 sec^{-1}. Assuming that this depopulating frequency by ambipolar diffusion applies to N_2^+, O_2^+, NO^+, and electrons, the relative importance of this depopulating process to other depopulating processes will now be discussed.

For N_2^+, the principal depopulating reaction is charge transfer with O_2. Since the rate constant* is $1 \times 10^{-10}\ cm^3/sec$,[7,8,9] the depopulating frequency by charge transfer at 1 torr total pressure of air is $6.44 \times 10^5\ sec^{-1}$.

**Rate constants are given in Appendix A.*

For O_2^+, the major depopulating reactions are positive charge rearrangement with N_2, charge transfer with NO, and ion-ion mutual neutralization with O_2^-. Using the rate constants given in Appendix A and number densities of 2.57×10^{16} cm^{-3}, 1.12×10^{10} cm^{-3}, and 1.96×10^{8} cm^{-3} for N_2, NO, and O_2^-, respectively, the depopulating frequency for O_2^+ is approximately 26.3 sec^{-1}.

For NO^+, the major depopulating reactions are ion-ion mutual neutralization with O_2^- and dissociative recombination. Using the rate constants given in Appendix A and an electron density of 1.05×10^{7} cm^{-3}, the depopulating frequency is 7.76 sec^{-1}.

For electrons the principal depopulating reaction is three-body attachment to O_2. For an O_2 density 6.44×10^{15} cm^{-3} and a rate constant of 2.42×10^{-30} cm^6/sec at 300^oK,[10] the depopulating frequency is 100 sec^{-1}.

Hence, the depopulating frequencies for N_2^+, O_2^+, NO^+, and electrons by reaction processes are all at least an order of magnitude greater than the depopulating frequency by ambipolar diffusion. The experimental observations[6] also have shown that depopulation by diffusion is negligible for pressures above 1 torr. As a result, the use of a computer code which does not consider diffusion is justified.

III. DESCRIPTION OF THE COMPUTER CODE

The computer code solves a set of simultaneous differential equations for 15 species and 166 reactions using a fourth order Runge-Kutta technique with variable mesh. The general form of the differential equation for a particular species y, taking into account all the reactions j which involve this species, can be expressed by

$$\frac{dy}{dt} = \sum_j F_j(y) - y \sum_i R_i(y) , \qquad (3)$$

where $\sum_j F_j(y)$ is the total populating rate including the initial production

$q(y)$ by external sources and $y \sum_i R_i(y)$ is the total depopulating rate. Thus $F_j(y)$ is the rate at which species y is formed by reaction j and $R_i(y)$ is the frequency at which species y is removed by reaction i.

For example, consider one reaction, the associative detachment process

$$A^- + B \rightarrow AB + e \; . \tag{4}$$

Two species are formed, AB and e, and two species are removed, A^- and B. Therefore, two formation terms and two removal terms exist for this reaction. These are:

$F(e) = k_4 \, [A^-][B]$, the rate at which species e is formed

$F(AB) = k_4 \, [A^-][B]$, the rate at which species AB is formed

$R(A^-) = k_4 \, [B]$, the frequency at which species A^- is removed

$R(B) = k_4 \, [A^-]$, the frequency at which species B is removed

The number density of species y is denoted by the brackets and k_4 is the reaction rate constant for Reaction (4).

The computer code incorporates the following 15 species in the solution: e, NO_2^-, O^-, O_2^-, O_3^-, N_2^+, NO^+, O^+, O_2^+, N, NO, N_2O, NO_2, O, and O_3. The symbol M is used to denote total number density in some reactions. The computer code assumes a constant reservoir of N_2, and O_2 is available. If desired, the computer code allows species O to be held constant.

The 166 reactions and their rate constants are given in Appendix A in the order they are used in the computer code. The rate constants are those given by Keneshea and Fowler.[5] A few of these constants are known to be incorrect. However, in the interest of having a consistent set for comparison with other work, the incorrect values have not been changed. Since this report is interested in the solutions at $300^{\circ}K$, the rate constants are given at $300^{\circ}K$. If the constant has a temperature dependence, this temperature dependence is given. To omit any reaction in the computer code, it is only necessary to set the rate constant to zero. In Appendix B, these 166 reactions have been arranged to show the reactions which form and remove species y.

The numerical approach employed by the computer code meets the following requirements:

- Allows for a variable time increment
- Prevents truncation errors from accumlating too rapidly
- Determines when a species approaches a steady state, i.e., reaches quasi-equilibrium
- Allows a species that has reached quasi-equilibrium to continue to change

Initially, the complete set of 15 differential equations are integrated ignoring the requirement of conservation of charge. After the first successful integration, charge balance is maintained by always computing the concentration of the largest positive ion from the charge-balance equation. The charge-balance equations state that the sum of the positive ion concentrations equals the sum of the negative ion concentrations plus the electron density.

When a species approaches a steady state, its differential equation is removed from the set by setting its derivative to zero. Once a species has reached quasi-equilibrium, the algebraic equation resulting from setting the derivative to zero replaces the differential equation and is solved by the method of successive substitutions. Once a differential equation has been removed from the set, the solution from then on is obtained by iteration between the differential and algebraic sets. This technique allows the number density of the species to change until the species reaches its true equilibrium value.

A description of the computer program is given in Appendix C, and the Fortran statements are given in Appendix D, as adapted to run on the BRL Electronic Scientific Computer (BRLESC).

IV. SOLUTIONS

The computer code has been given input information which allows a comparison to be made with the G. C. Dewey experiment.[6] For these calculations the production term q(y) is zero for all species except N_2^+, O_2^+, and electrons. The production is given by

$$q(y) = K(y)\, pi \ ,$$

where p is the gas pressure in torr, i is the irradiating beam current density measured in the cavity in microampere per square meter, and K(y) has been determined[6] as

$$K(O_2^+) = (5.10 \pm 0.10) \times 10^{11} \ (\text{cm } \mu\text{A torr/sec})^{-1}$$

and

$$K(N_2^+) = (5.70 \pm 0.40) \times 10^{11} \ (\text{cm } \mu\text{A torr/sec})^{-1} \ .$$

The irradiating electron beam current density in the cavity is the product of the Van de Graaff accelerator beam current which has undergone scattering into a square-meter area, and the transmission coefficient of the aluminum foil which forms one end of the cavity containing the gas. The transmission coefficient has been determined to be 0.288.

For 4:1 mixtures of N_2 and O_2 with a total pressure of 1 torr at 300°K, the number density of N_2 is 2.57×10^{16} cm^{-3}, and the number density of O_2 is 6.44×10^{15} cm^{-3}. For a Van de Graaff accelerator beam current density of 100 microamperes per square meter, the initial production terms are

$$q(N_2^+) = 1.31 \times 10^{9} \ \text{cm}^{-3} \ \text{sec}^{-1} \ ,$$

$$q(O_2^+) = 2.94 \times 10^{8} \ \text{cm}^{-3} \ \text{sec}^{-1} \ ,$$

and

$$q(e) = 1.61 \times 10^{9} \ \text{cm}^{-3} \ \text{sec}^{-1} \ .$$

Lower accelerator beam current densities naturally give lower initial production terms. Solutions have been obtained for accelerator beam current densities of 0.1, 1.0, 10, and 100 microamperes per square meter.

This corresponds to q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, and 1.61×10^9 cm^{-3} sec^{-1}. Solutions have been obtained using the rate constants given in Appendix A with the exception that the photodetachment and photodissociation reaction rates were set to zero.* The solutions out to 100 seconds are shown in Figures 2 through 16. Since the solutions were plotted by an automatic plotter, certain notation changes were made. These are: Q(E) denotes q(e), 1.61(9) denotes 1.61×10^9, and NO2- denotes NO_2^- with similar notations for other species. Zero time corresponds to the start of the continuous irradiation of the cavity with only N_2 and O_2 present.

The solutions show character which depends on the value of the electron beam current density. The automatic plotter plots in short, straight-line segments. Thus, character of this type should be ignored. Characteristics that cannot be ignored, however, are (1) the time needed to approach a steady-state condition if one is approached, (2) the rate at which the number density is increasing or decreasing, and (3) the time of maximum number density.

If the number density of a species is directly proportional to the irradiating beam current density, the curves for the four current densities would all fall on top of each other since each curve has been multiplied by the appropriate power of ten. This occurs only for N_2^+ as shown by Figure 7. The reason for this is that N_2^+ is formed solely by the irradiating electron beam and removed by charge transfer with O_2 which has a constant reservoir independent of the irradiating electron beam.

If the curves for lower values of q(e) fall above the curve for $q(e) = 1.61 \times 10^9$ cm^{-3} sec^{-1}, the number density is less than directly proportional to the irradiating beam current density. If the curves fall below, the number density is more than directly proportional.

**Inclusion of photodetachment and photodissociative reactions makes little difference because of the intense ionization.*

The dependence of the number densities on irradiating beam current density is more directly shown by Figure 17. Here the number densities at approximately 22 seconds are shown as a function of the irradiating beam current density. Solid lines are used for neutrals. Dashed lines are used for positive ions. Dash-dot lines are used for negatively charged species. As shown in this figure, the atomic oxygen concentration is the largest of the 15 time-varying species for a beam current density of 100 microamperes per square meter but decreases rapidly at lower beam current densities until it approaches the atomic nitrogen concentration at 0.1 microampere per square meter. However, the atomic oxygen concentration is artifically high since three-body recombination with O_2 (Reactions 153 and 154 of Appendix A) has been neglected. The O_3 concentration is too small for the same reason. While the neglect of these reactions and incorrect values for the rate constants for other reactions affect the number densities of the species, the general dependence of number density on the irradiating electron beam will remain as shown.

V. CONCLUSIONS

The following conclusions are made:

1. Any time a mixture of N_2 and O_2 are irradiated by an ionizing source, chemical kinetics produces an abundance of species. The number densities of the various species depend upon the magnitude of the ionizing radiation, the initial number densities, and the rate constants for the various reactions.

2. The charge transfer of N_2^+ with O_2 is rapid enough that N_2^+ normally will not be the dominant ion. Subsequent reactions of O_2^+ with N_2 and NO to produce NO^+ give the result that NO^+ will be the dominant positive ion whenever a mixture of N_2 and O_2 are subjected to ionizing radiation. This contradicts the statement of Hirsh et al[6] that "at pressures above 1 torr, the positive ion spectra observed in 4:1 mixtures are dominated by two species, N_2^+ and NO^+." However, Hirsh (private communication) now says that these measurements were in error.

3. The large number density of NO produced by the chemical kinetics implies that the number density of NO in the ionosphere could be quite large.

4. Many of the species do not reach a steady-state condition within 100 seconds.

5. Only the number density of N_2^+ is linearly dependent on the irradiating electron beam current density.

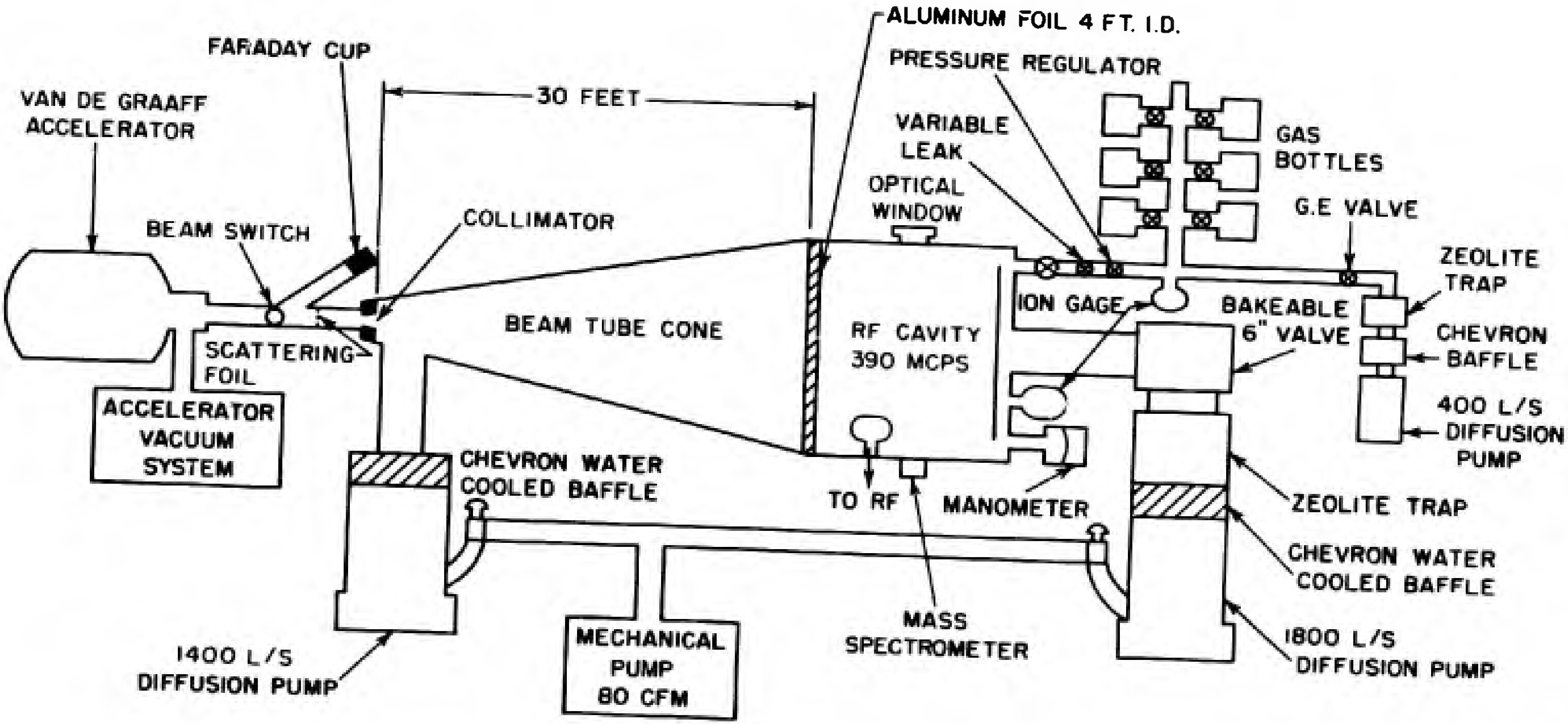

Figure 1. Schematic diagram of experimental system at the G. C. Dewey Corporation (Reference 6)

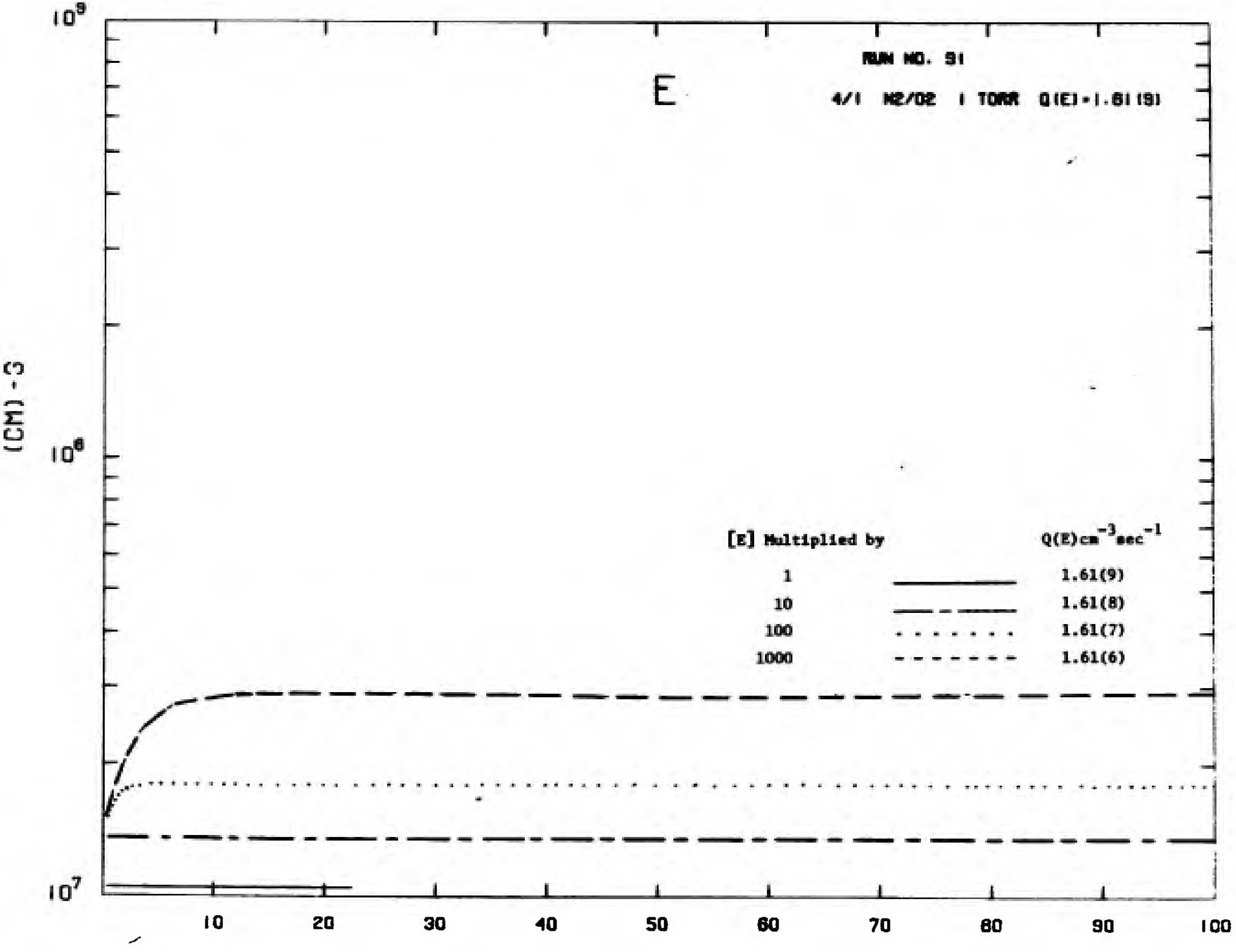

Figure 2. Electron density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

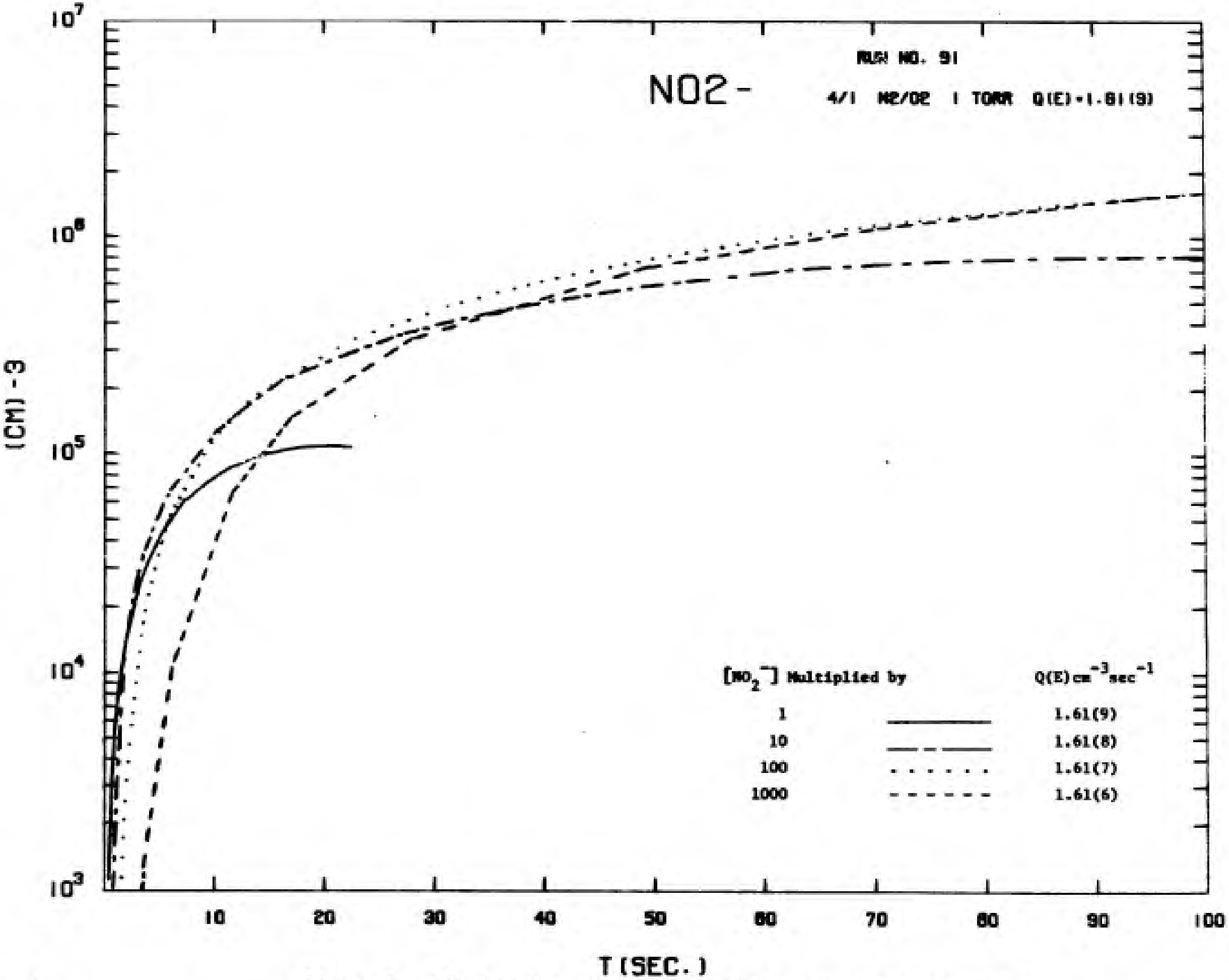

Figure 3. NO_2^- density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

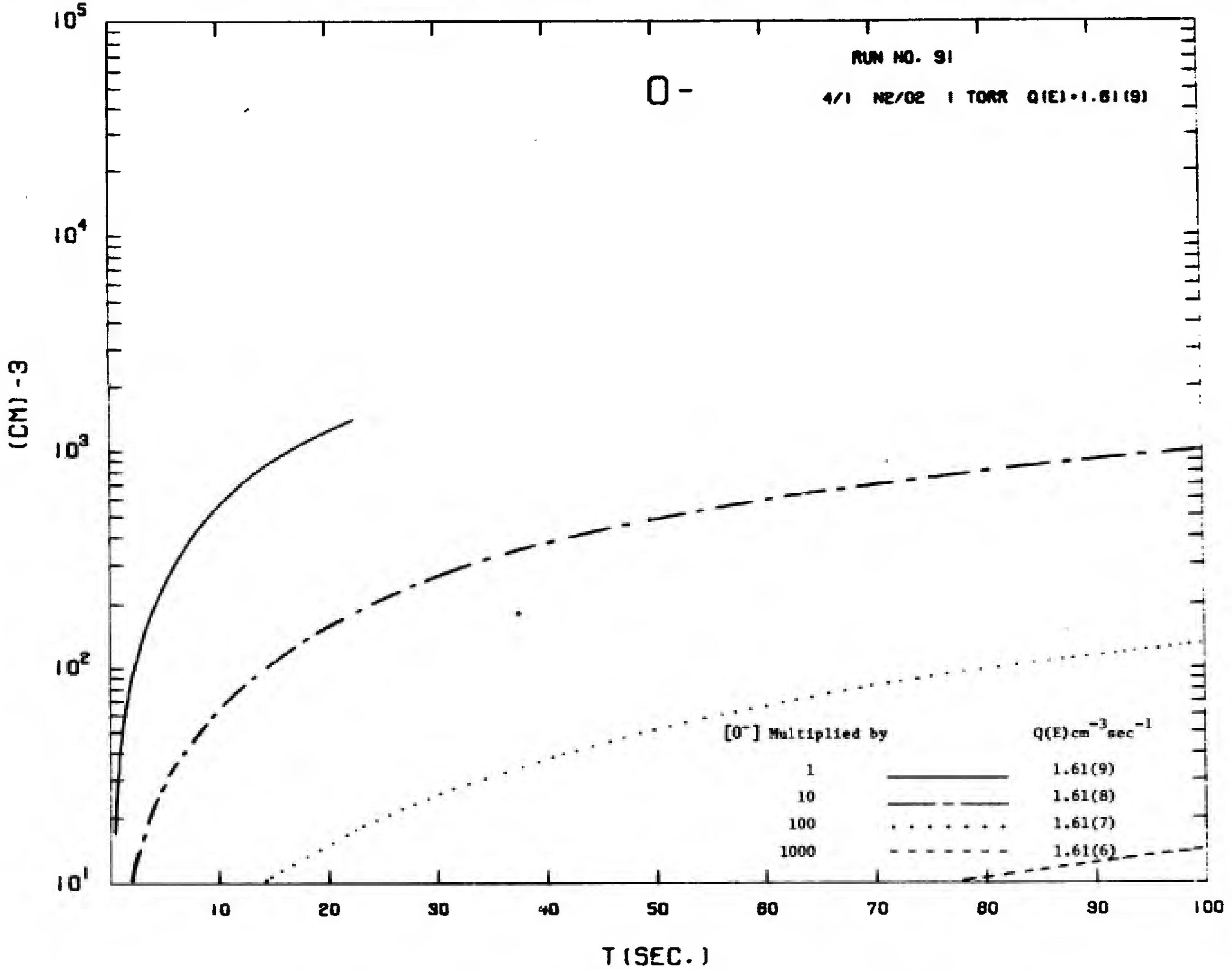

Figure 4. O^- density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

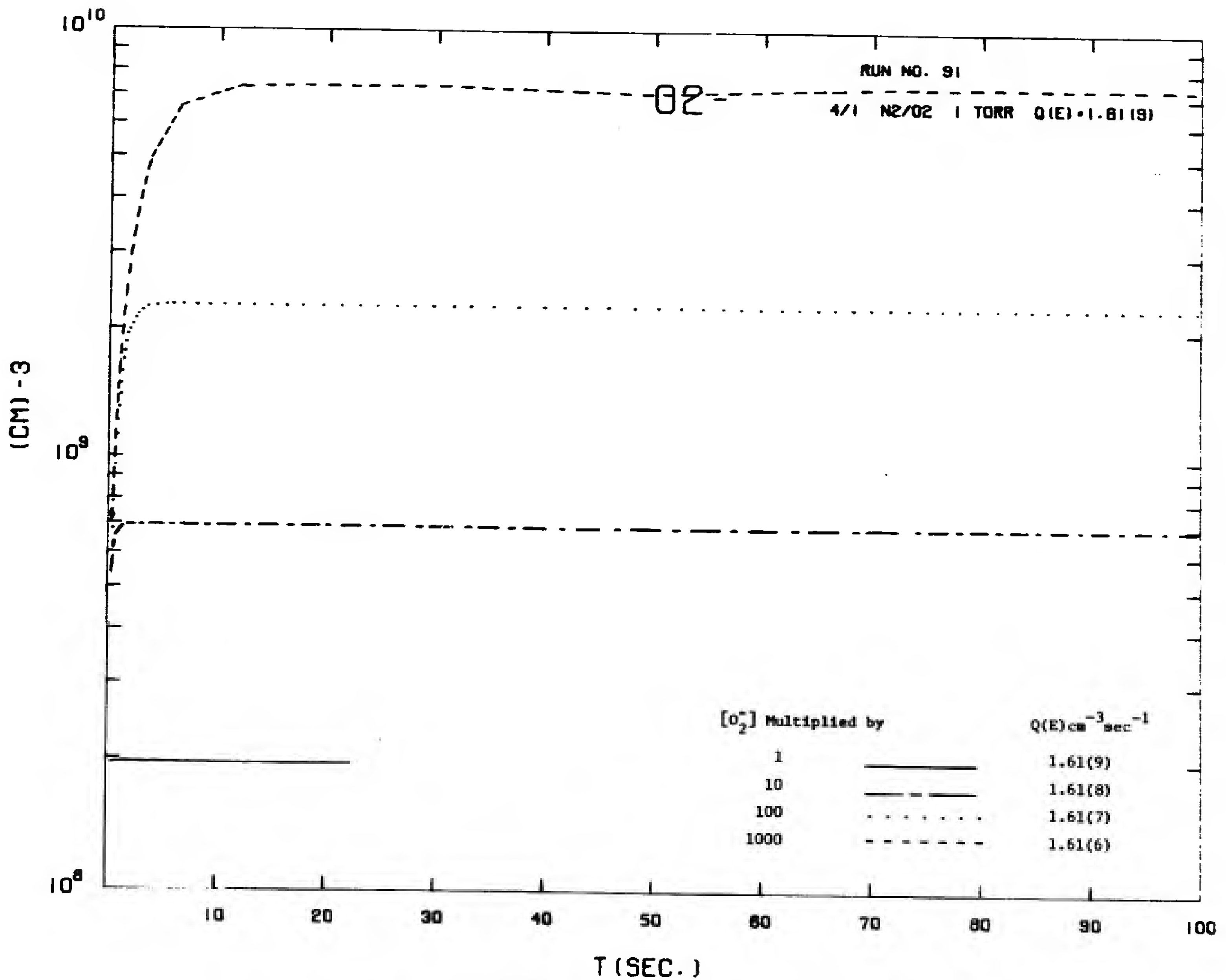

Figure 5. O_2^- density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

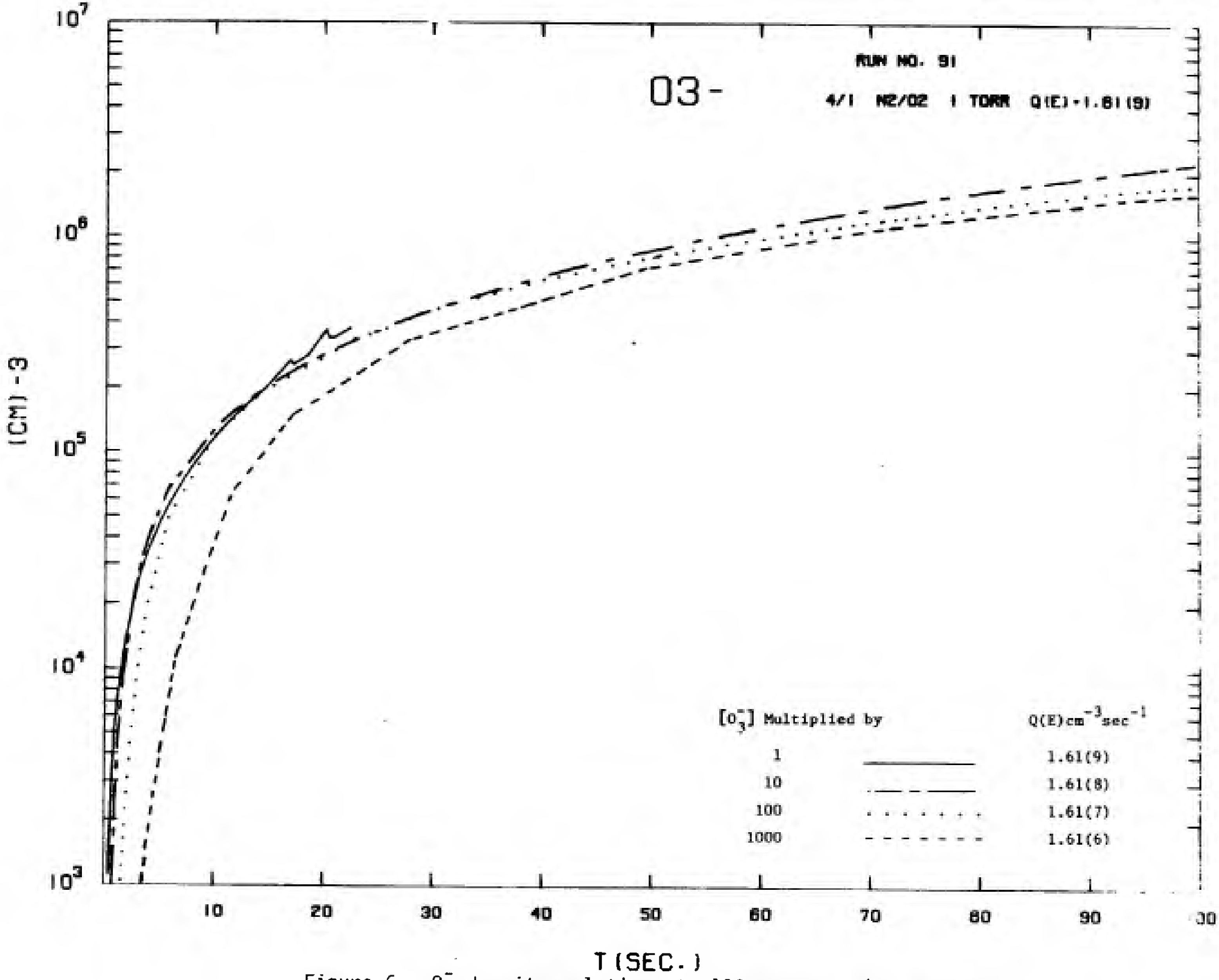

Figure 6. O_3^- density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

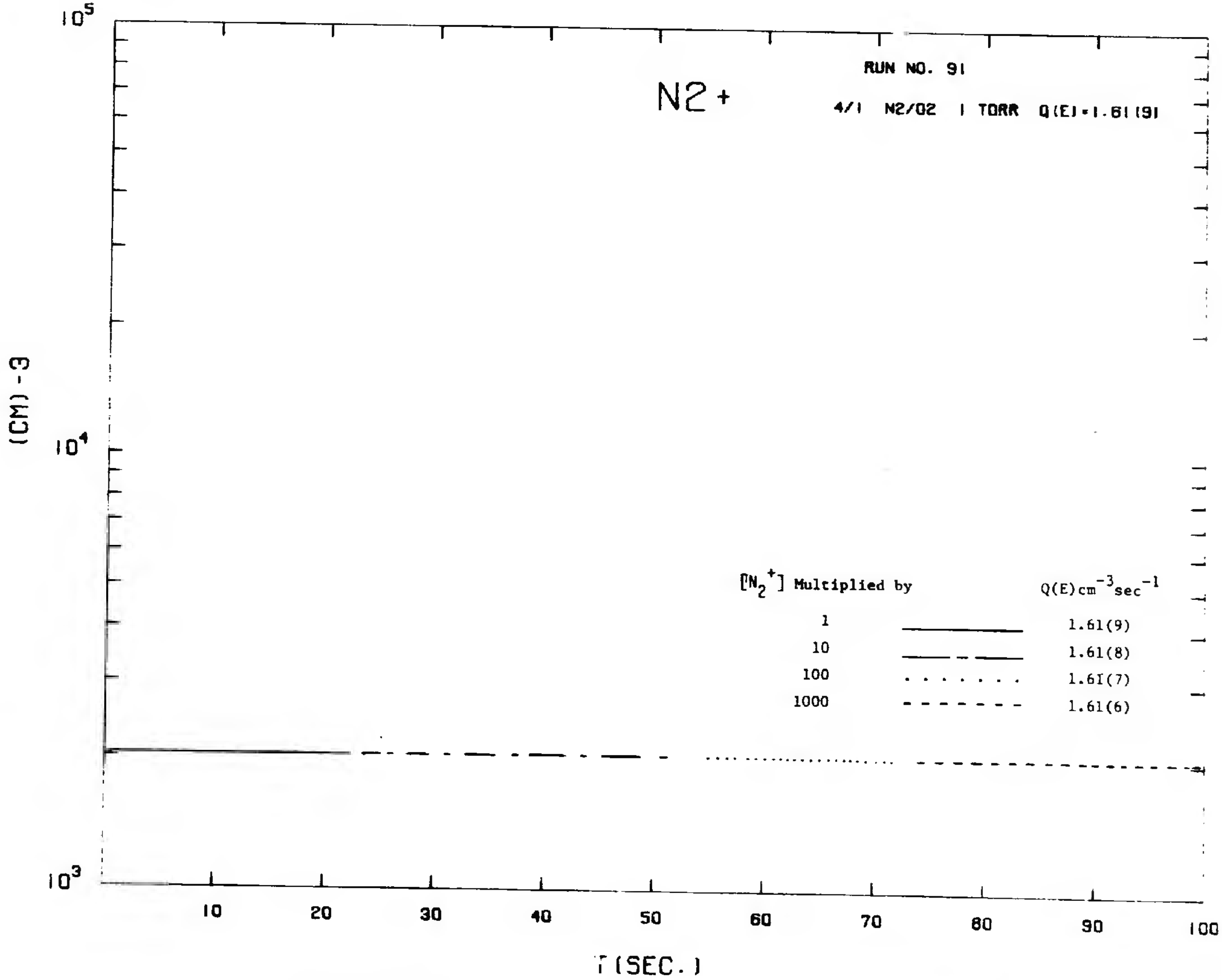

Figure 7. N_2^+ density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

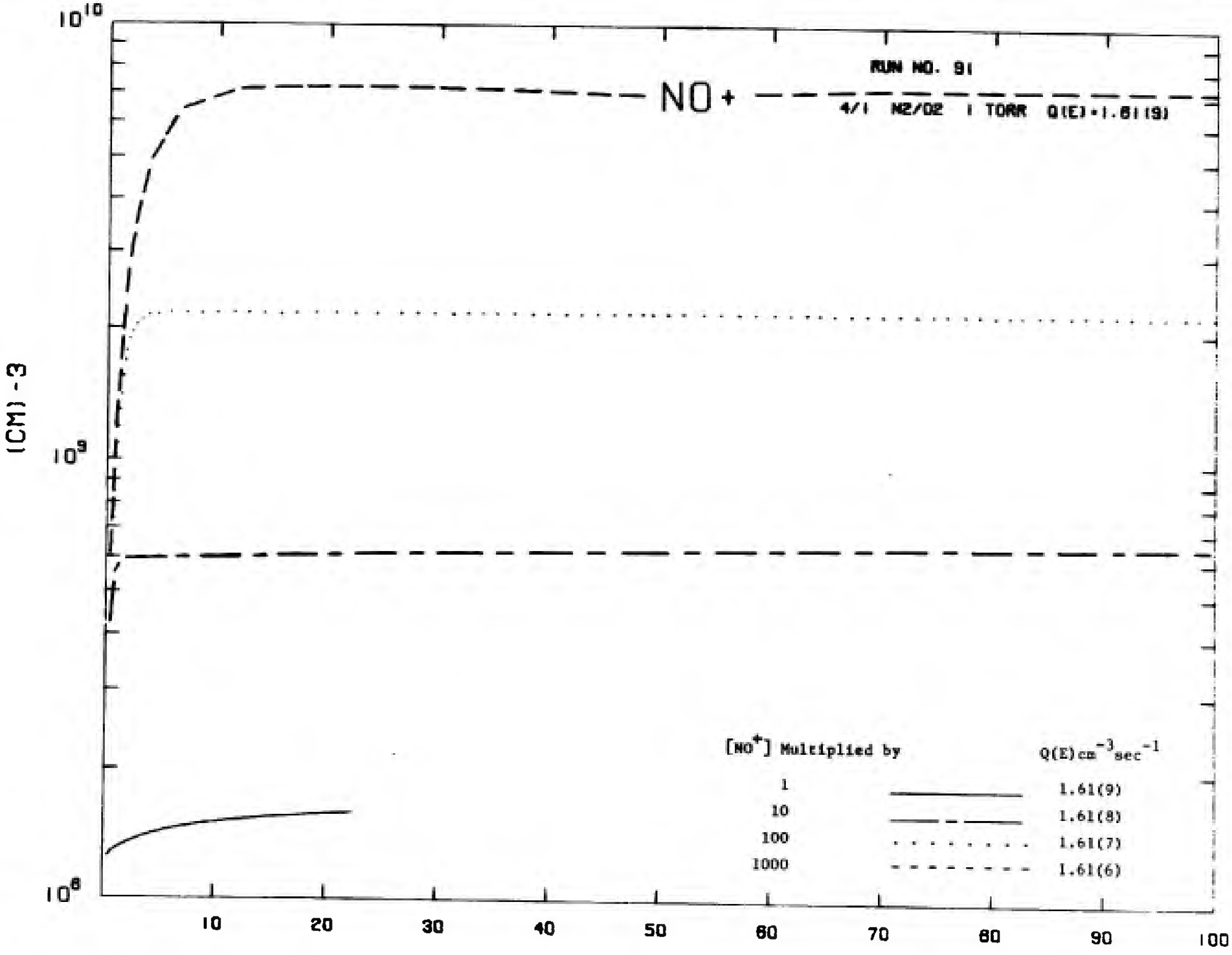

Figure 8. NO^+ density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

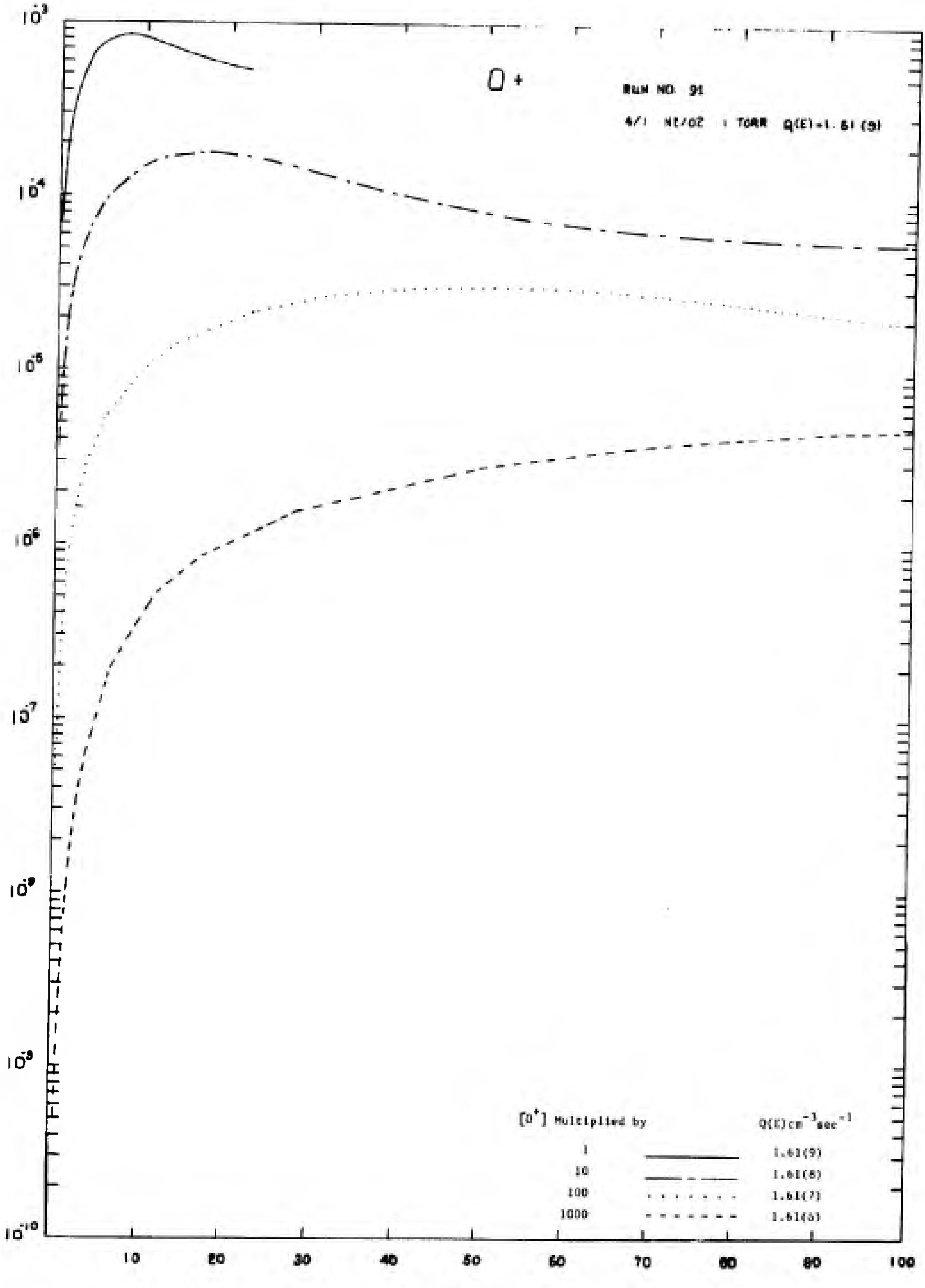

Figure 9. O^+ density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

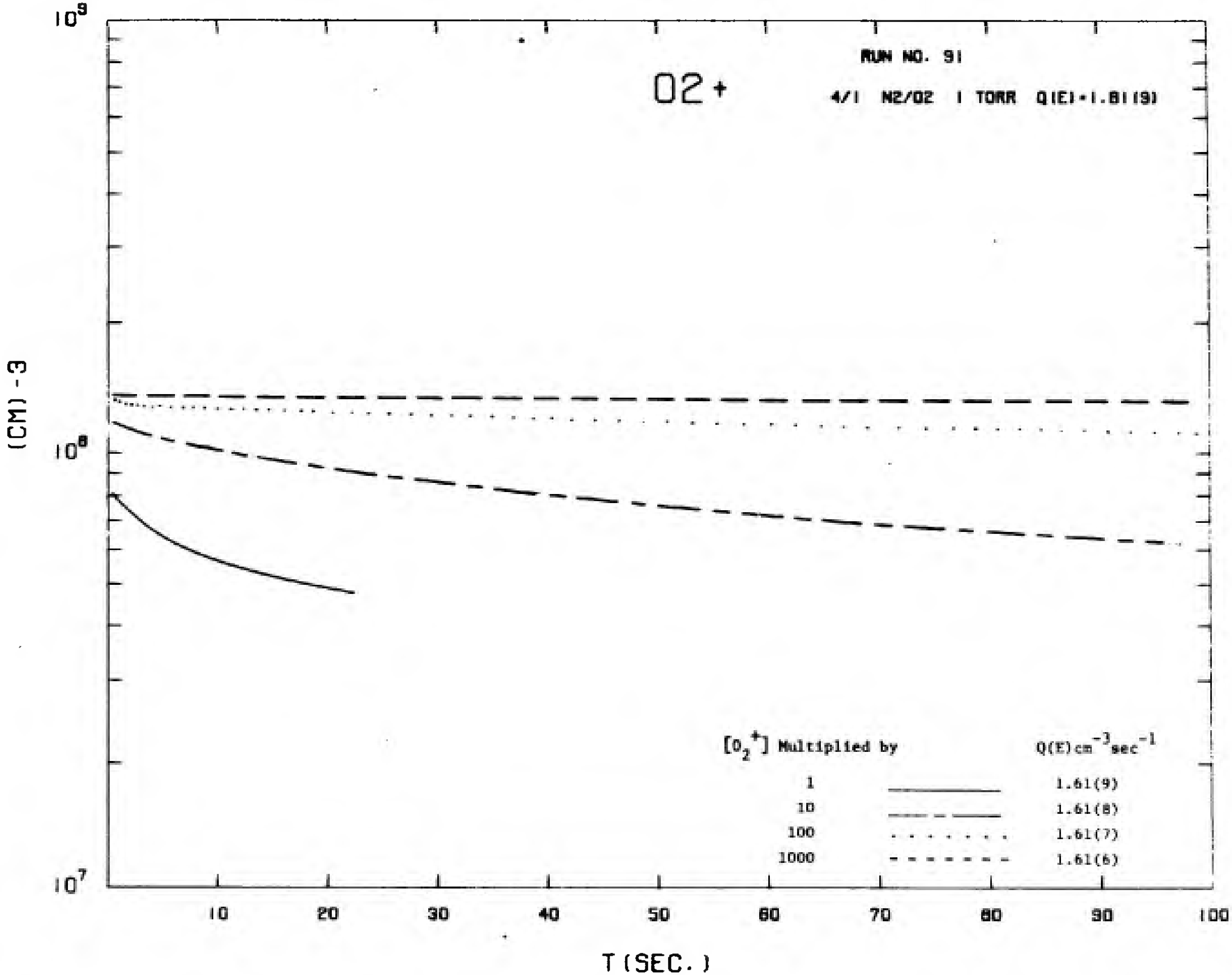

Figure 10. O_2^+ density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

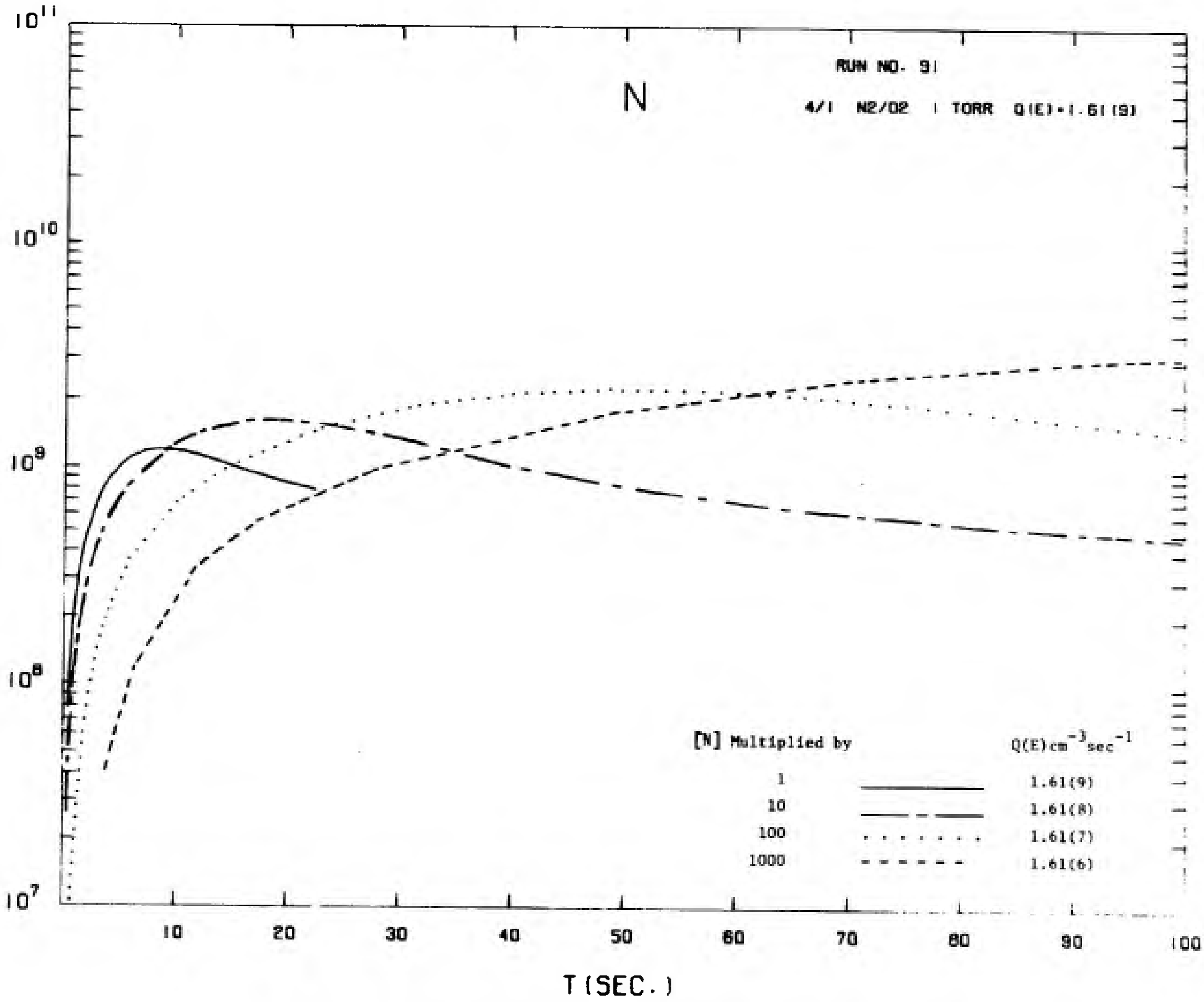

Figure 11. N density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

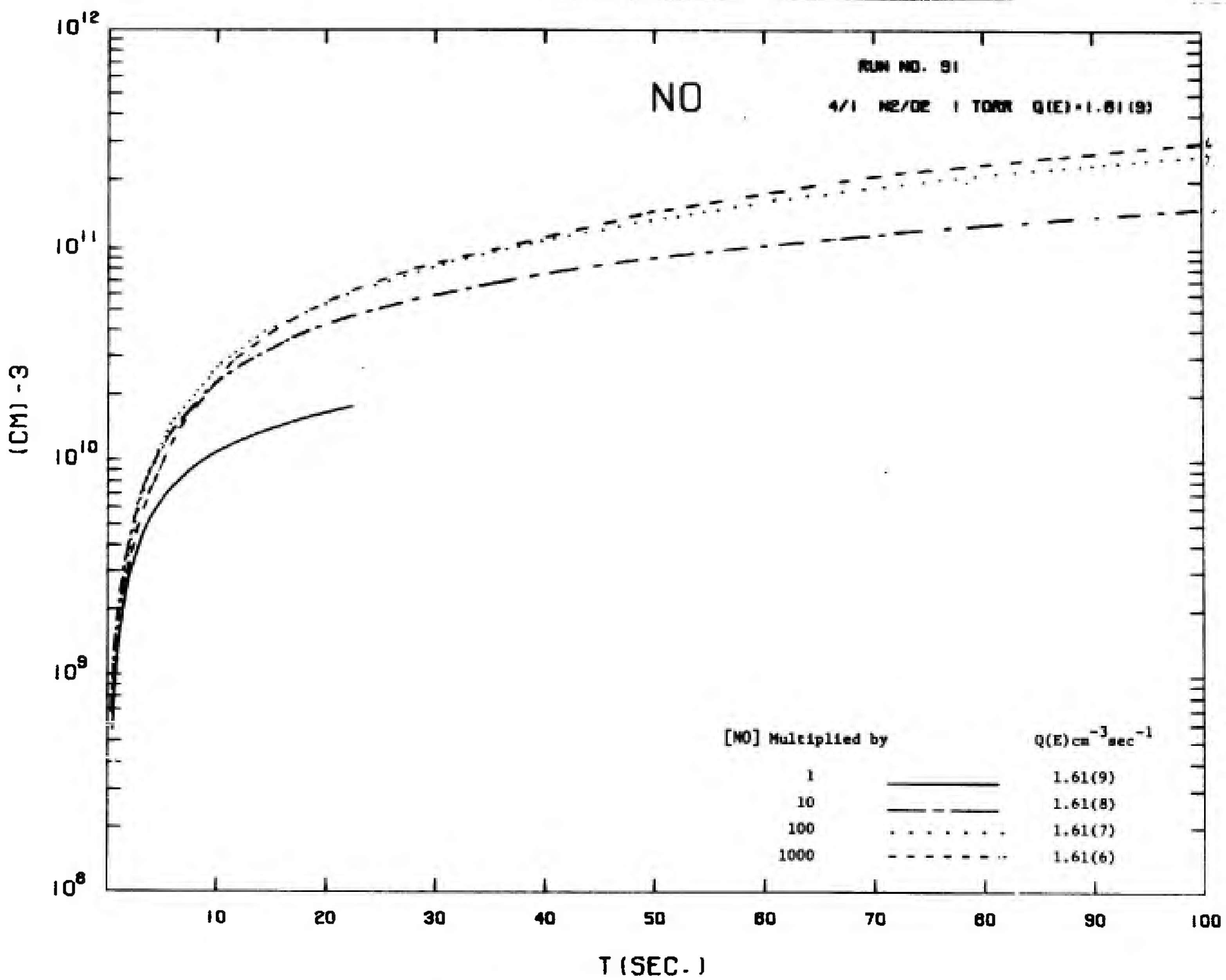

Figure 12. NO density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

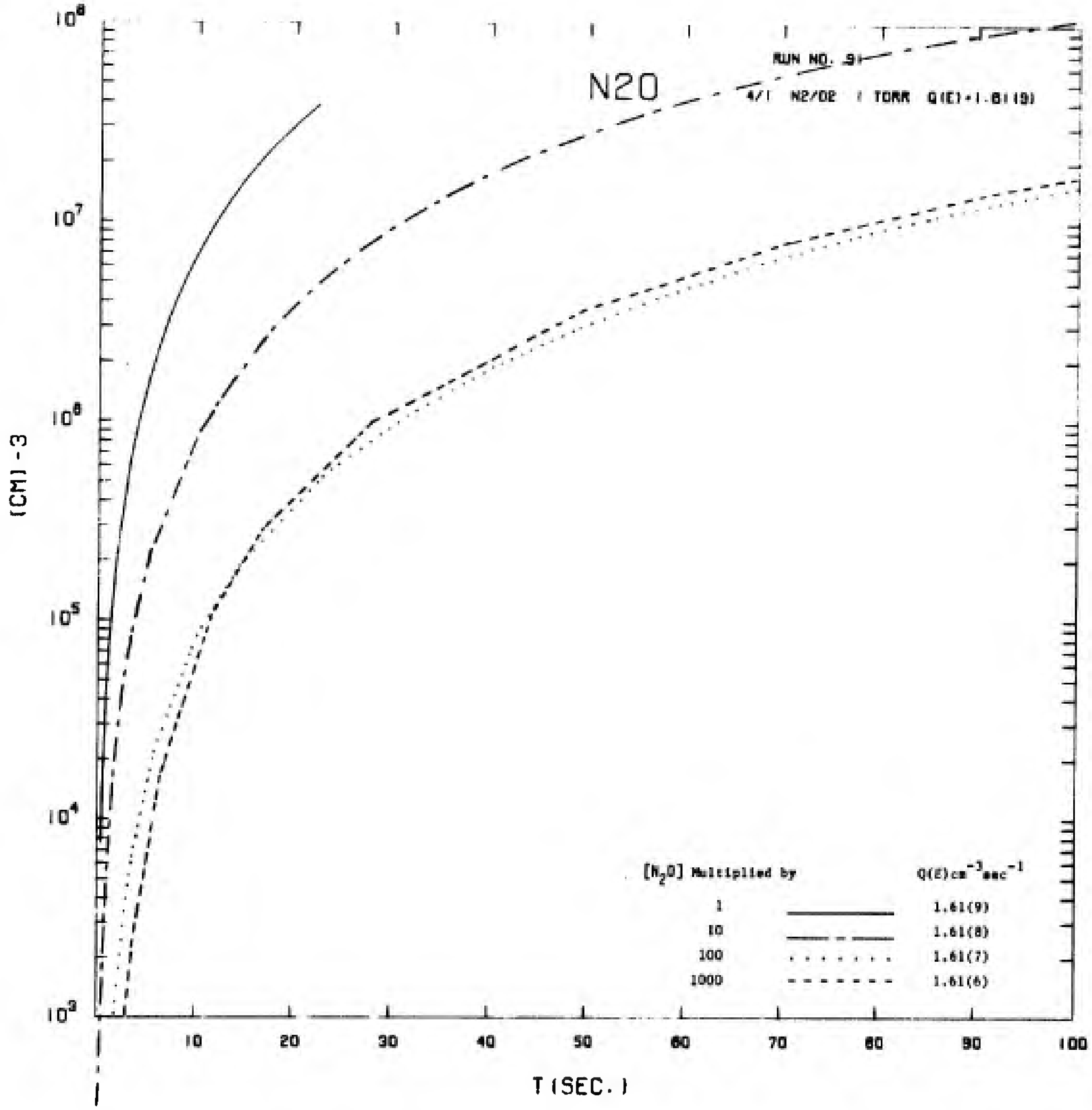

Figure 13. N_2O density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

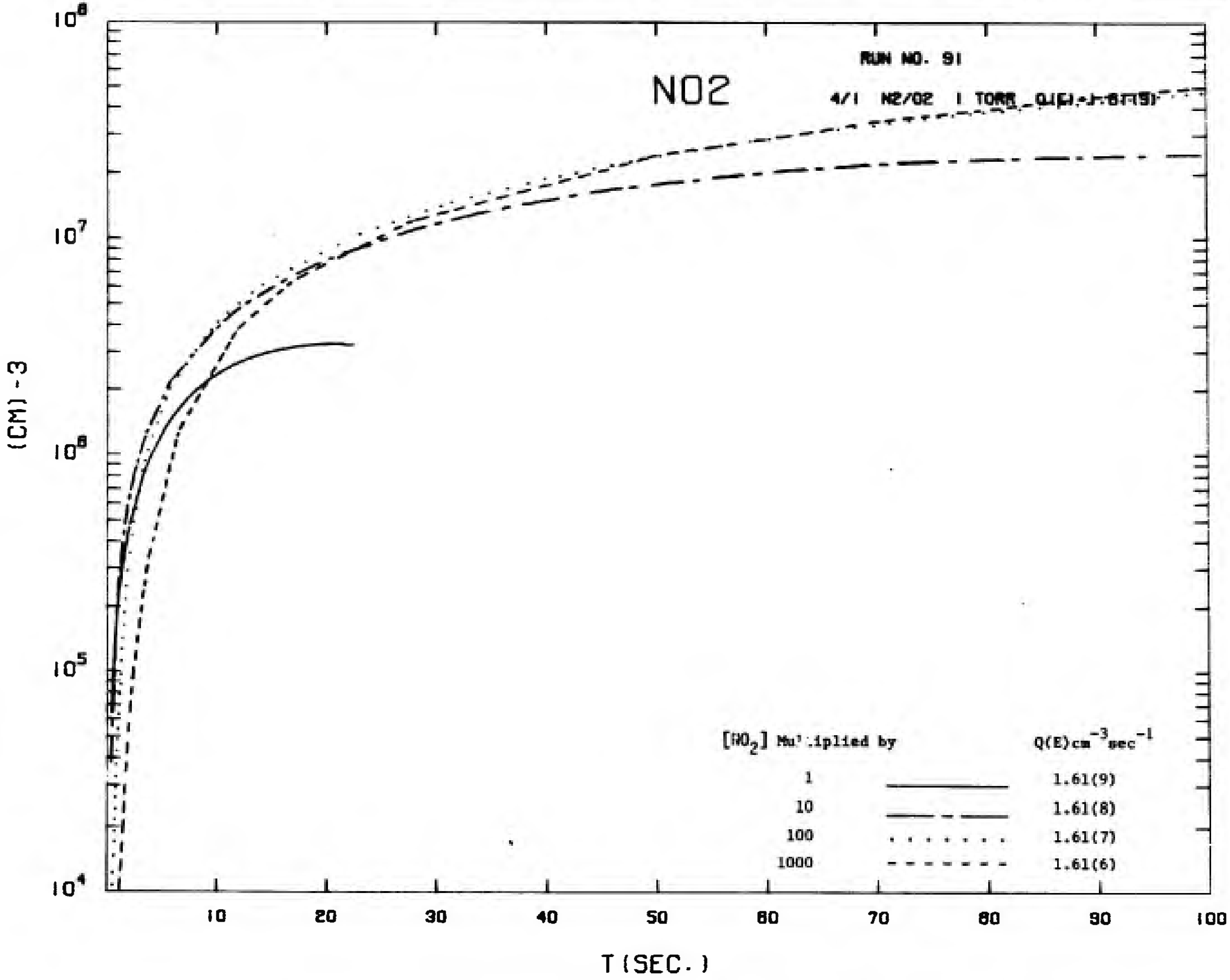

Figure 14. NO_2 density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

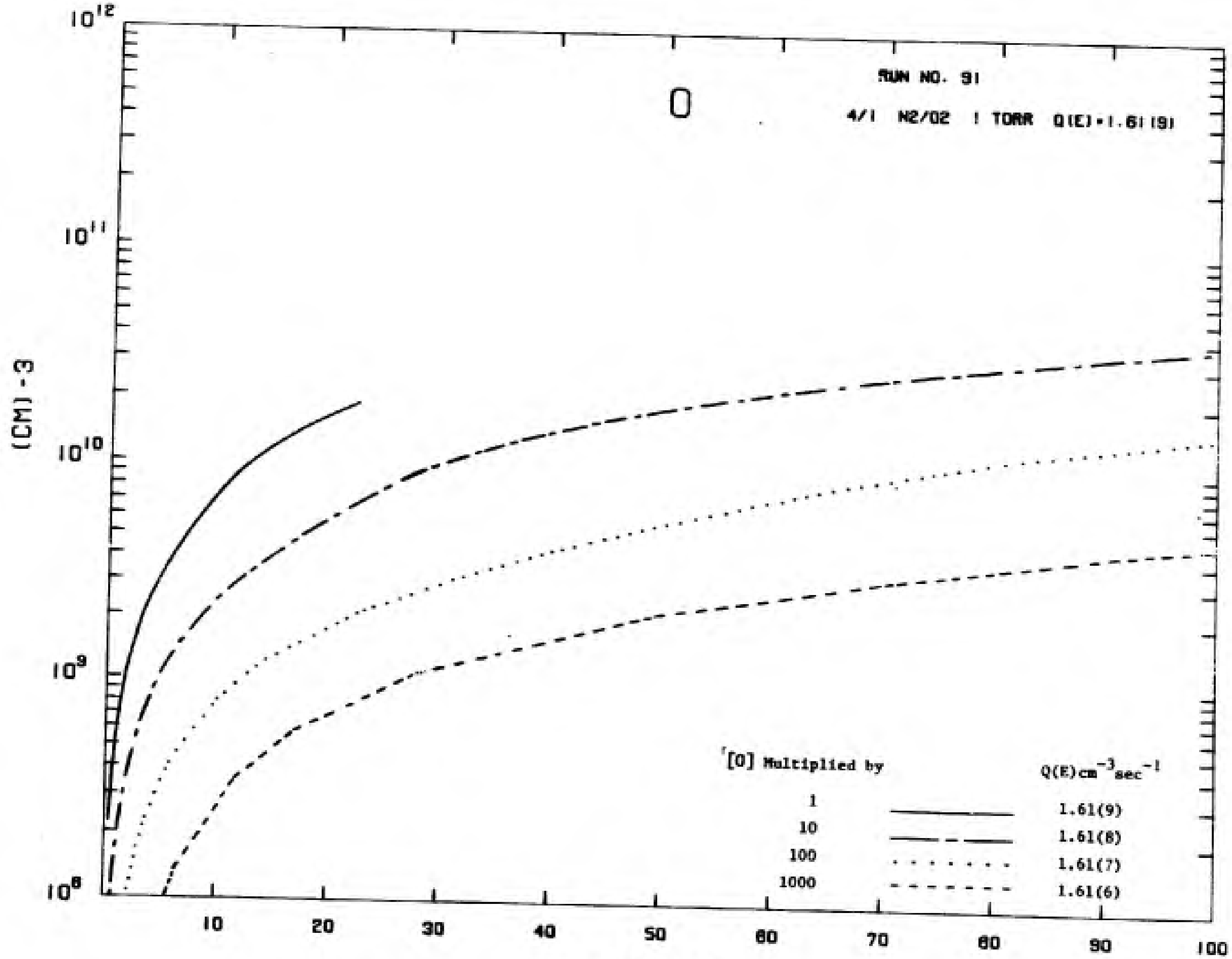

Figure 15. O density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

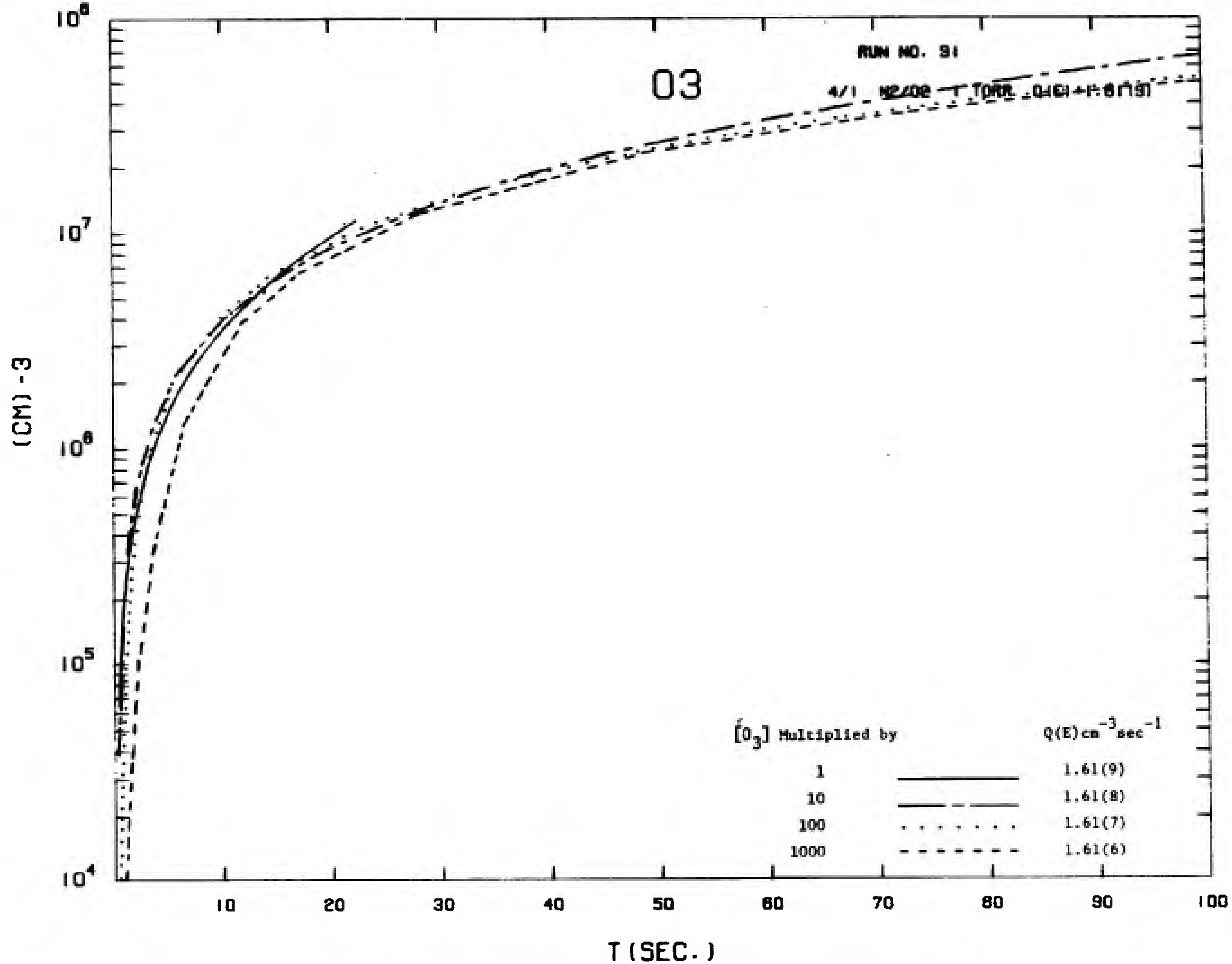

Figure 16. O_3 density solutions to 100 sec for q(e) values of 1.61×10^6, 1.61×10^7, 1.61×10^8, 1.61×10^9 cm^{-3} sec^{-1}

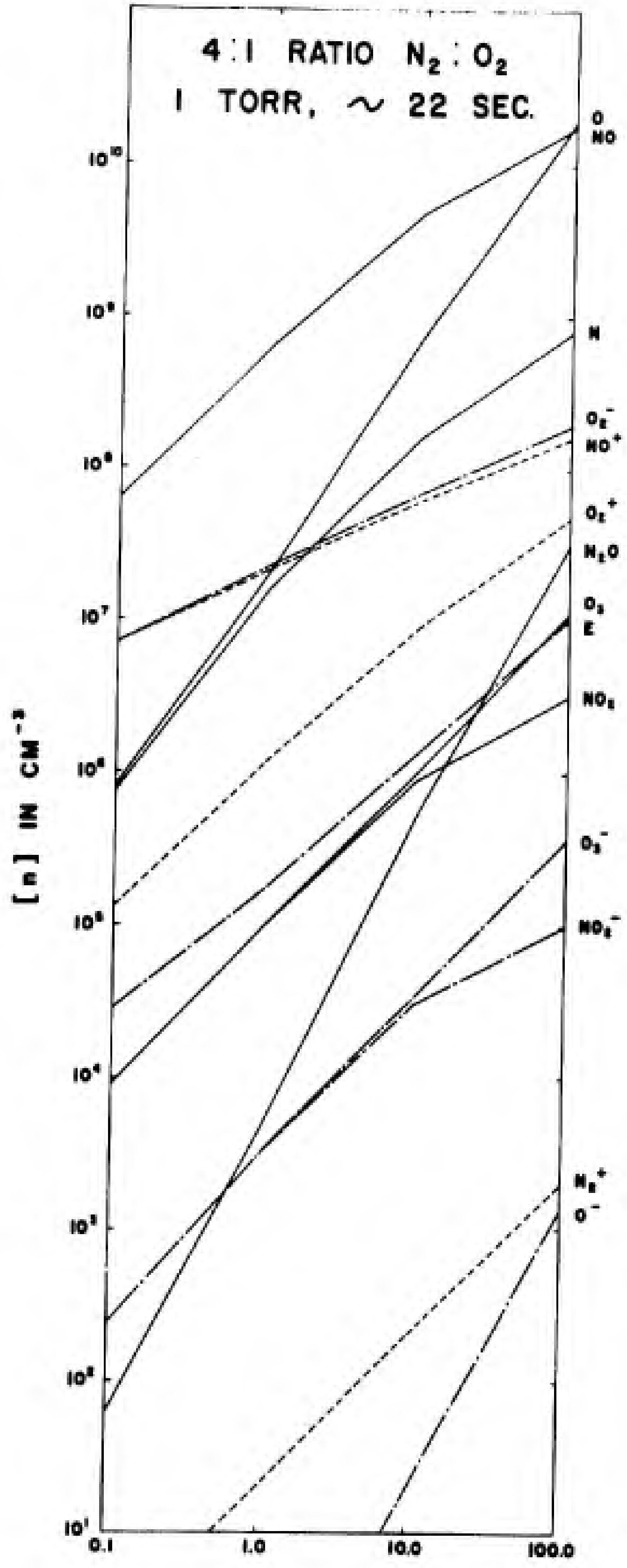

Figure 17. Beam current density in microampere per square meter

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APPENDIX A

REACTIONS AND REACTION RATE CONSTANTS

(Reactions are numbered as used in program)

Reaction No.	Reaction	Rate Constant at 300^oK	Rate Constant
1	$O_2^- + h\nu \rightarrow O_2 + e$	$0.44\ sec^{-1}$	
2	$O^- + h\nu \rightarrow O + e$	$1.4\ sec^{-1}$	
3	$NO_2^- + h\nu \rightarrow NO_2 + e$	$0.04\ sec^{-1}$	
4	$O_3^- + h\nu \rightarrow O_3 + e$	$0.04\ sec^{-1}$	
5	$O_2^- + O_2 \rightarrow O_2 + O_2 + e$	$3.35x10^{-17}\ cm^3/sec$	$9 \times 10^{-15} T^2 e^{-5100/T}$
6	$O_2^- + N_2 \rightarrow N_2 + O_2 + e$	$1.34 \times 10^{-18}\ cm^3/sec$	$3.6 \times 10^{-16} T^2 e^{-5100/T}$
7	$O_2^- + O \rightarrow O + O_2 + e$	$1.34 \times 10^{-18}\ cm^3/sec$	$3.6 \times 10^{-16} T^2 e^{-5100/T}$
8	$O^- + O \rightarrow O_2 + e$	$1 \times 10^{-13}\ cm^3/sec$	
9	$O^- + O_2 \rightarrow O_3 + e$	$1.57 \times 10^{-20}\ cm^3/sec$	$1 \times 10^{-13} e^{-4700/T}$
10	$O^- + N \rightarrow NO + e$	$1 \times 10^{-13}\ cm^3/sec$	
11	$O^- + N_2 \rightarrow N_2O + e$	$1 \times 10^{-13}\ cm^3/sec$	
12	$O^- + NO \rightarrow NO_2 + e$	$1 \times 10^{-13}\ cm^3/sec$	
13	$O^- + O_3 \rightarrow O_2 + O_2 + e$	$1 \times 10^{-13}\ cm^3/sec$	
14	$O_2^- + N \rightarrow NO_2 + e$	$1 \times 10^{-13}\ cm^3/sec$	
15	$O_2^- + O \rightarrow O_3 + e$	$1 \times 10^{-13}\ cm^3 sec$	
16	$O + e \rightarrow O^- + h\nu$	$1.31 \times 10^{-15}\ cm^3/sec$	
17	$O_2 + e \rightarrow O_2^- + h\nu$	$1 \times 10^{-19}\ cm^3/sec$	
18	$NO_2 + e \rightarrow NO_2^- + h\nu$	$1 \times 10^{-17}\ cm^3/sec$	

Reaction No.	Reaction	Rate Constant at 300°K	Rate Constant
19	$O_3 + e \rightarrow O_3^- + h\nu$	1×10^{-17} cm^3/sec	
20	$O_3 + e \rightarrow O^- + O_2$	1×10^{-11} cm^3/sec	
21	$O_3 + e \rightarrow O_2^- + O$	3.78×10^{-22} cm^3/sec	$1 \times 10^{-11}\ e^{-7200/T}$
22	$O + e + O_2 \rightarrow O^- + O_2$	1×10^{-31} cm^6/sec	
23	$O + e + N_2 \rightarrow O^- + N_2$	1×10^{-31} cm^6/sec	
24	$O_2 + e + O_2 \rightarrow O_2^- + O_2$	2.42×10^{-30} cm^6/sec	$1.4 \times 10^{-31} T^{0.5}$
25	$O_2 + e + N_2 \rightarrow O_2^- + N_2$	1×10^{-31} cm^6/sec	$5.8 \times 10^{-33} T^{0.5}$
26	$N_2^+ + e \rightarrow N + N$	3.0×10^{-7} cm^3/sec	$9 \times 10^{-5} T^{-1}$
27	$NO^+ + e \rightarrow N + O$	2.0×10^{-7} cm^3/sec	$6 \times 10^{-5} T^{-1}$
28	$O_2^+ + e \rightarrow O + O$	2.0×10^{-7} cm^3/sec	$6 \times 10^{-5} T^{-1}$
29	$O^+ + e + M \rightarrow O + M$	1.92×10^{-28} cm^6/sec	$1 \times 10^{-24} T^{-1.5}$
30	$O_2^+ + e + M \rightarrow O_2 + M$	1.92×10^{-26} cm^6/sec	$1 \times 10^{-22} T^{-1.5}$
31	$N_2^+ + e + M \rightarrow N_2 + M$	1.92×10^{-26} cm^6/sec	$1 \times 10^{-22} T^{-1.5}$
32	$NO^+ + e + M \rightarrow NO + M$	1.92×10^{-26} cm^6/sec	$1 \times 10^{-22} T^{-1.5}$
33	$NO^+ + e + M \rightarrow N + O + M$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$
34	$O^+ + e \rightarrow O + h\nu$	4.06×10^{-12} cm^3/sec	$2.2 \times 10^{-10} T^{-0.7}$
35	$O_2^+ + e \rightarrow O_2 + h\nu$	1×10^{-12} cm^3/sec	
36	$N_2^+ + e \rightarrow N_2 + h\nu$	1×10^{-12} cm^3/sec	
37	$NO^+ + e \rightarrow NO + h\nu$	1×10^{-12} cm^3/sec	
38	$O^- + NO^+ \rightarrow O + NO$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
39	$O^- + N_2^+ \rightarrow O + N_2$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
40	$O^- + O_2^+ \rightarrow O + O_2$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$

Reaction No.	Reaction	Rate Constant at 300°K	Rate Constant
41	$O^- + O^+ \rightarrow O + O$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
42	$O_2^- + O^+ \rightarrow O_2 + O$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
43	$O_2^- + O_2^+ \rightarrow O_2 + O_2$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
44	$O_2^- + N_2^+ \rightarrow O_2 + N_2$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
45	$O_2^- + NO^+ \rightarrow O_2 + NO$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
46	$O_3^- + O_2^+ \rightarrow O_3 + O_2$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
47	$O_3^- + NO^+ \rightarrow O_3 + NO$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
48	$NO_2^- + NO^+ \rightarrow NO_2 + NO$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
49	$NO_2^- + O^+ \rightarrow NO_2 + O$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
50	$NO_2^- + O_2^+ \rightarrow NO_2 + O_2$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
51	$O_3^- + O^+ \rightarrow O_3 + O$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
52	$O^- + O^+ + N \rightarrow O_2 + N$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$
53	$O^- + O_2^+ + M \rightarrow O_3 + M$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$
54	$O^- + N_2^+ + M \rightarrow N_2O + M$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$
55	$O^- + NO^+ + M \rightarrow NO_2 + M$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$
56	$O^- + O^+ + O_2 \rightarrow O_2 + O_2$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$
57	$O^- + O^+ + N_2 \rightarrow O_2 + N_2$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$
58	$O^- + O^+ + O \rightarrow O_2 + O$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$
59	$O_2^- + O_2^+ + M \rightarrow O_2 + O_2 + M$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$
60	$O_2^- + N_2^+ + M \rightarrow O_2 + N_2 + M$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$

Reaction No.	Reaction	Rate Constant at 300°K	Rate Constant
61	$O_2^- + NO^+ + M \rightarrow O_2 + NO + M$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$
62	$O_2^- + O^+ + M \rightarrow O_3 + M$	1.92×10^{-27} cm^6/sec	$1 \times 10^{-23} T^{-1.5}$
63	$O_2^- + O \rightarrow O_2 + O^-$	1×10^{-12} cm^3/sec	
64	$O^- + O_3 \rightarrow O + O_3^-$	1×10^{-9} cm^3/sec	
65	$O^- + NO_2 \rightarrow O + NO_2^-$	1×10^{-9} cm^3/sec	
66	$O_2^- + O_3 \rightarrow O_2 + O_3^-$	1×10^{-9} cm^3/sec	
67	$O_2^- + NO_2 \rightarrow O_2 + NO_2^-$	1×10^{-9} cm^3/sec	
68	$NO_2^- + O_3 \rightarrow NO_2 + O_3^-$	1×10^{-9} cm^3/sec	
69	$N_2^+ + O \rightarrow N_2 + O^+$	1×10^{-12} cm^3/sec	
70	$O^+ + O_2 \rightarrow O + O_2^+$	4×10^{-11} cm^3/sec	
71	$O^+ + NO \rightarrow O + NO^+$	2.4×10^{-11} cm^3/sec	
72	$O_2^+ + NO \rightarrow O_2 + NO^+$	8×10^{-10} cm^3/sec	
73	$N_2^+ + O_2 \rightarrow N_2 + O_2^+$	1×10^{-10} cm^3/sec	
74	$N_2^+ + N \rightarrow N_2 + N^+$	0 cm^3/sec	
75	$N_2^+ + NO \rightarrow N_2 + NO^+$	5×10^{-12} cm^3/sec	
76	$O^+ + NO_2 \rightarrow O + NO_2^+$	0 cm^3/sec	
77	$O^+ + O \rightarrow O_2^+ + h\nu$	1×10^{-16} cm^3/sec	
78	$O^+ + N \rightarrow NO^+ + h\nu$	1×10^{-18} cm^3/sec	
79	$O^+ + N_2 \rightarrow N_2O^+ + h\nu$	0 cm^3/sec	
80	$O^+ + NO \rightarrow NO_2^+ + h\nu$	0 cm^3/sec	

Reaction No.	Reaction			Rate Constant at 300^oK	Rate Constant
81	$O_2^+ + O$	→	$O_3^+ + h\nu$	0 cm^3/sec	
82	$NO^+ + O$	→	$NO_2^+ + h\nu$	0 cm^3/sec	
83	$O^+ + N_2$	→	$NO^+ + N$	3×10^{-12} cm^3/sec	
84	$O^+ + NO$	→	$O_2^+ + N$	3×10^{-12} cm^3/sec	
85	$O_2^+ + N$	→	$O^+ + NO$	3.82×10^{-15} cm^3/sec	$3 \times 10^{-12}e^{-2000/T}$
86	$O_2^+ + N_2$	→	$NO^+ + NO$	4.54×10^{-16} cm^3/sec	$1 \times 10^{-11}e^{-3000/T}$
87	$O_2^+ + N$	→	$NO^+ + O$	1.8×10^{-10} cm^3/sec	
88	$N_2^+ + O$	→	$NO^+ + N$	2.5×10^{-10} cm^3/sec	
89	$N_2^+ + O_2$	→	$NO^+ + NO$	8.57×10^{-17} cm^3/sec	$1 \times 10^{-11}e^{-3500/T}$
90	$O^+ + O + M$	→	$O_2^+ + M$	1×10^{-29} cm^6/sec	
91	$O^+ + N + M$	→	$NO^+ + M$	1×10^{-29} cm^6/sec	
92	$O^+ + N_2 + M$	→	$N_2O^+ + M$	0 cm^6/sec	
93	$N + N + M$	→	$N_2 + M$	2.0×10^{-32} cm^6/sec	$6 \times 10^{-30}T^{-1}$
94	$N + O + M$	→	$NO + M$	1.15×10^{-32} cm^6/sec	$2 \times 10^{-31}T^{-0.5}$
95	$NO + O + M$	→	$NO_2 + M$	0 cm^6/sec	
96	$O + O_2 + M$	→	$O_3 + M$	0 cm^6/sec	
97	$N + N + N_2$	→	$N_2 + N_2$	0 cm^6/sec	
98	$N + N + N$	→	$N_2 + N$	0 cm^6/sec	
99	$N + O$	→	$NO + h\nu$	2×10^{-17} cm^3/sec	
100	$NO + O$	→	$NO_2 + h\nu$	6.4×10^{-17} cm^3/sec	

Reaction No.	Reaction			Rate Constant at 300°K	Rate Constant
101	$N + NO$	→	$N_2O + h\nu$	1×10^{-22} cm^3/sec	
102	$N + O_2$	→	$NO_2 + h\nu$	1×10^{-22} cm^3/sec	
103	$O + O_2$	→	$O_3 + h\nu$	1×10^{-21} cm^3/sec	
104	$O + O_3$	→	$O_2 + O_2$	4.42×10^{-14} cm^3/sec	$5 \times 10^{-10} e^{-2800/T}$
105	$N + O_3$	→	$NO + O_2$	0 cm^3/sec	
106	$NO_2 + O$	→	$NO + O_2$	5.13×10^{-12} cm^3/sec	$3 \times 10^{-11} e^{-530/T}$
107	$N + NO_2$	→	$O_2 + N_2$	1.47×10^{-23} cm^3/sec	$2 \times 10^{-13} e^{-7000/T}$
108	$N + NO_2$	→	$NO + NO$	4×10^{-12} cm^3/sec	
109	$N + NO$	→	$O + N_2$	2.5×10^{-11} cm^3/sec	
110	$N + O_2$	→	$NO + O$	4.35×10^{-22} cm^3/sec	$3 \times 10^{-16} T^{1.5} e^{-6600/T}$
111	$O_3^- + NO_2$	→	$O_3 + NO_2^-$	1×10^{-9} cm^3/sec	
112	$O^- + O_2$	→	$O_3^- + h\nu$	1×10^{-15} cm^3/sec	
113	$O_2^- + O_2 + N_2$	→	$NO_2^- + NO_2$	5.78×10^{-42} cm^6/sec	$1 \times 10^{-34} e^{-5000/T}$
114	$O_3^- + N_2$	→	$NO_2^- + NO$	1.62×10^{-23} cm^3/sec	$1 \times 10^{-17} e^{-4000/T}$
115	$O_2^+ + NO_2$	→	$NO^+ + O_3$	1×10^{-11} cm^3/sec	
116	$O_2^- + NO^+$	→	$NO_2 + O$	1×10^{-11} cm^3/sec	
117	$O_2^- + NO^+$	→	$N + O_3$	1×10^{-11} cm^3/sec	
118	$O_2^- + NO^+$	→	$N + O + O_2$	1×10^{-13} cm^3/sec	
119	$O_2^- + N_2^+$	→	$NO + NO$	1×10^{-11} cm^3/sec	
120	$O_2^- + N_2^+$	→	$NO_2 + N$	1×10^{-13} cm^3/sec	

Reaction No.	Reaction			Rate Constant at 300°K	Rate Constant
121	$O_2^- + N_2^+$	→	$N + N + O + O$	0 cm^3/sec	
122	$NO_2^- + NO^+$	→	$NO_3 + N$	0 cm^3/sec	
123	$NO_2^- + NO^+$	→	$N + NO + O_2$	1×10^{-13} cm^3/sec	
124	$O_2^- + N_2^+$	→	$N_2O + O$	1×10^{-13} cm^3/sec	
125	$NO_2^- + NO^+$	→	$O_3 + N_2$	5.78×10^{-21} cm^3/sec	$1 \times 10^{-13} e^{-5000/T}$
126	$O_3^- + NO^+$	→	$N + O_2 + O_2$	1×10^{-13} cm^3/sec	
127	$O_3^- + NO^+$	→	$NO_2 + O_2$	1×10^{-13} cm^3/sec	
128	$NO + NO + O_2$	→	$NO_2 + NO_2$	0 cm^6/sec	
129	$NO + h\nu$	→	$N + O$	6×10^{-8} cm^3/sec	
130	$O_3 + h\nu$	→	$O + O_2$	5.34×10^{-3} cm^3/sec	
131	$NO_2 + h\nu$	→	$NO + O$	3×10^{-3} cm^3/sec	
132	$N_2O + h\nu$	→	$N + NO$	5.55×10^{-8} cm^3/sec	
133	$N_2O + h\nu$	→	$O + N_2$	4.08×10^{-7} cm^3/sec	
134	$O^+ + N_2O$	→	$O + N_2O^+$	0 cm^3/sec	
135	$N_2^+ + N_2$	→	$N_4^+ + h\nu$	0 cm^3/sec	
136	$O + O + O_2$	→	$O_2 + O_2$	2.89×10^{-33} cm^6/sec	$5 \times 10^{-32} T^{-0.5}$
137	$O + O + O$	→	$O + O_2$	1.15×10^{-32} cm^6/sec	$2 \times 10^{-31} T^{-0.5}$
138	$O + O + N_2$	→	$O_2 + N_2$	2.89×10^{-33} cm^6/sec	$5 \times 10^{-32} T^{-0.5}$
139	$O + O$	→	$O_2 + h\nu$	1×10^{-21} cm^3/sec	
140	$N_2 + O$	→	$N_2O + h\nu$	1×10^{-24} cm^3/sec	

Reaction No.	Reaction		Rate Constant at 300°K	Rate Constant
141	$NO_2^- + N_2^+$	→ $N_2O + NO$	1×10^{-13} cm^3/sec	
142	$O_3^- + N_2^+$	→ $N_2O + O_2$	1×10^{-13} cm^3/sec	
143	$O_2 + h\nu$	→ $O + O$	0 cm^3/sec	
144	$O + e + O_2$	→ $O_2^- + O$	3.29×10^{-32} cm^6/sec	$1.9 \times 10^{-33} T^{0.5}$
145	$NO_2 + e + O_2$	→ $NO_2^- + O_2$	6×10^{-28} cm^6/sec	
146	$NO_2 + e + N_2$	→ $NO_2^- + N_2$	4×10^{-29} cm^6/sec	
147	$NO_2^- + N_2^+$	→ $NO_2 + N_2$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
148	$O_3^- + N_2^+$	→ $N_2 + O_3$	2.89×10^{-8} cm^3/sec	$5 \times 10^{-7} T^{-0.5}$
149	$O^- + NO + M$	→ $NO_2^- + M$	1×10^{-30} cm^6/sec	
150	$O_2^- + N + M$	→ $NO_2^- + M$	1×10^{-30} cm^6/sec	
151	$O^- + O_2 + O_2$	→ $O_3^- + O_2$	3.33×10^{-31} cm^6/sec	$1 \times 10^{-28} T^{-1}$
152	$N + N$	→ $N_2 + h\nu$	1×10^{-24} cm^3/sec	
153	$O + O_2 + O_2$	→ $O_2 + O_3$	0 cm^6/sec	
154	$O + O_2 + N_2$	→ $O_3 + N_2$	0 cm^6/sec	
155	$O + O + O_2$	→ $O + O_3$	6.5×10^{-34} cm^6/sec	
156	$O + N_2 + M$	→ $N_2O + M$	6.68×10^{-48} cm^6/sec	$2 \times 10^{-33} e^{-10000/T}$
157	$NO + O + O_2$	→ $NO_2 + O_2$	0 cm^6/sec	
158	$NO + O + N_2$	→ $NO_2 + N_2$	0 cm^6/sec	
159	$N + O_2 + M$	→ $NO_2 + M$	4.54×10^{-38} cm^6/sec	$1 \times 10^{-33} e^{-3000/T}$
160	$N + NO + M$	→ $N_2O + M$	3.34×10^{-48} cm^6/sec	$1 \times 10^{-33} e^{-10000/T}$

Reaction No.	Reaction			Rate Constant at 300°K	Rate Constant
161	$O + N_2$	→	$N + NO$	5.17×10^{-65} cm^3/sec	$1 \times 10^{-10} e^{-37500/T}$
162	$NO + O$	→	$N + O_2$	1.15×10^{-40} cm^3/sec	$7.1 \times 10^{-17} T^{1.5} e^{-19000/T}$
163	$N_2O + O$	→	$NO + NO$	1.88×10^{-12} cm^3/sec	$2 \times 10^{-10} e^{-1400/T}$
164	$N_2O + O$	→	$O_2 + N_2$	1.43×10^{-30} cm^3/sec	$5 \times 10^{-11} e^{-13500/T}$
165	$N + NO_2$	→	$N_2O + O$	2×10^{-11} cm^3/sec	
166	$NO + O_3$	→	$NO_2 + O_2$	1.47×10^{-14} cm^3/sec	$8 \times 10^{-13} e^{-1200/T}$

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APPENDIX B

FORMATION AND REMOVAL TERMS FOR EACH SPECIES

$$\frac{d(e)}{dt} = \sum F(e) - e\sum R(e)$$

REACTIONS

Forming (e)

$PNE \rightarrow$ external source

$NO_2^- + h\nu \rightarrow NO_2 + e$

$O^- + h\nu \rightarrow O + e$

$O^- + N \rightarrow NO + e$

$O^- + N_2 \rightarrow N_2O + e$

$O^- + NO \rightarrow NO_2 + e$

$O^- + O \rightarrow O_2 + e$

$O^- + O_2 \rightarrow O_3 + e$

$O^- + O_3 \rightarrow O_2 + O_2 + e$

$O_2^- + h\nu \rightarrow O_2 + e$

$O_2^- + N \rightarrow NO_2 + e$

$O_2^- + N_2 \rightarrow N_2 + O_2 + e$

$O_2^- + O \rightarrow O + O_2 + e$

$O_2^- + O \rightarrow O_3 + e$

$O_2^- + O_2 \rightarrow O_2 + O_2 + e$

$O_3^- + h\nu \rightarrow O_3 + e$

Removing (e)

$e + N_2^+ \rightarrow N + N$

$e + N_2^+ \rightarrow N_2 + h\nu$

$e + N_2^+ + M \rightarrow N_2 + M$

$e + NO^+ \rightarrow N + O$

$e + NO^+ \rightarrow NO + h\nu$

$e + NO^+ + M \rightarrow N + O + M$

$e + NO^+ + M \rightarrow NO + M$

$e + O^+ \rightarrow O + h\nu$

$e + O^+ + M \rightarrow O + M$

$e + O_2^+ \rightarrow O + O$

$e + O_2^+ \rightarrow O_2 + h\nu$

$e + O_2^+ + M \rightarrow O_2 + M$

$e + NO_2 \rightarrow NO_2^- + h\nu$

$e + NO_2 + N_2 \rightarrow NO_2^- + N_2$

$e + NO_2 + O_2 \rightarrow NO_2^- + O_2$

$e + O \rightarrow O^- + h\nu$

$e + O + N_2 \rightarrow O^- + N_2$

$e + O + O_2 \rightarrow O^- + O_2$

$e + O + O_2 \rightarrow O_2^- + O$

$e + O_2 \rightarrow O_2^- + h\nu$

$e + O_2 + N_2 \rightarrow O_2^- + N_2$

$e + O_2 + O_2 \rightarrow O_2^- + O_2$

Forming (e)

Removing (e)

$$e + O_3 \rightarrow O^- + O_2$$

$$e + O_3 \rightarrow O_2^- + O$$

$$e + O_3 \rightarrow O_3^- + h\nu$$

$$\frac{d(NO_2^-)}{dt} = \sum F(NO_2^-) - NO_2^- \sum R(NO_2^-)$$

REACTIONS

Forming (NO_2^-)			Removing (NO_2^-)		
$O^- + NO + M$	$\rightarrow$	$NO_2^- + M$	$NO_2^- + h\nu$	$\rightarrow$	$NO_2 + e$
$O_2^- + N + M$	$\rightarrow$	$NO_2^- + M$	$NO_2^- + N_2^+$	$\rightarrow$	$NO_2 + N_2$
$O_2^- + NO_2$	$\rightarrow$	$NO_2^- + O_2$	$NO_2^- + N_2^+$	$\rightarrow$	$N_2O + NO$
$O_2^- + O_2 + N_2$	$\rightarrow$	$NO_2^- + NO_2$	$NO_2^- + NO^+$	$\rightarrow$	$N + NO + O_2$
$O_3^- + N_2$	$\rightarrow$	$NO_2^- + NO$	$NO_2^- + NO^+$	$\rightarrow$	$NO_2 + NO$
$O_3^- + NO_2$	$\rightarrow$	$NO_2^- + O_3$	$NO_2^- + NO^+$	$\rightarrow$	$NO_3 + N$
$NO_2 + e$	$\rightarrow$	$NO_2^- + h\nu$	$NO_2^- + NO^+$	$\rightarrow$	$O_3 + N_2$
$NO_2 + e + N_2$	$\rightarrow$	$NO_2^- + N_2$	$NO_2^- + O^+$	$\rightarrow$	$NO_2 + O$
$NO_2 + e + O_2$	$\rightarrow$	$NO_2^- + O_2$	$NO_2^- + O_2^+$	$\rightarrow$	$NO_2 + O_2$
$NO_2 + O^-$	$\rightarrow$	$NO_2^- + O$	$NO_2^- + O_3$	$\rightarrow$	$NO_2 + O_3^-$

$$\frac{d(O^-)}{dt} = \sum F(O^-) - O^- \sum R(O^-)$$

REACTIONS

Forming (O^-)

$O_2^- + O$	$\rightarrow$	$O^- + O_2$
$O + e$	$\rightarrow$	$O^- + h\nu$
$O + e + N_2$	$\rightarrow$	$O^- + N_2$
$O + e + O_2$	$\rightarrow$	$O^- + O_2$
$O_3 + e$	$\rightarrow$	$O^- + O_2$

Removing (O^-)

$O^- + h\nu$	$\rightarrow$	$O + e$
$O^- + N_2^+$	$\rightarrow$	$O + N_2$
$O^- + N_2^+ + M$	$\rightarrow$	$N_2O + M$
$O^- + NO^+$	$\rightarrow$	$O + NO$
$O^- + NO^+ + M$	$\rightarrow$	$NO_2 + M$
$O^- + O^+$	$\rightarrow$	$O + O$
$O^- + O^+ + N$	$\rightarrow$	$O_2 + N$
$O^- + O^+ + N_2$	$\rightarrow$	$O_2 + N_2$
$O^- + O^+ + O$	$\rightarrow$	$O_2 + O$
$O^- + O^+ + O_2$	$\rightarrow$	$O_2 + O_2$
$O^- + O_2^+$	$\rightarrow$	$O + O_2$
$O^- + O_2^+ + M$	$\rightarrow$	$O_3 + M$
$O^- + N$	$\rightarrow$	$NO + e$
$O^- + N_2$	$\rightarrow$	$N_2O + e$
$O^- + NO$	$\rightarrow$	$NO_2 + e$
$O^- + NO + M$	$\rightarrow$	$NO_2^- + M$
$O^- + NO_2$	$\rightarrow$	$NO_2^- + O$
$O^- + O$	$\rightarrow$	$O_2 + e$
$O^- + O_2$	$\rightarrow$	$O_3 + e$
$O^- + O_2$	$\rightarrow$	$O_3^- + h\nu$
$O^- + O_2 + O_2$	$\rightarrow$	$O_3^- + O_2$
$O^- + O_3$	$\rightarrow$	$O + O_3^-$
$O^- + O_3$	$\rightarrow$	$O_2 + O_2 + e$

$$\frac{d(O_2^-)}{dt} = \sum F(O_2^-) - O_2^- \sum R(O_2^-)$$

REACTIONS

Forming (O_2^-)

$O_2 + e$	$\rightarrow$	$O_2^- + h\nu$
$O_2 + e + N_2$	$\rightarrow$	$O_2^- + N_2$
$O_2 + e + O$	$\rightarrow$	$O_2^- + O$
$O_2 + e + O_2$	$\rightarrow$	$O_2^- + O_2$
$O_3 + e$	$\rightarrow$	$O_2^- + O$

Removing (O_2^-)

$O_2^- + h\nu$	$\rightarrow$	$O_2 + e$
$O_2^- + N_2^+$	$\rightarrow$	$N_2 + O_2$
$O_2^- + N_2^+$	$\rightarrow$	$N + N + O + O$
$O_2^- + N_2^+$	$\rightarrow$	$NO + NO$
$O_2^- + N_2^+$	$\rightarrow$	$NO_2 + N$
$O_2^- + N_2^+$	$\rightarrow$	$N_2O + O$
$O_2^- + N_2^+ + M$	$\rightarrow$	$O_2 + N_2 + M$
$O_2^- + NO^+$	$\rightarrow$	$NO + O_2$
$O_2^- + NO^+$	$\rightarrow$	$NO_2 + O$
$O_2^- + NO^+$	$\rightarrow$	$N + O_3$
$O_2^- + NO^+$	$\rightarrow$	$N + O_2 + O$
$O_2^- + NO^+ + M$	$\rightarrow$	$NO + O_2 + M$
$O_2^- + O^+$	$\rightarrow$	$O + O_2$
$O_2^- + O^+ + M$	$\rightarrow$	$O_3 + M$
$O_2^- + O_2^+$	$\rightarrow$	$O_2 + O_2$
$O_2^- + O_2^+ + M$	$\rightarrow$	$O_2 + O_2 + M$
$O_2^- + N$	$\rightarrow$	$NO_2 + e$
$O_2^- + N + M$	$\rightarrow$	$NO_2^- + M$
$O_2^- + N_2$	$\rightarrow$	$O_2 + N_2 + e$
$O_2^- + N_2 + O_2$	$\rightarrow$	$NO_2^- + NO_2$
$O_2^- + NO_2$	$\rightarrow$	$NO_2^- + O_2$

Forming (O_2^-)

Removing (O_2^-)

$$O_2^- + O \rightarrow O^- + O_2$$

$$O_2^- + O \rightarrow O_2 + O + e$$

$$O_2^- + O \rightarrow O_3 + e$$

$$O_2^- + O_2 \rightarrow O_2 + O_2 + e$$

$$O_2^- + O_3 \rightarrow O_3^- + O_2$$

$$\frac{d(O_3^-)}{dt} = \sum(O_3^-) - O_3^- \sum R(O_3^-)$$

REACTIONS

Forming (O_3^-)			Removing (O_3^-)		
$O^- + O_2$	$\rightarrow$	$O_3^- + h\nu$	$O_3^- + h\nu$	$\rightarrow$	$O_3 + e$
$O^- + O_2 + O_2$	$\rightarrow$	$O_3^- + O_2$	$O_3^- + N_2^+$	$\rightarrow$	$N_2 + O_3$
$O^- + O_3$	$\rightarrow$	$O_3^- + O$	$O_3^- + N_2^+$	$\rightarrow$	$N_2O + O_2$
$O_3 + e$	$\rightarrow$	$O_3^- + h\nu$	$O_3^- + NO^+$	$\rightarrow$	$O_3 + NO$
$O_3 + NO_2^-$	$\rightarrow$	$O_3^- + NO_2$	$O_3^- + NO^+$	$\rightarrow$	$N + O_2 + O_2$
$O_3 + O_2^-$	$\rightarrow$	$O_3^- + O_2$	$O_3^- + NO^+$	$\rightarrow$	$NO_2 + O_2$
			$O_3^- + O^+$	$\rightarrow$	$O + O_3$
			$O_3^- + O_2^+$	$\rightarrow$	$O_2 + O_3$
			$O_3^- + N_2$	$\rightarrow$	$NO_2^- + NO$
			$O_3^- + NO_2$	$\rightarrow$	$NO_2^- + O_3$

$$\frac{d(N_2^+)}{dt} = \sum F(N_2^+) - N_2^+ \sum R(N_2^+)$$

REACTIONS

Forming (N_2^+)

PN2	$\rightarrow$	external source

Removing (N_2^+)

$N_2^+ + e \rightarrow N + N$

$N_2^+ + e \rightarrow N_2 + h\nu$

$N_2^+ + e + M \rightarrow N_2 + M$

$N_2^+ + NO_2^- \rightarrow N_2 + NO_2$

$N_2^+ + NO_2^- \rightarrow N_2O + NO$

$N_2^+ + O^- \rightarrow O + N_2$

$N_2^+ + O^- + M \rightarrow N_2O + M$

$N_2^+ + O_2^- \rightarrow N_2 + O_2$

$N_2^+ + O_2^- \rightarrow NO + NO$

$N_2^+ + O_2^- \rightarrow NO_2 + N$

$N_2^+ + O_2^- \rightarrow N + N + O + O$

$N_2^+ + O_2^- \rightarrow N_2O + O$

$N_2^+ + O_2^- + M \rightarrow N_2 + O_2 + M$

$N_2^+ + O_3^- \rightarrow N_2O + O_2$

$N_2^+ + O_3^- \rightarrow N_2 + O_3$

$N_2^+ + N \rightarrow N_2 + N^+$

$N_2^+ + N_2 \rightarrow N_4^+ + h\nu$

$N_2^+ + NO \rightarrow N_2 + NO^+$

$N_2^+ + O \rightarrow O^+ + N_2$

$N_2^+ + O \rightarrow NO^+ + N$

$N_2^+ + O_2 \rightarrow O_2^+ + N_2$

$N_2^+ + O_2 \rightarrow NO^+ + NO$

$$\frac{d(NO^+)}{dt} = \sum F(NO^+) - NO^+ \sum R(NO^+)$$

REACTIONS

Forming (NO^+)			Removing (NO^+)		
PNO	→	external source	$NO^+ + e$	→	$N + O$
$N_2^+ + NO$	→	$NO^+ + N_2$	$NO^+ + e$	→	$NO + h\nu$
$N_2^+ + O$	→	$NO^+ + N$	$NO^+ + e + M$	→	$N + O + M$
$N_2^+ + O_2$	→	$NO^+ + NO$	$NO^+ + e + M$	→	$NO + M$
$O^+ + N$	→	$NO^+ + h\nu$	$NO^+ + NO_2^-$	→	$N + NO + O_2$
$O^+ + N + M$	→	$NO^+ + M$	$NO^+ + NO_2^-$	→	$N + NO_3$
$O^+ + N_2$	→	$NO^+ + N$	$NO^+ + NO_2^-$	→	$N_2 + O_3$
$O^+ + NO$	→	$NO^+ + O$	$NO^+ + NO_2^-$	→	$NO + NO_2$
$O_2^+ + N$	→	$NO^+ + O$	$NO^+ + O^-$	→	$NO + O$
$O_2^+ + N_2$	→	$NO^+ + NO$	$NO^+ + O^- + M$	→	$NO_2 + M$
$O_2^+ + NO$	→	$NO^+ + O_2$	$NO^+ + O_2^-$	→	$N + O + O_2$
$O_2^+ + NO_2$	→	$NO^+ + O_3$	$NO^+ + O_2^-$	→	$N + O_3$
			$NO^+ + O_2^-$	→	$NO + O_2$
			$NO^+ + O_2^-$	→	$NO_2 + O$
			$NO^+ + O_2^- + M$	→	$NO + O_2 + M$
			$NO^+ + O_3^-$	→	$N + O_2 + O_2$
			$NO^+ + O_3^-$	→	$NO + O_3$
			$NO^+ + O_3^-$	→	$NO_2 + O_2$
			$NO^+ + O$	→	$NO_2^+ + h\nu$

$$\frac{d(O^+)}{dt} = \sum F(O^+) - O^+ \sum R(O^+)$$

REACTIONS

Forming (O^+)

PO	→	external source
$N_2^+ + O$	→	$O^+ + N_2$
$O_2^+ + N$	→	$O^+ + NO$

Removing (O^+)

$O^+ + e$	→	$O + h\nu$
$O^+ + e + M$	→	$O + M$
$O^+ + NO_2^-$	→	$NO_2 + O$
$O^+ + O^-$	→	$O + O$
$O^+ + O^- + O$	→	$O_2 + O$
$O^+ + O^- + N$	→	$O_2 + N$
$O^+ + O^- + N_2$	→	$O_2 + N_2$
$O^+ + O^- + O_2$	→	$O_2 + O_2$
$O^+ + O_2^-$	→	$O + O_2$
$O^+ + O_2^- + M$	→	$O_3 + M$
$O^+ + O_3^-$	→	$O + O_3$
$O^+ + N$	→	$NO^+ + h\nu$
$O^+ + N + M$	→	$NO^+ + M$
$O^+ + N_2$	→	$N_2O^+ + h\nu$
$O^+ + N_2$	→	$NO^+ + N$
$O^+ + N_2 + M$	→	$N_2O^+ + M$
$O^+ + NO$	→	$NO^+ + O$
$O^+ + NO$	→	$NO_2^+ + h\nu$
$O^+ + NO$	→	$O_2^+ + N$
$O^+ + N_2O$	→	$N_2O^+ + O$
$O^+ + NO_2$	→	$NO_2^+ + O$
$O^+ + O$	→	$O_2^+ + h\nu$
$O^+ + O + M$	→	$O_2^+ + M$
$O^+ + O_2$	→	$O + O_2^+$

$$\frac{d(O_2^+)}{dt} = \sum F(O_2^+) - O_2^+ \sum R(O_2^+)$$

REACTIONS

Forming (O_2^+)

PO_2	→	external source
$N_2^+ + O_2$	→	$O_2^+ + N_2$
$O^+ + NO$	→	$O_2^+ + N$
$O^+ + O$	→	$O_2^+ + h\nu$
$O^+ + O + M$	→	$O_2^+ + M$
$O^+ + O_2$	→	$O_2^+ + O$

Removing (O_2^+)

$O_2^+ + e$	→	$O + O$
$O_2^+ + e$	→	$O_2 + h\nu$
$O_2^+ + e + M$	→	$O_2 + M$
$O_2^+ + NO_2^-$	→	$NO_2 + O_2$
$O_2^+ + O^-$	→	$O + O_2$
$O_2^+ + O^- + M$	→	$O_3 + M$
$O_2^+ + O_2^-$	→	$O_2 + O_2$
$O_2^+ + O_2^- + M$	→	$O_2 + O_2 + M$
$O_2^+ + O_3^-$	→	$O_2 + O_3$
$O_2^+ + N$	→	$NO^+ + O$
$O_2^+ + N$	→	$O^+ + NO$
$O_2^+ + N_2$	→	$NO^+ + NO$
$O_2^+ + NO$	→	$NO^+ + O_2$
$O_2^+ + NO_2$	→	$NO^+ + O_3$
$O_2^+ + O$	→	$O_3^+ + h\nu$

$$\frac{d(N)}{dt} = \sum F(N) - N\sum R(N)$$

REACTIONS

Forming (N)

$NO_2^- + NO^+$	$\rightarrow$	$N + NO_3$
$NO_2^- + NO^+$	$\rightarrow$	$N + NO + O_2$
$O_2^- + N_2^+$	$\rightarrow$	$N + NO_2$
$O_2^- + N_2^+$	$\rightarrow$	$N + N + O + O$
$O_2^- + NO^+$	$\rightarrow$	$N + O_3$
$O_2^- + NO^+$	$\rightarrow$	$N + O_2 + O$
$O_3^- + NO^+$	$\rightarrow$	$N + O_2 + O_2$
$N_2^+ + e$	$\rightarrow$	$N + N$
$N_2^+ + O$	$\rightarrow$	$NO^+ + N$
$NO^+ + e$	$\rightarrow$	$N + O$
$NO^+ + e + M$	$\rightarrow$	$N + O + M$
$O^+ + N_2$	$\rightarrow$	$NO^+ + N$
$O^+ + NO$	$\rightarrow$	$N + O_2^+$
$N_2 + O$	$\rightarrow$	$N + NO$
$NO + h\nu$	$\rightarrow$	$N + O$
$NO + O$	$\rightarrow$	$N + O_2$
$N_2O + h\nu$	$\rightarrow$	$N + NO$

Removing (N)

$N + O^-$	$\rightarrow$	$NO + e$
$N + O_2^-$	$\rightarrow$	$NO_2 + e$
$N + O_2^- + M$	$\rightarrow$	$NO_2^- + M$
$N + N_2^+$	$\rightarrow$	$N^+ + N_2$
$N + O^+$	$\rightarrow$	$NO^+ + h\nu$
$N + O^+ + M$	$\rightarrow$	$NO^+ + M$
$N + O_2^+$	$\rightarrow$	$NO^+ + O$
$N + O_2^+$	$\rightarrow$	$O^+ + NO$
$N + N$	$\rightarrow$	$N_2 + h\nu$
$N + N + M$	$\rightarrow$	$N_2 + M$
$N + N + N$	$\rightarrow$	$N_2 + N$
$N + N + N_2$	$\rightarrow$	$N_2 + N_2$
$N + NO$	$\rightarrow$	$N_2 + O$
$N + NO$	$\rightarrow$	$N_2O + h\nu$
$N + NO + M$	$\rightarrow$	$N_2O + M$
$N + NO_2$	$\rightarrow$	$N_2 + O_2$
$N + NO_2$	$\rightarrow$	$NO + NO$
$N + NO_2$	$\rightarrow$	$N_2O + O$
$N + O$	$\rightarrow$	$NO + h\nu$
$N + O + M$	$\rightarrow$	$NO + M$
$N + O_2$	$\rightarrow$	$NO + O$
$N + O_2$	$\rightarrow$	$NO_2 + h\nu$
$N + O_2 + M$	$\rightarrow$	$NO_2 + M$
$N + O_3$	$\rightarrow$	$NO + O_2$

$$\frac{d(NO)}{dt} = \sum F(NO) - NO \sum R(NO)$$

REACTIONS

Forming (NO)

$NO_2^- + N_2^+$	$\rightarrow$	$NO + N_2O$
$NO_2^- + NO^+$	$\rightarrow$	$NO + NO_2$
$NO_2^- + NO^+$	$\rightarrow$	$NO + O_2 + N$
$NO^+ + e$	$\rightarrow$	$NO + h\nu$
$NO^+ + e + M$	$\rightarrow$	$NO + M$
$N_2^+ + O_2$	$\rightarrow$	$NO + NO^+$
$O_2^+ + N$	$\rightarrow$	$NO + O^+$
$O_2^+ + N_2$	$\rightarrow$	$NO + NO^+$
$O^- + N$	$\rightarrow$	$NO + e$
$O^- + NO^+$	$\rightarrow$	$NO + O$
$O_2^- + NO^+ + M$	$\rightarrow$	$NO + O_2 + M$
$O_2^- + N_2^+$	$\rightarrow$	$NO + NO$
$O_3^- + N_2$	$\rightarrow$	$NO + NO_2^-$
$O_3^- + NO^+$	$\rightarrow$	$NO + O_3$
$N + O$	$\rightarrow$	$NO + h\nu$
$N + O + M$	$\rightarrow$	$NO + M$
$N + O_2$	$\rightarrow$	$NO + O$
$N + O_3$	$\rightarrow$	$NO + O_2$
$N + NO_2$	$\rightarrow$	$NO + NO$
$NO_2 + O$	$\rightarrow$	$NO + O_2$
$NO_2 + h\nu$	$\rightarrow$	$NO + O$
$N_2O + h\nu$	$\rightarrow$	$NO + N$

Removing (NO)

$NO + O^-$	$\rightarrow$	$NO_2 + e$
$NO + O^- + M$	$\rightarrow$	$NO_2^- + M$
$NO + N_2^+$	$\rightarrow$	$N_2 + NO^+$
$NO + O^+$	$\rightarrow$	$O + NO^+$
$NO + O^+$	$\rightarrow$	$NO_2^+ + h\nu$
$NO + O^+$	$\rightarrow$	$N + O_2^+$
$NO + O_2^+$	$\rightarrow$	$NO^+ + O_2$
$NO + N$	$\rightarrow$	$N_2O + h\nu$
$NO + N$	$\rightarrow$	$N_2 + O$
$NO + N + M$	$\rightarrow$	$N_2O + M$
$NO + h\nu$	$\rightarrow$	$N + O$
$NO + NO + O_2$	$\rightarrow$	$NO_2 + NO_2$
$NO + O$	$\rightarrow$	$NO_2 + h\nu$
$NO + O$	$\rightarrow$	$O_2 + N$
$NO + O + M$	$\rightarrow$	$NO_2 + M$
$NO + O + N_2$	$\rightarrow$	$NO_2 + N_2$
$NO + O + O_2$	$\rightarrow$	$NO_2 + O_2$
$NO + O_3$	$\rightarrow$	$NO_2 + O_2$

Forming (NO)			Removing (NO)
$O + N_2$	→	$NO + N$	
$O + N_2O$	→	$NO + NO$	
$O_2^- + NO^+$	→	$NO + O_2$	

$$\frac{d(N_2O)}{dt} = \sum F(N_2O) - N_2O \sum R(N_2O)$$

REACTIONS

Forming (N_2O)

$O^- + N_2$	$\rightarrow$	$N_2O + e$
$O^- + N_2^+ + M$	$\rightarrow$	$N_2O + M$
$O_2^- + N_2^+$	$\rightarrow$	$N_2O + O$
$N_2^+ + NO_2^-$	$\rightarrow$	$N_2O + NO$
$N_2^+ + O_3^-$	$\rightarrow$	$N_2O + O_2$
$N + NO_2$	$\rightarrow$	$N_2O + O$
$N + NO + M$	$\rightarrow$	$N_2O + M$
$NO + N$	$\rightarrow$	$N_2O + h\nu$
$O + N_2$	$\rightarrow$	$N_2O + h\nu$
$O + N_2 + M$	$\rightarrow$	$N_2O + M$

Removing (N_2O)

$N_2O + h\nu$	$\rightarrow$	$NO + N$
$N_2O + h\nu$	$\rightarrow$	$N_2 + O$
$N_2O + O^+$	$\rightarrow$	$O + N_2O^+$
$N_2O + O$	$\rightarrow$	$NO + NO$
$N_2O + O$	$\rightarrow$	$O_2 + N_2$

$$\frac{d(NO_2)}{dt} = \sum F(NO_2) - NO_2 \sum R(NO_2)$$

REACTIONS

Forming (NO_2)

$NO_2^- + h\nu$	$\rightarrow$	$NO_2 + e$
$NO_2^- + N_2^+$	$\rightarrow$	$NO_2 + N_2$
$NO_2^- + NO^+$	$\rightarrow$	$NO_2 + NO$
$NO_2^- + O^+$	$\rightarrow$	$NO_2 + O$
$NO_2^- + O_2^+$	$\rightarrow$	$NO_2 + O_2$
$NO_2^- + O_3$	$\rightarrow$	$NO_2 + O_3^-$
$O^- + NO^+ + M$	$\rightarrow$	$NO_2 + M$
$O_2^- + N_2^+$	$\rightarrow$	$NO_2 + N$
$O_2^- + NO^+$	$\rightarrow$	$NO_2 + O$
$O_2^- + O_2 + N_2$	$\rightarrow$	$NO_2 + NO_2^-$
$O_3^- + NO^+$	$\rightarrow$	$NO_2 + O_2$
$N + O_2 + M$	$\rightarrow$	$NO_2 + M$
$N + O_2^-$	$\rightarrow$	$NO_2 + e$
$N + O_2$	$\rightarrow$	$NO_2 + h\nu$
$NO + O^-$	$\rightarrow$	$NO_2 + e$
$NO + NO + O_2$	$\rightarrow$	$NO_2 + NO_2$
$NO + O$	$\rightarrow$	$NO_2 + h\nu$
$NO + O + M$	$\rightarrow$	$NO_2 + M$
$NO + O_3$	$\rightarrow$	$NO_2 + O_2$
$O + NO + N_2$	$\rightarrow$	$NO_2 + N_2$
$O + NO + O_2$	$\rightarrow$	$NO_2 + O_2$

Removing (NO_2)

$NO_2 + e$	$\rightarrow$	$NO_2^- + h\nu$
$NO_2 + e + N_2$	$\rightarrow$	$NO_2^- + N_2$
$NO_2 + e + O_2$	$\rightarrow$	$NO_2^- + O_2$
$NO_2 + h\nu$	$\rightarrow$	$NO + O$
$NO_2 + O^-$	$\rightarrow$	$NO_2^- + O$
$NO_2 + O_2^-$	$\rightarrow$	$NO_2^- + O_2$
$NO_2 + O_3^-$	$\rightarrow$	$NO_2^- + O_3$
$NO_2 + O^+$	$\rightarrow$	$NO_2^+ + O$
$NO_2 + O_2^+$	$\rightarrow$	$NO^+ + O_3$
$NO_2 + N$	$\rightarrow$	$NO + NO$
$NO_2 + N$	$\rightarrow$	$N_2 + O_2$
$NO_2 + N$	$\rightarrow$	$N_2O + O$
$NO_2 + O$	$\rightarrow$	$NO + O_2$

$$\frac{d(O)}{dt} = \sum F(O) - O\sum R(O)$$

REACTIONS

Forming (O)			Removing (O)		
$NO_2^- + O^+$	$\rightarrow$	$O + NO_2$	$O + e$	$\rightarrow$	$O^- + h\nu$
$O^- + h\nu$	$\rightarrow$	$O + e$	$O + O^-$	$\rightarrow$	$O_2 + e$
$O^- + N_2^+$	$\rightarrow$	$O + N_2$	$O + O_2^-$	$\rightarrow$	$O_3 + e$
$O^- + NO^+$	$\rightarrow$	$O + NO$	$O + O_2^-$	$\rightarrow$	$O^- + O_2$
$O^- + O^+$	$\rightarrow$	$O + O$	$O + N_2^+$	$\rightarrow$	$O^+ + N_2$
$O^- + O_2^+$	$\rightarrow$	$O + O_2$	$O + N_2^+$	$\rightarrow$	$NO^+ + N$
$O^- + NO_2$	$\rightarrow$	$O + NO_2^-$	$O + NO^+$	$\rightarrow$	$NO_2^+ + h\nu$
$O^- + O_3$	$\rightarrow$	$O + O_3^-$	$O + O^+$	$\rightarrow$	$O_2^+ + h\nu$
$O_2^- + N_2^+$	$\rightarrow$	$O + O + N + N$	$O + O^+ + M$	$\rightarrow$	$O_2^+ + M$
$O_2^- + N_2^+$	$\rightarrow$	$O + N_2O$	$O + O_2^+$	$\rightarrow$	$O_3^+ + h\nu$
$O_2^- + NO^+$	$\rightarrow$	$O + N + O_2$	$O + N$	$\rightarrow$	$NO + h\nu$
$O_2^- + NO^+$	$\rightarrow$	$O + NO_2$	$O + N + M$	$\rightarrow$	$NO + M$
$O_2^- + O^+$	$\rightarrow$	$O + O_2$	$O + N_2$	$\rightarrow$	$NO + N$
$O_3^- + O^+$	$\rightarrow$	$O + O_3$	$O + N_2$	$\rightarrow$	$N_2O + h\nu$
$NO^+ + e$	$\rightarrow$	$O + N$	$O + N_2 + e$	$\rightarrow$	$O^- + N_2$
$NO^+ + e + M$	$\rightarrow$	$O + N + M$	$O + N_2 + M$	$\rightarrow$	$N_2O + M$
$O^+ + e$	$\rightarrow$	$O + h\nu$	$O + NO$	$\rightarrow$	$NO_2 + h\nu$
$O^+ + e + M$	$\rightarrow$	$O + M$	$O + NO$	$\rightarrow$	$O_2 + N$
$O^+ + NO$	$\rightarrow$	$O + NO^+$	$O + NO + M$	$\rightarrow$	$NO_2 + M$
$O^+ + NO_2$	$\rightarrow$	$O + NO_2^+$	$O + NO + N_2$	$\rightarrow$	$NO_2 + N_2$
$O^+ + N_2O$	$\rightarrow$	$O + N_2O^+$	$O + NO + O_2$	$\rightarrow$	$NO_2 + O_2$

Forming (0)

$O^+ + O_2$	$\rightarrow$	$O + O_2^+$
$O_2^+ + e$	$\rightarrow$	$O + O$
$N + O_2^+$	$\rightarrow$	$NO^+ + O$
$N + NO$	$\rightarrow$	$O + N_2$
$N + NO_2$	$\rightarrow$	$O + N_2O$
$N + O_2$	$\rightarrow$	$O + NO$
$NO + h\nu$	$\rightarrow$	$O + N$
$N_2O + h\nu$	$\rightarrow$	$O + N_2$
$NO_2 + h\nu$	$\rightarrow$	$O + NO$
$O_2 + h\nu$	$\rightarrow$	$O + O$
$O_3 + h\nu$	$\rightarrow$	$O + O_2$
$O_3 + e$	$\rightarrow$	$O + O_2^-$

Removing (0)

$O + N_2O$	$\rightarrow$	$NO + NO$
$O + N_2O$	$\rightarrow$	$O_2 + N_2$
$O + NO_2$	$\rightarrow$	$NO + O_2$
$O + O$	$\rightarrow$	$O_2 + h\nu$
$O + O + O$	$\rightarrow$	$O_2 + O$
$O + O + N_2$	$\rightarrow$	$O_2 + N_2$
$O + O + O_2$	$\rightarrow$	$O_2 + O_2$
$O + O_2$	$\rightarrow$	$O_3 + h\nu$
$O + O_2 + e$	$\rightarrow$	$O^- + O_2$
$O + O_2 + M$	$\rightarrow$	$O_3 + M$
$O + O_2 + N_2$	$\rightarrow$	$O_3 + N_2$
$O + O_2 + O$	$\rightarrow$	$O_3 + O$
$O + O_2 + O_2$	$\rightarrow$	$O_3 + O_2$
$O + O_3$	$\rightarrow$	$O_2 + O_2$

$$\frac{d(O_3)}{dt} = \sum F(O_3) - O_3 \sum R(O_3)$$

REACTIONS

Forming (O_3)

$NO_2^- + NO^+ \rightarrow O_3 + N_2$

$O^- + O_2 \rightarrow O_3 + e$

$O_2^- + NO^+ \rightarrow O_3 + N$

$O_2^- + O^+ + M \rightarrow O_3 + M$

$O_2^- + O \rightarrow O_3 + e$

$O_3^- + h\nu \rightarrow O_3 + e$

$O_3^- + N_2^+ \rightarrow O_3 + N_2$

$O_3^- + NO^+ \rightarrow O_3 + NO$

$O_3^- + O^+ \rightarrow O_3 + O$

$O_3^- + O_2^+ \rightarrow O_3 + O_2$

$O_3^- + NO_2 \rightarrow O_3 + NO_2^-$

$O_2^+ + O^- + M \rightarrow O_3 + M$

$O_2^+ + NO_2 \rightarrow O_3 + NO^+$

$O + O_2 \rightarrow O_3 + h\nu$

$O + O_2 + M \rightarrow O_3 + M$

$O + O_2 + N_2 \rightarrow O_3 + N_2$

$O + O_2 + O \rightarrow O_3 + O$

$O + O_2 + O_2 \rightarrow O_3 + O_2$

Removing (O_3)

$O_3 + e \rightarrow O^- + O_2$

$O_3 + e \rightarrow O_2^- + O$

$O_3 + e \rightarrow O_3^- + h\nu$

$O_3 + h\nu \rightarrow O + O_2$

$O_3 + NO_2^- \rightarrow O_3^- + NO_2$

$O_3 + O^- \rightarrow O + O_3^-$

$O_3 + O^- \rightarrow O_2 + O_2 + e$

$O_3 + O_2^- \rightarrow O_3^- + O_2$

$O_3 + N \rightarrow NO + O_2$

$O_3 + NO \rightarrow NO_2 + O_2$

$O_3 + O \rightarrow O_2 + O_2$

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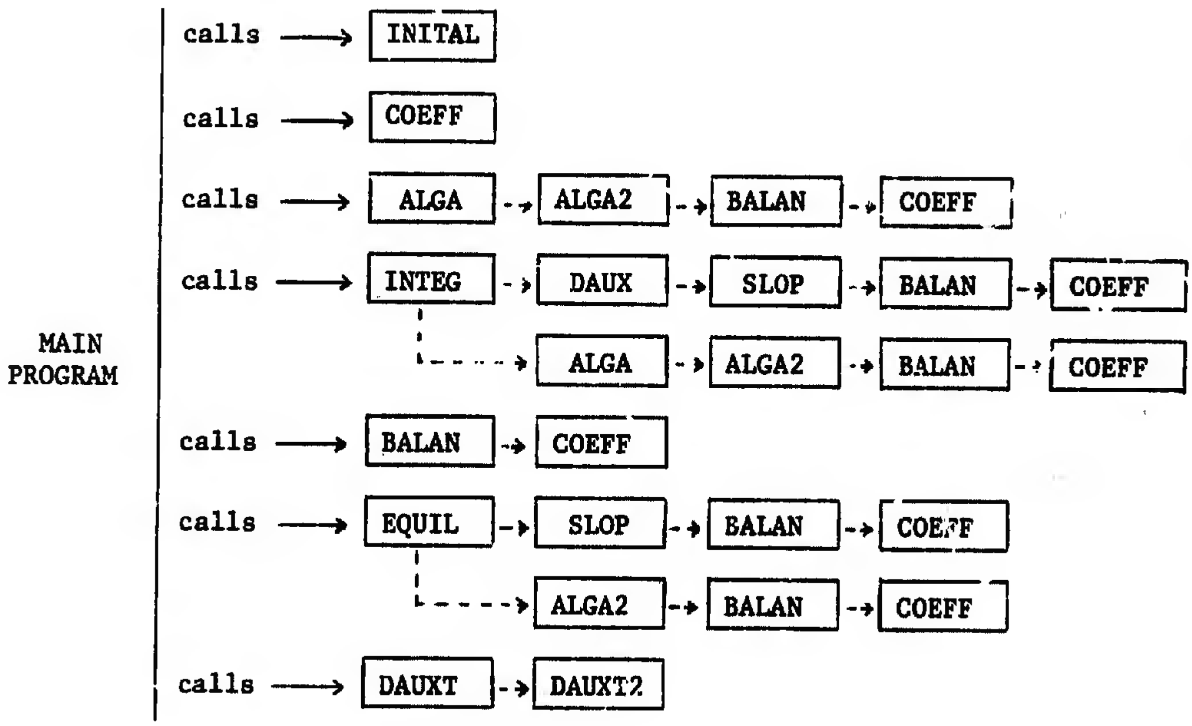
APPENDIX C

DESCRIPTION OF COMPUTER PROGRAM

The Fortran program consists of a Main Program and 11 subroutines; namely, INITIAL, COEFF, BALAN, INTEG, ALGA, ALGA2, SLOP, DAUX, EQUIL, DAUXT, and DAUXT2.

The figure shows how each subroutine is used by another. From this it can be seen that the program is rather complex and skips around a great deal from one subroutine to another.



Flow chart of subroutine usage

MAIN PROGRAM

Purpose: Control the flow of computations

Input Data - Cards

Output Data - Tapes 3 and 9.

Tape 3 → For print out of histories.

Tape 9 → Referred to in program as tape 6; for BRLESC runs designated as tape 9. All output except histories is put on this tape. Data stored on temporary tapes 1 and 4 is transferred to this tape before a run is terminated.

Two temporary tapes are used in running the program.

Tape 1 → For storing time, number densities of NO, N NO_2, O_3, NO^+, N_2O, O, and production.

Tape 4 → For storing time, number densities of O_2, N_2 and values of Key_y (y = 1 - NUMB).

A. INITIALIZATION OF SYSTEM AND INPUT

Initial setting of variables

$CHI = 1 \cdot 10^{-20}$	Lowest value to which a species may decay.
NOCOM = 166	Total number of reaction rates used in the program. If additional reactions are to be included, the program must be changed. If any one of the 166 reactions is to be omitted, set the reaction rate in input data to zero.
ENDE = 0.0	Lower limit on electron density.
ITER = 30	Maximum number of iterations allowed in iteration subroutine (ALGA).

LAM = 5	Keeps track of largest positive species.
KOUNT = 0	Counter for number of times tape 4 is written on.
MOUNT = 0	Counter for number of times tape 1 is written on.
KNT = 0	Counter for number of lines to write on a page.
JAKE = 1	Keeps track of integrating mesh Δt. Used in ALGA and INTEG subroutines. If JAKE = 2, Δt is vanishing in integration. If JAKE > 2, Δt is vanishing in iteration.
JUMP = 1	After first integration, if any species is in equilibrium, the integrating mesh is cut back to $\Delta t/2$ and JUMP is set equal to 2 where it remains for rest of solution.
JACK = 1	After a successful integration, JACK is set to two. It will remain two until largest positive species changes at which time it is reset to one before continuing with integration. After a successful integration with this new largest positive species, JACK gets set to two and continues to be set in this manner throughout the solution.
KLOT = 0	Counter for number of times Δt remains constant, maximum allowed = 10.
TIME = $1 \cdot 10^{-6}$	Used in DAUXT subroutine if histories are to be printed every time cycle.
NUMB = 15 or 14	Number of variable species or number of differential equations solved by the program. If option KB4 = 0 species 0 is held constant and NUMB = 14.

Following locations are used for keeping track of the status of any species y during run time (y = 1 - NUMB).

$LOCK_y$ = 0	Counter to keep track of number of times quasi-equilibrium test is satisfied. Each time this test is satisfied one is added to $LOCK_y$. $LOCK_y$ must be satisfied three times before a species is put in equilibrium (this satisfies the condition of the second derivative being zero).
KEY_y = 1	Initially set equal to one. The KEY_y values will give the status of any species during run time and are used throughout the program for branching purposes.

If KEY_y = 1	Species is not in equilibrium.
KEY_y = 2	Species is in quasi-equilibrium.
KEY_y = 3	Species has decayed below CHI.
KEY_y = 4	Species is the largest of the positive species.

TREG(J+3) (J = 1 - NUMB)	Location where number densities at time t are stored.
TTREG(J+3) (J = 1 - NUMB)	Location where previous integrated results are stored.

Input Data in CGS System

Cards 1-33 Floating point formal ± x.xxxxxE±xx (1P6E12.5)

Card 1 Columns

Columns		
1-12	Eubar	Criteria used in integration subroutine
13-24	Elbar	Criteria used in iteration subroutine
25-36	Del	Criteria used in EQUIL subroutine for testing equilibrium status of a species
37-48	Epsi	Not used
49-60	Endt	Total time over which you desire results

Cards 2-29	166 reaction rates	
Card 30 Columns		
1-12	Alt	Altitude in cm. If altitude is zero program will halt.
13-24	D	Total number density cm^{-3}
25-36	DO2	Number density of molecular oxygen
37-48	DO	Number density of atomic oxygen
49-60	DN2	Number density of molecular nitrogen
61-72	T	Temperature in degrees Kelvin at given altitude
Card 31 Columns	Number Density of	
1-12	e	
13-24	O^-	
25-36	O_2^-	
37-48	O_3^-	
49-60	NO_2^-	
61-72	O^+	
Card 32 Columns		
1-12	O_2^+	
13-24	N_2^+	
25-36	NO	
37-48	N	
49-60	NO_2	
61-72	O_3	

Card 33 Columns

1-12	N_2O	Number density
13-24	Prod	Constant part of external source function
25-36	XMAS	Criteria on Δt used in EQUIL subroutine

Card 34 Integer format ±x±x±x±x±x±x±x±x (8I2) for following options:

Options:

KB1 = 0	All log output
KB1 = 1*	Time decimal output, number densities log output
KB1 = 2	All decimal output
KB2 = 0	Prints out histories of reactions
KB2 = 1	No histories printed
KB3 = 0	Changes rate constant for next run
KB3 = 1	Uses same rate constants as last run
KB3 = 2	Reads new criteria and changes rate constants
KB4 = 0	Specie O is held constant
KB4 = 1	Differential equation for O is included in the solution
KB5 = 0	Prints histories every time step
KB5 = 1	Prints histories every time cycle
KB6 = 1	Reads another point card after an error
KB7 = 1	Constant production for O, NO, N_2 and e If this is not wanted, omit this card from input data.

If data is to be plotted by Plot Code (FORAST Code for Calcomp Plotter) this option must be 1.

Cards 35-36 Alphabetic format, 40 characters or less stating title of plot. A requirement of the BRLESC PLOTTING CODE is that a > symbol must appear after last character of the title. The first <u>ten</u> characters must be as listed below in order for plot code to work.

Columns	1	2	3	4	5	6	7	8	9	10 --------41
35	b	b	b	R	U	N	b	N	0	. -------- >
36	4	/	1	b	b	N	2	/	0	2 -------- >

where b is a blank column.

There will be no card 37 in input data if option KB7 = 0

Card 37 Floating point format ±x.xxxxxE±xx (1P5E12.5)

Columns		
1-12	PO	Constant production for 0^+
13-24	PNO	Constant production for NO^+
25-36	PN2	Constant production for N_2^+
37-48	PO2	Constant production for 0_2^+
49-60	PNE	Constant production for e

Following locations are reserved for use in integration subroutine:

where N = NUMB (number of equations in solution)

LINT (2N+4 to 3N+3)	Current initial $y_{n,o}$ preserved
I2NT (3N+4 to 4N+3)	$y_{n,1}$
K2NT (4N+4 to 5N+3)	$y_{n,2}$
J2NT (5N+4 to 6N+3)	$y_{n,3}$
N2NT (6N+4 to 7N+3)	Current initial value working area
KINT (7N+4 to 8N+3)	Current initial $y_{n,o}$ preserved
MINT (8N+4)	Current t_o preserved

NINT (8N+5) Current initial Δt

I3NT (8N+6) Current t_o working area

The INITAL and COEFF subroutines are called here.

If KB7 = 1 the PRODUC subroutine (AFCRL-63) which has been incorporated here as part of the MAIN program is ignored and transfer is to B.

If KB7 = 0 a constant rate of production of ion-pairs/cm^3/sec (PROD) is read into the program. (See card #33 input)

This production represents the number of electrons produced by some source other than the chemical reactions themselves and is partitioned among the positive ions as follows:

$q(e)$ = PNE = PROD

$q(O^+)$ = PO = K · DO

$q(O_2^+)$ = PO_2 = K · DO2

$q(N_2^+)$ = PN_2 = K · DN2

$q(NO^+)$ = PNO = K · DNO

where $K = (a_i + b_i t + c_i t_2)$ (i = neutral species)

$a_i = \frac{PROD}{TOT}$ $b_i = c_i = 0$ t = time

TOT = DO + DO2 = DN2 (total number density of neutral species O, O_2 and N_2)

If a sharp change is required in source function it can be accomodated here by giving values to b_i and c_i.

B. PREPARE OUTPUT TAPES AND WRITE RATE CONSTANTS AND INITIAL CONDITIONS

Initial conditions are put on output tapes along with reaction rates read into COB region and actual rate constants used in CON region.

C. INTEGRATION OF EQUATIONS STARTS HERE

From statement 5 on, the solution actually starts. If all species are in quasi-equilibrium ALGA is called and iteration takes place; otherwise INTEG is called and integration takes place. The overall solution is obtained by iteration between the differential and algebraic sets.

After a successful integration, the largest positive species is determined. The BALAN subroutine is called where the number densities of the largest positive species, N_2 and O_2 are computed. Before integration is continued the following five tests are made:

1. Test (KLOT) to determine if time increment Δt is constant for more than 10 passes.

KLOT > 10 — an error print ("the increment is constant at $1 \cdot 10^{-6}$sec.") is written on tape 9. Data on temporary tapes 1 and 4 is transferred to tape 9 and run is terminated.

KLOT $\leq$ 10 — The number densities of O_2 and N_2 and KEY_y (y = 1 - NUMB) are put on temporary tape 4.

2. Test (JAKE) to see if integrating mesh is vanishing in either iteration or integration subroutines.

If integrating mesh is vanishing, i.e.

JAKE = 2 — an error print ("the integrating mesh is vanishing in integration" at ....sec.")

JAKE > 2 — an error print ("the integrating mesh is vanishing in iteration at --- sec.")
Data on temporary tapes 1 and 4 is transferred to output tape 9 and run is terminated.

If integrating mesh is not vanishing JACK is set to 2 and transfer is made to EQUIL subroutine.

3. In EQUIL subroutine all species are tested for quasi-equilibrium. (See EQUIL subroutine).

4. Test (CHI) to see if any species y has decayed below CHI. If so, KEY_y is set to 3 and the number density of corresponding species y is set to zero. Once a KEY position has been set to 3, it remains there for remainder of solution.

5. Test (PROD) if PNE = 0 and $\frac{y_e \text{ computed}}{y_e \text{ initial}} < .001$, the KEY values and number densities for species e, O^-, and O_2^- are set to 3 and zero, respectively.

The computed number densities for all species are put into TTREG region and used for comparison with next integration results.

D. OUTPUT OF RESULTS START HERE

The results of this integration are put on output tapes, 1, 4 and 9 in form specified by options.

If there is not a constant production, the production is brought up to date here with latest times and number densities (as described earlier in this main program).

If KB2 = 0 subroutine DAUXT is called where histories are computed and recorded on tape 3.

E. DECISION TO CONTINUE INTEGRATION

1. If run time is not complete, the largest positive species y is determined from charge balance equation.

a. If the largest positive species y has changed from previous integration, proper settings are made for KEY_y and LAM. JACK is reset to 1 and integration continued.

b. If the largest positive species y has not changed from previous integration, all previous settings of LAM, KEY_y and JACK remain unchanged and integration is continued.

2. If run time is finished, all results on temporary tapes 1 and 4 are transferred to output tape 9. The next case is initiated depending on the setting of option KB3.

Initial Subroutine

Purpose: To set up initial conditions on differential equations.

Transfer to this subroutine from the MAIN program is made once at the beginning of the solution.

TREG(2) = 0.0	Initial time for independent variable t (sec.)
TREG(3) = $1 \cdot 10^{-6}$	Initial mesh Δt. If it is known that a species will reach quasi-equilibrium before $1 \cdot 10^{-6}$ seconds, it will save computer time if the initial mesh Δt is set to smaller value here.
TREG [4 to (NUMB+3)]	Initial number densities of the 15 species are put into this region. Dependent variables y_i.

Compute

1. TOTO = Total neutral density of oxygen.

2. TOTN = Total neutral density of nitrogen.

COEFF Subroutine

Purpose: To compute actual rate constants used in the program and to compute common terms in the differential equations that remain constant for any given time.

Transfer to this subroutine is from MAIN program or from subroutine BALAN.

The setting of a sense light allows this subroutine to compute the rate constants once (Part I). Thereafter, when this subroutine is called, only the common terms of differential equations that remain constant for any given solution will be computed (Part II).

PART I - The rate constants read into the computer in the COB region are independent of temperature. Those rate constants that are temperature dependent are multiplied by their temperature dependent factor. The actual rate constants used are put in the CON region. Rate constants read into (COB) and rate constants used in (CON) are both printed on output tape 9.

PART II - To save computer time, the common terms of the equations that remain constant for any given solution are computed and put into the YURI region to be used later in the SLOP and ALGA2 subroutines, where formation and removal terms are computed. PART II is done every time BALAN subroutine is called.

If additional reactions are incorporated in the solution, this subroutine must be changed.

Integration Subroutine

Purpose: To solve the differential equations

Transfer to this subroutine is from the MAIN program.

The fourth-order, Runge-Kutta technique with variable mesh is used for solving the system of 15, first-order, differential equations. This method does not require evaluation of derivatives beyond the first. Approximations are obtained by evaluating the first derivative four times. The method is stable and self-starting; only functional values at a single previous point are required to obtain functional values ahead. The error in each step is of the order h^5 where h is the length of the interval.

Given the system of n first-order ordinary differential equations in y as functions of t and y_n.

$$\frac{dy_i}{dt} = f_i(t, y_1, y_2, \ldots\ldots y_n) \qquad i = 1, 2, \ldots\ldots n$$

The values of any y_i at time t is determined from a previously calculated value by

$$y_{n,1} = y_{n,o} + \Delta y$$

where the first increment in y is computed from formulas

$$k_{n,1} = f_n(t_o, y_{1,o}, y_{2,o}, \ldots\ldots y_{n,o})h$$

$$k_{n,2} = f_n[(t_0 + \frac{h}{2}), (y_{1,0} + \frac{k_{1,1}}{2}), (y_{2,0} + \frac{k_{2,2}}{2}), \ldots\ldots (y_{n,0} + \frac{k_{n,1}}{2})]h$$

$$k_{n,3} = f_n [(t_0 + \frac{h}{2}), (y_{1,0} + \frac{k_{1,2}}{2}), (y_{2,0} + \frac{k_{2,2}}{2}), \ldots\ldots (y_{n,0} + \frac{k_{n,2}}{2})]h \qquad (1)$$

$$k_{n,4} = f_n [(t_0 + \frac{h}{2}), (y_{1,0} + k_{1,3}), (y_{2,0} + k_{2,3}), \ldots\ldots (y_{n,0} + k_{n,3})] h$$

$$\Delta y = 1/6 (k_{n,1} + 2k_{n,2} + 2k_{n,3} + k_{n,4})$$

$$t_1 = t_o + h \qquad y_1 = y_o + \Delta y$$

The increment of the functions are calculated once for all, using formulas (1). The calculations for the first increment are exactly the same as for any other increment.

Starting with initial values y_o, t_o the solution for y_1, t_1 is as follows:

$y_{n,1}$, $t_o+\Delta t$ is computed using initial conditions $y_{n,o}$, t_o and a time increment Δt

$y_{n,2}$, $t_o+2\Delta t$ is computed using $y_{n,1}$, $t_o+\Delta t$ as initial values with same increment Δt

$y_{n,3}$, $t_o+2\Delta t$ is computed using $y_{n,o}$, t_o as initial values with a time increment of $2 \cdot \Delta t$

The relative difference between $y_{n,2}$ and $y_{n,3}$ is computed and the following test made:

$$\frac{|y_{n,2} - y_{n,3}|}{y_{n,2}} < \varepsilon$$

where ε is some number < 1 which gives required accuracy in the integration.. If all species meet this criteria, the solution is $y_{n,2}$.

Upon entering this subroutine, the current initial conditions are preserved and at the beginning of each integration cycle, time t and the integrating mesh, Δt, are tested.

If either (a) or (b) is satisfied integration takes place.

(a) $t < 5 \times 10^{-6}$

(b) $t \geq 5 \times 10^{-6}$ and $\Delta t \geq 1 \times 10^{-15}$.

If $t \geq 5 \times 10^{-6}$ and $\Delta t < 1 \times 10^{-15}$ the integrating mesh is vanishing in this subroutine. JAKE is set equal to 2 and return is to the MAIN program where data on temporary tapes 1 and 4 are transferred to output tape 9, a comment is then written on tape 9 "Integrating mesh is vanishing in INT at t = x.xxxxxsec.," and run is terminated.

In the process of integration, those species not in quasi-equilibrium are integrated in manner described above. After each derivative evaluation the following tests are made:

1. If the number density of any species not in quasi-equilibrium is negative anywhere along the way, the integrating mesh is cut back (see below).

2. The status of each species is tested and, if in quasi-equilibrium, transfer is made to the ALGA subroutine where number densities for these species in quasi-equilibrium are computed by iteration of algebraic set. Upon each return to the integration subroutine, variables JAM and JAKE, set in ALGA, are tested.

3. If JAKE $\leq$ 2 and JAM = 1 the criteria of iteration subroutine is satisfied. The iterated values of species in quasi-equilibrium replace their corresponding y_o and integration is continued.

4. If JAKE $\leq$ 2 and JAM = 2 some species are not in quasi-equilibrium. For those that are, the iteration criteria was not met so the integrating mesh is cut back (see below).

5. If JAKE > 2, criteria was not satisfied in ALGA subroutine. The integrating mesh is vanishing. Integration is terminated and return is to main program where data on temporary tapes 1 and 4 are transferred

to output tape 9, a comment is written on tape 9 "Integrating mesh vanishing in ALGA at t = x.xxxxxsec.," and run is terminated.

After a complete integration cycle for those species in quasi-equilibrium $y_{n,2}$ is the solution: for species not in quasi-equilibrium the relative difference between $y_{n,2}$ and $y_{n,3}$ is computed and following test made:

$$\frac{|y_{n,2} - y_{n,3}|}{y_{n,2}} < \varepsilon \qquad n = 1 \rightarrow \text{number}$$

where ε is some number < 1 which gives required accuracy in the integration.

If the relative difference for all species not in quasi-equilibrium is $< \varepsilon$, the solution is $y_{n,2}$ and the integration is complete. The integrating mesh is doubled and control returns to MAIN program.

If any relative difference is $> \varepsilon$, accuracy is being lost, so integrating mesh is cut back.

Cut Back in Integrating Mesh

The integrating mesh will be cut back in this subroutine if one of the following conditions exist:

1. The number density of any species is negative.
2. JAKE < 3 and JAM = 2
3. $$\frac{|y_{n,2} - y_{n,3}|}{y_{n,2}} > \varepsilon \qquad n = 1 \rightarrow \text{number}$$

The cut back in the integrating mesh depends on the setting of variable JACK.

JACK = 1 JACK will be 1 if it is the initial integration, or if it is the first integration after most abundant species has changed; otherwise, JACK will be 2. When JACK = 1 the integrating mesh is halved, current initial conditions reset and integration repeated. The integrating mesh is cut back but is not allowed to be cut back below initial mesh.

JACK = 2 When JACK = 2, the routine allows the integrating mesh to be halved three times and if trouble still exists, the mesh will be cut back in steps of 10. After each cutback, the current initial conditions are reset and integration is repeated. Likewise, the integrating mesh is not allowed to be cut back below initial mesh.

Upon completion of an integration, time is in TREG(2), solutions for this time are in TREG(4 to N+3) and Δt for next integration is in TREG(3).

ALGA Subroutine (Iteration)

Purpose: To solve algebraic equations

$$y_i = \frac{\sum F_j(y_i)}{\sum R_j(y_i)} \qquad i = 1 \rightarrow \text{NUMB}$$

for species in quasi-equilibrium by method of successive substitutions.

Transfer is made to this subroutine from the MAIN program if all species are in quasi-equilibrium; otherwise, transfer is from the integration subroutine (INTEG).

Before iteration of algebraic equations takes place, subroutine ALGA2 is called where all Key_i are tested and FORM(i) and REMV(i) computed for species i in quasi-equilibrium.

Iteration starts with an initial value $y_{i,o}$ and employs the recurrence formula

$$y_{i,k+1} = f(y_{i,k})$$

After each iteration the (k+1) values are compared to the previous k value

$$(1-\delta) \leq \frac{y_{i,k}}{y_{i,(k+1)}} < (1+\delta)$$

where δ or EUBAR is some number < 1 that determines digital accuracy of iterated results.

Iteration continues for all species in quasi-equilibrium. The setting of variables JAM and JAKE determine what takes place on return to integration subroutine.

JAM = 1 JAM gets set equal to one when the above criteria is satisfied within preset number of iterations (30) for all species that are in quasi-equilibrium. The iterated values replace $y_{i,o}$ and return is to integration subroutine.

JAM = 2 JAM gets set equal to two when the criteria is not satisfied for all species that are in quasi-equilibrium, and some of the species still have not reached quasi-equilibrium status. The iterated values replace $y_{i,o}$ and return is to integration subroutine.

JAKE = 3 JAKE gets set equal to three when the integrating mesh is vanishing in this subroutine. All species are in quasi-equilibrium and iteration is not successful for all of them. The time increment is halved; initial time reset to $t_o - \Delta t/2$. If Δt is not less than the initial integrating mesh, the initial $y_{i,o}$ are restored and iteration repeated. If cut back in time causes Δt to become smaller than initial integrating mesh, JAKE is set to 3; return is to the integration subroutine where return is made to the MAIN program and run is terminated. Comment written on output tape.

"Integrating mesh is vanishing in ALGA at x.xxx sec."

DAUX Subroutine

Purpose: To compute derivative values.

Transfer to this subroutine is from the integration subroutine (INTEG).

This routine computes derivatives using the formation and removal terms computed in SLOP subroutine, which is called on entering this subroutine.

$$\frac{dy_i}{dt} = \text{FORM}\ (y_i) - y_i\ \text{REMV}\ (y_i) \qquad i - 1 \rightarrow \text{NUMB}$$

If any species is in quasi-equilibrium, i.e., $KEY_i = 2$, its derivative is set to zero.

If there is a production term for species NO or O it is subtracted from their respective number densities.

SLOP Subroutine

Purpose: To compute formation and removal terms, $\sum F_j(y_i)$ and $\sum R_j(y_i)$, for species not in quasi-equilibrium, i.e., $KEY_i = 1$.

Transfer is made to this subroutine from subroutines DAUX and EQUIL. Before the formation and removal terms are computed in this subroutine, subroutine BALAN is called where number densities of the largest positive species, N_2 and O_2 are computed, plus the constant terms in YURI block computed in Part II of the COEFF subroutine.

Each species is tested for quasi-equilibrium and for any $KEY_i = 1$. The sum of all reaction rates j, forming and removing a particular species i, are put into FORM(i) and REMV(i), respectively.

$$FORM(i) = \sum F_j(y_i) \qquad i = 1 \rightarrow NUMB$$

$$REMV(i) = \sum R_j(y_i)$$

For the largest positive species the production and removal term is set to zero and its KEY_i value to 4.

This subroutine must be changed if additional reactions are incorporated.

ALGA2 Subroutine

Purpose: To compute the formation and removal terms, $\sum F_j(y_i)$ and $\sum R_j(y_i)$, for species in quasi-equilibrium, i.e. $KEY_i = 2$.

Transfer is made to this subroutine from subroutines ALGA and EQUIL. Subroutine BALAN is called where the number densities of the largest positive species, N_2 and O_2 are computed, plus constant terms in YURI block computed in Part II of COEFF subroutine.

This subroutine is similar to the SLOP subroutine. Each species is tested for quasi-equilibrium and for any $KEY_i = 2$. The production and removal terms FORM(i) and REMV(i) are computed.

BALAN Subroutine

Purpose: To compute largest positive species from charge balance equation.

Transfer is made to this subroutine from the MAIN program or from subroutines SLOP or ALGA2.

The setting of variable LAM indicates which positive species is largest.

If LAM = 1, O^+ is largest positive species.

If LAM = 2, O_2^+ is largest positive species.

If LAM = 3, N_2^+ is largest positive species.

If LAM = 4, NO^+ is largest positive species.

Depending on it's setting, the largest positive species is computed from the charge balance equation.

$$\sum y^+ = e + \sum y^- .$$

The number density of N_2 and O_2 is computed. If either or both are negative, their number density is set to zero.

COEFF subroutine is called where terms in YURI region are computed.

EQUIL Subroutine

Purpose: To test each species i for quasi=equilbrium and set corresponding KEY_i.

Transfer to this subroutine is from the MAIN program after a successful integration.

This subroutine calls SLOP and ALGA2 where formation and removal terms for all species are computed.

After each successful integration, a test for quasi-equilibrium is made. Two conditions must be satisfied before a species is considered in quasi-equilibrium:

1. $\frac{di}{dt} = 0$

2. $\frac{d^2i}{dt^2} = 0$

The steady state of a species i may be expressed by:

$$\frac{di}{dt} = \sum F_j(i) - i\sum R_j(i) = 0$$

This equation states that for a species to be in equilibrium its first derivative is zero. This is a necessary condition but not sufficient. A situation could exist whereby the first derivative is negative and, as time increases, the derivative passes through zero and becomes positive. When this happens, it does not necessarily mean that the species has reached equilibirum when it passes through zero. Therefore, it is also necessary for the second derivative to be zero. Rather than compute the second derivative, it is considered to be zero if the criteria on the first derivative is satisfied after three successive integrations.

The differential equation is removed from the set when a species starts to oscillate around a steady value. Because of the oscillations in the solution at quasi-equilibrium, the derivative value is not allowed to become exactly zero. Since equilibrium implies a balance between formation and removal terms, these terms are used to establish a criteria on the first derivative.

The first necessary condition for quasi-equilibrium is considered fulfilled if one of the following criteria is satisfied.

$$\left|\frac{\Delta y_i}{\Delta t}\right| > .001, \text{ and } \frac{\left|\frac{\Delta y_i}{\Delta t}\right|}{y_i\sum R_j(y_i)} < \delta$$

or

$$\frac{\Delta y_i}{\Delta t} \leqq .001, \ \Delta t > \text{XMAS and } \left|1 - \frac{\sum F_j(y_i)}{y\sum R_j(y_i)}\right| \leqq \delta$$

where $\delta < 1$.

If test is satisfied, variable $LOCK_i$ is increased by 1. If test is not satisfied, variable $LOCK_i$ is set equal to zero. Once Key_i has been set to 3 for any species, it remains that way for remainder of solution.

KEY_i will be 4 for the most abundant positive ion.

All KEY_i are tested $j = 1 \rightarrow NUMB$

If $KEY_i < 3$ and $LOCK_i < 3$ then KEY_i set to 1

If $KEY_i < 3$ and $LOCK_i \geq 3$, then KEY_i set to 2 and species is considered in equilibrium or has reached the quasi-equilibrium state. Return is to MAIN program, where results of integration are put on output tape and decision to continue integration made.

The selection of a value for δ is of importance for two reasons.

1. If δ is too small, the differential equations will never be removed from the set because oscillations in densities will never meet criteria.

2. If δ is too large, the differential equations will be removed before iterations of algebraic set of equations can converge.

Once a species has been put in quasi-equilibrium, the solution from then on is dependent upon this assumption. If a differential equation is removed too soon, it is possible to get an erroneous solution.

DAUXT and DAUXT2 Subroutines

Purpose: To compute histories of the reactions.

Transfer is made to this subroutine from the MAIN program if option KB2=0.

The histories of the reactions are obtained by computing the rate of each reaction each time it is used. The behavior of any particular reaction can be studied from its history. Computation of this information is optional.

If KB2=0 and KB5=0, histories will be printed every time step.
If KB2=0 and KB5=1, histories will be printed every time cycle.
If KB2=1, histories will not be printed.

The printout of histories is on tape 3. The program is set up to run one case after another and histories might be desired on some cases and not on others; therefore, tape 3 must be furnished.

Subroutine DAUXT2 is a continuation of subroutine DAUXT. Transfer is made to subroutine DAUXT2 at the end of subroutine DAUXT.

APPENDIX D

FORTRAN STATEMENTS OF COMPUTER CODE

```
* B151
$          MAXT(20) MINS
$       MAXO(99999)LINES$$$
*       RTTORC
*       LIST
CSOLUTION OF THE REACTION RATE EQUATIONS IN THE IONOSPHERE 15 SPECIES
C       ZERO ALTITUDE TO END COMPUTATIONS
C       IF RESULTS ARE TO BE PLOTTED FOLLOWING RESTRICTIONS ARE NECESSARY
C       KB1=1.  THE FIRST TITLE CARD MUST HAVE RUN NO. IN COLUMNS 4-10
C       THE SECOND TITLE CARD MUST HAVE 4/1  N2/O2 IN COLUMNS 1-10
C       ANY OTHER COMMENTS MAY APPEAR IN COLUMNS 11-35
C       A > SYMBOL MUST BE LAST CHARACTER
C       KB1=0 FOR ALL LOG OUTPUT
C       KB1=1 FOR TIME AS DECIMAL OUTPUT NUMBER DENSITIES LOG OUTPUT
C       KB1=2 FOR ALL DECIMAL OUTPUT
C       KB2=0 CALLS DAUXT.
C       KB3=0 CHANGES RATE CONSTANTS FOR NEXT RUN.
C       KB3=1 USES THE SAME RATE CONSTANTS AS LAST RUN
C       KB3=2 READS NEW CRITERIA AND CHANGES RATE CONSTANT
C       KB4=0  O HELD CONSTANT.
C       KB4=1  O EQUATION IN SYSTEM.
C       KB5=1 PRINTS DAUXT ONLY ONCE EVERY TIME CYCLE.
C       KB6=1 READS ANOTHER POINT CARD AFTER AN ERROR.
C       KB7=1  IF YOU WANT A CONSTANT PRODUCTION FOR O,NO, N2, O2, AND E
C                A CARD WITH THESE VALUES MUST BE INSERTED IN INPUT DATA
C       KB8=1   WANT TO DO ANOTHER CYCLE WITH OUTPUT OF THIS RUN AS INPUT
C       UNITS OF INPUT PARAMETERS ARE CGS.
C
      COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175
     1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)
      COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2
     1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,K
     2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5,NSKIP,EPSI,IFAIL,TOTO,T
     3OTN,DEL,XMAS,KB4,B5,KB7
      COMMON KKK,DDD
      DIMENSION DONT(20),TITLE(12),TTREG(20),TITL(12)
      EQUIVALENCE(DO2,DZ2),(DO,DZ)
      REAL LOGT
      LOGT(QOOOFL)=0.43429448*ALOG(QOOOFL)
C
C       INITIALIZATION OF SYSTEM AND INPUT.
   37 REWIND 1
      REWIND 3
      REWIND 4
      CALL SETMSI(2)
      CHI=1.0E-20
      NOCOM=166
      ENDE=0.0
      ITER=30
   24 READ(5,50)        EUBAR,ELBAR,DEL,EPSI,ENDT,B4
   20 READ(5,50)       (COB(J),J=1,NOCOM)
    1 READ(5,50)      ALT,D,DO2,DO,DN2,T
      READ(5,50)      (BEGIN(J),J=1,13),PROD,XMAS
      READ(5,1100)      KB1,KB2,KB3,KB4,KB5,KB6,KB7,KB8
```

```
      READ(5,440)     (TITLE(N),N=1,12)
      READ(5,440)     (TITL (N),N=1,12)
      KKK=0
      IF(KB7 .EQ.0) GOTO 13
      READ(5,50)   PO,PNO,PN2,PO2,PNE
        PROD=PNE
      TOTAL=PROD
   13 DNO=BEGIN(9)
      CALL SLITE (2)
      TIME=1.0E-6
      JUMP=1
      KOUNT=0
      MOUNT=0
      KNT=0
      JAKE=1
      JACK=1
      LAM=5
      NSKIP=1
      KLOT=0
      DO 1000 J=1,148
 1000 TREG(J)=0.0
      IF(ALT .EQ. 0.0) GO TO 99
      IF(KB4 .EQ. 0) GO TO 408
  407 NUMB=15
      GO TO 409
  408 NUMB=14
  409 LINT=((2*NUMB)+4)
      I2NT=((3*NUMB)+4)
      K2NT=((4*NUMB)+4)
      J2NT=((5*NUMB)+4)
      N2NT=((6*NUMB)+4)
      KINT=((7*NUMB)+4)
      MINT=((8*NUMB)+4)
      NINT=((8*NUMB)+5)
      I3NT=((8*NUMB)+6)
      DO 45 J=1,NUMB
      TTREG(J+3)=0.0
      LOCK(J)=0
   45 KEY(J)=1
      CALL INITAL
      CALL COEFF
      IF(KB7 .EQ. 1) GOTO 439
      TREG(1)=TREG(2)*TREG(2)
      DENO=DZ
      DENNO=DNO
      DENO2=DZ2
      DENN2=DN2
      TOT=DZ2+DN2+DZ
      AO=PROD/TOT
      AN2=PROD/TOT
      AO2=PROD/TOT
      ANO=PROD/TOT
      PNE=PROD
      TOTAL=PROD
      BO=0
      CO=0
      BO2=0
      CO2=0
      BN2=0
      CN2=0
```

```
      BNO=0
      CNO=0
      PO=(AO+BO*TREG(2)+CO*TREG(1))*DENO
      PO2=(AO2+BO2*TREG(2)+CO2*TREG(1))*DENO2
      PN2=(AN2+BN2*TREG(2)+CN2*TREG(1))*DENN2
      PNO=(ANO+BNO*TREG(2)+CNO*TREG(1))*DENNO
C
C     PREPARE OUTPUT TAPES AND WRITE RATE CONSTANTS AND INITIAL
C     CONDITIONS.
C
  439 WRITE(6,441)      (TITLE(N),N=1,12)
      WRITE(6,440)      (TITL (N),N=1,12)
  441 FORMAT(1H1,12A6)
      WRITE(3,441)   (TITLE(N), N=1,12)
      WRITE(3,440)   (TITL(N),N=1,12)
      WRITE(3,1005)  D,DO2,DN2,DO,T
      WRITE(6,51)
      WRITE(6,52)ALT
      WRITE(6,1005)      D,DO2,DN2,DO,T
      IF(KB7 .EQ. 0) GOTO 442
      WRITE(6,443)           PO,PNO,PN2,PO2,PNE
      WRITE(3,443)  PO,PNO,PN2,PO2,PNE
  442 WRITE(6,68)
      IS=1
      DO 901 J=1,15
      IT=IS+4
      WRITE(6,900)(I,COB(I),I=IS,IT)
      WRITE(6,69)(I,CON(I),I=IS,IT)
      IS=IS+5
  901 CONTINUE
      WRITE(6,77)
      DO 91 J=1,18
      IT=IS+4
      WRITE(6,900) (I,COB(I),I=IS,IT)
      WRITE(6,69) (I,CON(I),I=IS,IT)
      IS=IS+5
   91 CONTINUE
      I=166
      WRITE(6,903)  I,COB(I)
      WRITE(6,902)  I,CON(I)
      WRITE(6,53)
      IF(KB1 .LE. 1) GOTO 8
    7 WRITE(6,75)      TREG(2),(TREG(J),J=4,11)
      IF(KB4 .EQ. 0) GO TO 411
      WRITE(1) TREG(2),(TREG(J),J=12,18),PROD
      GO TO 412
  411 WRITE(1) TREG(2),(TREG(J),J=12,17),DO,PROD
  412 MOUNT=MOUNT+1
      GO TO 5
    8 M=NUMB+3
      IF(KB1 .EQ. 0) GOTO 54
      I=3
      DONT(2)=TREG(2)
      GOTO 55
   54 I=2
   55 DO 16  J=I,M
      DEC=TREG(J)
      IF(DEC) 81,104,105
  104 DONT(J)=0.0
      GO TO 16
```

```
  105 DONT(J)=LOGT(DEC)
   16 CONTINUE
      IF(PROD) 81,3,4
    3 DPROD=0.0
      GO TO 9
    4 DPROD=LOGT(PROD)
    9 WRITE(6,75)      DONT(2),(DONT(J),J=4,11)
      IF(KB4 .EQ. 0) GO TO 414
  413 WRITE(1)      DONT(2),(DONT(J),J=12,18),DPROD
      GO TO 415
  414 DDO=LOGT(DO)
      WRITE(1)      DONT(2),(DONT(J),J=12,17),DDO,DPROD
  415 MOUNT=MOUNT+1
    5 DO 6 K=1,NUMB
      IF(KEY(K)-2) 10,6,6
    6 CONTINUE
      CALL ALGA
      TREG(3)=2.0*TREG(3)
      TREG(2)=TREG(2)+TREG(3)
      GO TO 12
C
C     INTEGRATION  OF EQUATIONS STARTS HERE.
C
   10 CALL INTEG
   12 CALL BALAN
      IF(TREG(3)-2.0E-6) 503,504,503
  504 KLOT=KLOT+1
      IF(KLOT-10) 505,505,506
  503 KLOT=0
  505 IF(KB1 .LE. 1) GOTO 514
      GO TO 517
  506 WRITE (6,507)
      GO TO 26
  514 DDO2=LOGT(DO2)
      DDN2=LOGT(DN2)
      IF(KB1 .EQ. 1) GOTO 62
      DONT(2)=LOGT(TREG(2))
      GOTO 63
   62 DONT(2)=TREG(2)
   63 WRITE(4) DONT(2),DDO2,DDN2,(KEY(J),J=1,NUMB)
      GO TO 515
  517 WRITE(4) TREG(2),DO2,DN2,(KEY(J),J=1,NUMB)
  515 KOUNT=KOUNT+1
      IF(JAKE-2) 25,29,11
   25 JACK=2
      CALL EQUIL
  519 GO TO (520,521),JUMP
  520 DO 522 J=1,NUMB
      IF(KEY(J)-2) 522,523,522
  522 CONTINUE
      GO TO 521
  523 FIRST=TREG(3)/2.0
      JUMP=2
  521 DO 46 J=1,NUMB
      IF(KEY(J)-3) 300,46,46
  300 IF(TREG(J+3)-TTREG(J+3)) 47,46,46
   47 IF(TREG(J+3)-CHI) 48,46,46
   48 KEY(J)=3
      TREG(J+3)=0.0
   46 CONTINUE
```

```
      IF(PNE) 600,601,600
  601 IF((TREG(4)/BEGIN(1))-1.0E-3) 602,600,600
  602 DO 603 J=1,3
      TREG(J+3)=0.0
  603 KEY(J)=3
  600 DO 83 J=1,NUMB
   83 TTREG(J+3)=TREG(J+3)
C
C     OUTPUT OF RESULTS STARTS HERE.
C
      IF(KNT-50) 2036,2037,2037
 2037 WRITE(6,53)
      KNT=0
 2036 KNT=KNT+1
      IF(KB1 .LE. 1) GOTO 19
   93 WRITE(6,75)      TREG(2),(TREG(J),J=4,11)
      IF(KB4 .EQ. 0) GO TO 419
      WRITE(1) TREG(2),(TREG(J),J=12,18),TOTAL
      GO TO 405
  419 WRITE(1)      TREG(2),(TREG(J),J=12,17),DO,TOTAL
      GO TO 405
   19 K=NUMB+3
      IF(KB1 .EQ. 0) GOTO 60
      I=3
      DONT(2)=TREG(2)
      GOTO 61
   60 I=2
   61 DO 28 J=I,K
      DEC=TREG(J)
      IF(DEC) 81,109,110
  109 DONT(J)=0.0
      GO TO 28
  110 DONT(J)=LOGT(DEC)
   28 CONTINUE
      IF(TOTAL) 81,114,115
  114 TOTL=0.0
      GO TO 2018
  115 TOTL=LOGT(TOTAL)
 2018 WRITE(6,75)      DONT(2),(DONT(J),J=4,11)
      IF(KB4 .EQ. 0) GO TO 421
  420 WRITE(1)      DONT(2),(DONT(J),J=12,18),TOTL
      GO TO 405
  421 DDO=LOGT(DO)
      WRITE(1)      DONT(2),(DONT(J),J=12,17),DDO,TOTL
  405 MOUNT=MOUNT+1
      IF(KB7 .EQ. 1) GOTO 18
      TREG(1)=TREG(2)*TREG(2)
      PO=(AO+BO*TREG(2)+CO*TREG(1))*DENO
      PO2=(AO2+BO2*TREG(2)+CO2*TREG(1))*DENO2
      PN2=(AN2+BN2*TREG(2)+CN2*TREG(1))*DENN2
      PNO=(ANO+BNO*TREG(2)+CNO*TREG(1))*DENNO
      PNE=PROD
      TOTAL=PNE
      TOT=DZ2+DN2+DZ
      DENNO=TREG(12)
      DENN2=DN2
      DENO2=DZ2
      IF(KB4 .EQ. 0) GOTO 43
      DENO=TREG(18)
      GOTO 18
```

```
   43 DENO=DZ
   18 IF(KB2 .EQ. 1) GO TO 15
   22 CALL DAUXT
C
C      DECISION TO CONTINUE INTEGRATION OR STOP IS MADE HERE.
C
   15 IF(TREG(4)-ENDE) 117,17,17
   17 IF(TREG(2)-ENDT) 100,117,117
  100 BIG=AMAX1(TREG(9),TREG(10),TREG(11),TREG(16))
      DO 203 J=1,3
      IF (BIG .EQ. TREG(J+8)) GO TO 204
  203 CONTINUE
      J=4
  204 IF(J-LAM) 205,206,205
  205 IF(LAM-4) 302,303,302
  303 KEY(13)=1
      GO TO 304
  302 KEY(LAM+5)=1
  304 JACK=1
  206 LAM=J
      GO TO 5
C
C      ERROR COMMENT OUTPUTS.
C
   29 WRITE(6,57)TREG(2)
      GOTO 26
   11 WRITE(6,58)TREG(2)
      GO TO 26
   81 WRITE(6,56)
      K=NUMB+3
      WRITE(6,59)      (TREG(J),J=2,K),TOTAL
      GO TO 26
  117 KB6=1
C
C      TRANSFER ALL RESULTS TO OUTPUT TAPE HERE.
C
   26 REWIND 1
      END FILE 3
      KNT=0
      WRITE(6,67)
      DO 150 K=1,MOUNT
      READ (1)     TREG(2),(TREG(J),J=12,17),DO,TOTAL
      WRITE(6,75)      TREG(2),(TREG(J),J=12,17),DO,TOTAL
      KNT=KNT+1
      IF(KNT-50) 150,150,34
   34 WRITE(6,67)
      KNT=0
  150 CONTINUE
      REWIND 1
      REWIND 4
      KNT=0
      IF(KB4 .EQ. 0) GO TO 425
      WRITE(6,73)
      GO TO 426
  425 WRITE(6,70)
  426 DO 21 K=1,KOUNT
      READ (4) TREG(2),DO2,DN2,(KEY(J),J=1,NUMB)
      IF(KB4 .EQ. 0) GO TO 423
      WRITE(6,72) TREG(2),DO2,DN2,(KEY(J),J=1,NUMB)
      GO TO 102
```

```
  423 WRITE(6,71) TREG(2),DO2,DN2,(KEY(J),J=1,NUMB)
  102 KNT=KNT+1
      IF(KNT-50) 21,21,2032
 2032 IF(KB4 .EQ. 0) GO TO 2033
      WRITE(6,73)
      GO TO 2035
 2033 WRITE(6,70)
 2035 KNT=0
   21 CONTINUE
      REWIND 4
      END FILE 6
      IF(KB8-1) 1050,700,1050
 1050 KB6=1
      GOTO 14
  700 KKK=KKK+1
      IF(KKK .EQ. 2) GOTO1050
      END FILE 3
        PROD=0
      KB7=0
      IF(KB1-1) 35,95,97
   95 M=NUMB+3
      JA=3
      TREG(2)=DONT(2)
      GOTO 36
   35 M=NUMB+3
      JA=2
   36 DO 96  J=JA,M
      DEC=10.0**DONT(J)
   96 TREG(J)=DEC
      DZ2=10.0**DDO2
      DN2=10.0**DDN2
   97 I=1
      DO 703  J=4,NUMB
      BEGIN(I)=TREG(J)
      I=I+1
  703 CONTINUE
      BEGIN(13)=TREG(17)
      IF(KB4 .EQ. 0) GOTO 98
      DO=TREG(18)
   98 DDD=TREG(16)
      D=DO+DN2+DO2
      GOTO  13
   14 IF(KB3-1) 23,1,24
   99 REWIND 3
      CALL EXIT
C
   50 FORMAT (1P6E12.5)
   51 FORMAT(58HOSOLUTION OF THE REACTION RATE EQUATIONS WITH 15 SPECIES
     1. )
  101 FORMAT(7H AT 521,2XI3,4XI3,1P3E14.7)
   52 FORMAT(11HOALTITUDE =1PE11.4,5H CM. )
   53 FORMAT(119H1 TIME (SEC)      N(E) /CC      N(O-) /CC     N(O2-) /CC  N
     1(O3-) /CC    N(NO2-) /CC    N(O+) /CC     N(O2+) /CC    N(N2+) /CC   )
   56 FORMAT(65HOTHE PROGRAM IN TRYING TO GENERATE THE LOG OF A NEGATIVE
     1 NUMBER. )
   57 FORMAT(45H THE INTERGRATING MESH IS VANISHING IN INT AT 1PE11.5,6H
     1 SEC. )
   58 FORMAT(47H THE INTERGRATING MESH IS VANISHING IN ALGA AT 1PE11.5,6
     1H SEC. )
   59 FORMAT(1P10F10.2)
```

```
   65 FORMAT(1H0,(5(2X4HCOB(,I3,2H)=1PE14.7)))
   66 FORMAT(1H0,(2X4HCOB(,I3,2H)=1PE14.7))
   67 FORMAT(118H1 TIME (SEC)     N(NO) /CC     N(N) /CC      N(NO2) /CC
     1N(O3) /CC     N(NO+) /CC    N(N2O) /CC     N(O) /CC    PRODUCTION   )
   68 FORMAT(22H0REACTION COEFFICIENTS)
   69 FORMAT(1H ,(5(2X4HCON(,I3,2H)=1PE14.7)))
     13- NO2- O+ O2+ N2+ NO  N  NO2  O3  NO+ N2O )
   71 FORMAT(1P3E13.5,16I4,1PE13.5)
   72 FORMAT(1P3E13.5,17I4,1PE13.5)
   73 FORMAT(102H1  TIME (SEC)  O2 DENSITY   N2 DENSITY     E  O-   O2- O
     13- NO2- O+ O2+ N2+ NO  N  NO2  O3  NO+ N2O  O  )
   75 FORMAT(1P10E13.5)
   77 FORMAT(1H1)
  440 FORMAT(12A6)
  507 FORMAT(42H THE INCREMENT IS CONSTANT AT 1.0E06 SEC. )
  900 FORMAT(1H0,(5(2X4HCOB(,I3,2H)=1PE14.7)))
  903 FORMAT(1H0,(2X4HCOB(,I3,2H)=1PE14.7))
  902 FORMAT(1H ,(2X4HCON(,I3,2H)=1PE14.7))
  125 FORMAT(15H0START TIME     ,A6)
  126 FORMAT(15H0FINISH TIME    ,A6)
 1005 FORMAT(16H0TOTAL DENSITY =1PE12.5,13H O2 DENSITY =1PE12.5,13H N2 D
     1ENSITY =1PE12.5,12H O DENSITY =1PE12.5,14H TEMPERATURE =0PF7.2)
  443 FORMAT(29H0CONSTANT PRODUCTION    Q(O+)=1PE9.2,10H    Q(NO+)=1PE9.2,
     110H    Q(N2+)=1PE9.2,10H    Q(O2+)=1PE9.2,8H    Q(E)=1PE9.2)
 1100 FORMAT(8I2)
      END
      SUBROUTINE INITAL
      COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175
     1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)
      COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2
     1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,K
     2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5,NSKIP,EPSI,IFAIL,TOTO,T
     3OTN,DEL,XMAS,KB4,B5,KB7
      COMMON KKK,DDD
      TREG(2)=0.0
      TREG(3)=1.0E-14
      FIRST=TREG(3)
      DO 1 J=1,12
      TREG(J+3)=BEGIN(J)
    1 CONTINUE
      IF(KKK-1) 5,4,5
    5 TREG(16)=0.0
      GO TO 6
    4 TREG(16)=DDD
    6 TREG(17)=BEGIN(13)
      TOTAL=PROD
      IF(KB4 .EQ. 0) GO TO 3
    2 TREG(18)=DO
    3 TOTO=TREG(5)+2.0*TREG(6)+3.0*TREG(7)+2.0*TREG(8)+TREG(9)+2.0*TREG(
     110)+TREG(12)+2.0*TREG(14)+3.0*TREG(15)+TREG(16)+TREG(17)+DO       +
     22.0*DO2
      TOTN=TREG(8)+2.0*TREG(11)+TREG(12)+TREG(13)+TREG(14)+TREG(16)+2.0*
     1TREG(17)+2.0*DN2
      RETURN
      END
      SUBROUTINE COEFF
C     BORTNERS 1963 REACTION RATES
      COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175
     1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)
      COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2
```

```
     1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,K
     2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5,NSKIP,EPSI,IFAIL,TOTO,T
     3OTN,DEL,XMAS,KB4,B5,KB7
      CALL SLITET(2,K000ZO)
      GO TO(17,18),K000ZO
   17 EX1=EXP(-5100.0/T)
      EX2=(T**1.5)
      EX3=(T**0.5)
      EX4=300.0/T
      EX5=(T**3.0)
      EX6=EXP(-500.0/T)
      EX7=EXP(-1250.0/T)
      EX8=EXP(-1000.0/T)
      EX9=EXP(-2000.0/T)
      DO 1 J=1,4
    1 CON(J)=COB(J)
      DO 15  J=5,7
   15 CON(J)=COB(J)*T*T*EX1
      CON(8)=COB(8)
      CON(9)=COB(9)*EXP(-4700.0/T)
      DO 2 J=10,20
    2 CON(J)=COB(J)
      CON(21)=COB(21)*EXP(-7200.0/T)
      DO 3 J=22,23
    3 CON(J)=COB(J)
      DO 9   J=24,25
    9 CON(J)=COB(J)*EX3
      DO 14   J=26,28
   14 CON(J)=COB(J)/T
      DO 4 J=29,33
    4 CON(J)=COB(J)/EX2
      CON(34)=COB(34)/(T**0.70)
      DO 5 J=35,37
    5 CON(J)=COB(J)
      DO 6 J=38,51
    6 CON(J)=COB(J)/EX3
      DO 12 J=52,62
   12 CON(J)=COB(J)/EX2
      DO 7 J=63,84
    7 CON(J)=COB(J)
      CON(85)=COB(85)*EXP(-2000.0/T)
      CON(86)=COB(86)*EXP(-3000.0/T)
      CON(88)=COB(88)
      CON(87)=COB(87)
      CON(89)=COB(89)*EXP(-3500.0/T)
      DO 13 J=90,92
   13 CON(J)=COB(J)
      CON(93)=COB(93)/T
      CON(94)=COB(94)/EX3
      DO 8 J=99,103
    8 CON(J)=COB(J)
      CON(104)=COB(104)*EXP(-2800.0/T)
      CON(106)=COB(106)*EXP(-530.0/T)
      CON(107)=COB(107)*EXP(-7000.0/T)
      CON(108)=COB(108)
      CON(109)=COB(109)
      CON(110)=COB(110)*EX2*EXP(-6600.0/T)
      DO 10 J=111,112
   10 CON(J)=COB(J)
      CON(113)=COB(113)*EXP(-5000.0/T)
```

```
      CON(114)=COB(114)*EXP(-4000.0/T)
      DO 11 J=115,124
   11 CON(J)=COB(J)
      CON(125)=COB(125)*EXP(-5000.0/T)
      DO 19 J=126,135
   19 CON(J)=COB(J)
      DO 20 J=136,138
   20 CON(J)=COB(J)/EX3
      DO 21 J=139,143
   21 CON(J)=COB(J)
      CON(128)=COB(128)*EXP(-4000.0/T)
      CON(144)=COB(144)*EX3
      CON(145)=COB(145)
      CON(146)=COB(146)
      CON(147)=COB(147)/EX3
      CON(148)=COB(148)/EX3
      CON(149)=COB(149)
      CON(150)=COB(150)
      CON(151)=COB(151)/T
      DO 16   J=152,155
   16 CON(J)=COB(J)
      CON(156)=COB(156)*EXP(-10000.0/T)
      CON(157)=COB(157)
      CON(158)=COB(158)
      CON(159)=COB(159)*EXP(-3000.0/T)
      CON(160)=COB(160)*EXP(-10000.0/T)
      CON(161)=COB(161)*EXP(-37500.0/T)
      CON(162)=COB(162)*EX2*EXP(-19000.0/T)
      CON(163)=COB(163)*EXP( -1400.0/T)
      CON(164)=COB(164)*EXP(-13500.0/T)
      CON(165)=COB(165)
      CON(166)=COB(166)*EXP(-1200.0/T)
   18 YURI(4)=DO2*(CON(17)+(DO2*CON(24))+(DN2*CON(25)))
      YURI(5)=CON(19)+CON(20)+CON(21)
      YURI(6)=(D*CON(29))+CON(34)
      YURI(7)=CON(28)+(D*CON(30))+CON(35)
      YURI(8)=CON(26)+(D*CON(31))+CON(36)
      YURI(9)=(D*CON(32))+CON(37)
      YURI(10)=CON(27)+(D*CON(33))
      YURI(11)=DO2*CON(112)
      YURI(12)=DN2*CON(114)
      YURI(13)=CON(47)          +CON(126)+CON(127)
      YURI(14)=CON(13)+CON(64)
      YURI(16)=(D*CON(53))+CON(40)
      YURI(17)=(D*CON(54))+CON(39)
      YURI(18)=(D*CON(55))+CON(38)
      YURI(19)=(D*CON(62))+CON(42)
      YURI(20)=(D*CON(59))+CON(43)
      YURI(21)=(CON(44)+(D*CON(60))+CON(119)+CON(120)+CON(121)+CON(124))
      YURI(22)=(D*CON(61))+CON(45)
      YURI(23)=DO2*(DN2*CON(113))
      YURI(24)=CON(48)+CON(123)
      YURI(26)=CON(85)+CON(87)
      YURI(27)=DN2*CON(83)
      YURI(28)=(D*CON(91))+CON(78)
      YURI(29)=CON(71)+CON(80)+CON(84)
      YURI(31)=DO2*CON(102)
      YURI(32)=2.0*DO2*CON(128)
      YURI(33)=CON(101)+CON(109)
      YURI(34)=CON(117)+CON(118)
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      YURI(35)=CON(107)+CON(108)
      YURI(36)=DN2*CON(86)
      YURI(38)=DO2*CON(9)
      YURI(42)=DO2*CON(73)
      YURI(47)=YURI(9)+YURI(10)
      YURI(48)=YURI(24)+CON(122)+CON(125)
      YURI(50)=CON(116)+YURI(22)+YURI(34)
      YURI(52)=DO2*CON(89)
      YURI(53)=DN2*CON(135)
      YURI(61)=CON(120)+(2.0*CON(121))
      YURI(62)=CON(122)+CON(123)
      YURI(63)=2.0*((D*CON(93))+(DN2*CON(97)))
      YURI(66)=DN2*CON(11)
      YURI(68)=YURI(31)+DO2*CON(110)
      YURI(72)=DO2*CON(110)
      YURI(74)=CON(15)+CON(63)
      YURI(75)=DO2*CON(22)+DN2*CON(23)
      YURI(76)=CON(77)+(D*CON(90))
      YURI(78)=D*CON(55)
      YURI(79)=D*CON(62)
      YURI(80)=D*CON(53)
      YURI(81)=D*CON(54)
      YURI(83)=CON(69)+CON(88)
      YURI(84)=CON(99)+(D*CON(94))
      YURI(85)=CON(100)+(D*CON(95))
      YURI(1)=(CON(1)+(DO2*CON(5))+(DN2*CON(6))+(DO*(CON(7)+CON(15))))
      YURI(2)=(DN2*CON(11))+(DO*CON(8))
      YURI(3)=DO*(CON(16)+(DO2*CON(22))+(DN2*CON(23)))
      YURI(15)=(CON(41)+(DO2*CON(56))+(DN2*CON(57))+(DO*CON(58)))
      YURI(25)=((DO2*CON(70))+(DO*(CON(77)+(D*CON(90)))))
      YURI(30)=DO*((D*CON(94))+CON(99))
      YURI(37)=DO*(CON(100)+(D*CON(95)))
      YURI(39)=DO*CON(63)
      YURI(40)=DO*CON(106)
      YURI(41)=DO*CON(69)
      YURI(43)=DO*CON(88)
      YURI(44)=YURI(3)+YURI(4)
      YURI(45)=CON(2)+YURI(2)+YURI(38)
      YURI(46)=YURI(45)+YURI(11)
      YURI(49)=YURI(1)+YURI(23)+YURI(39)
      YURI(51)=(DO*CON(81))+YURI(36)
      YURI(54)=CON(4)+YURI(12)
      YURI(55)=YURI(41)+YURI(43)+YURI(42)+YURI(52)
      YURI(56)=YURI(25)+YURI(27)+(DN2*(CON(79)+(D*CON(92))))
      YURI(57)=DO*CON(15)
      YURI(58)=DO*(DO2*(CON(103)+(D*CON(96))))
      YURI(59)=YURI(30)+YURI(72)
      YURI(60)=DO*CON(104)
      YURI(64)=YURI(30)+YURI(31)
      YURI(65)=DO*CON(82)
      YURI(67)=YURI(43)+YURI(52)
      YURI(69)=DO*(DN2*CON(140))
      YURI(70)=DO*CON(134)
      YURI(71)=DO2*CON(70)
      YURI(73)=2.0*DO2*CON(143)
      YURI(77)=YURI(30)+YURI(68)
      YURI(82)=CON(132)+CON(133)
      YURI(86)=DO2*(CON(103)+(D*CON(96)))+2.0*DO* (DO2*CON(136)+(DO*CON(
     1137))+(DN2*CON(138))+CON(139))+(DN2*CON(140))
      YURI(87)=DO*DO2*CON(144)
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      YURI(88)=DO2*CON(145)+DN2*CON(146)
      YURI(89)=D*CON(149)
      YURI(90)=DO2*DO2*CON(151)
      YURI(91)=D*CON(150)
      YURI(92)=DO*DN2*CON(161)
      YURI(93)=DO*CON(163)
      YURI(94)=DO*DO2*CON(157)+DO*DN2*CON(158)
      YURI(95)=DO*CON(162)
      YURI(96)=D*CON(160)
      YURI(97)=DO2*D*CON(159)
      YURI(98)=YURI(94)+YURI(95)
      YURI(99)=DO2*DN2*CON(154)+DO2*DO2*CON(153)+DO*DO2*CON(155)
      YURI(100)=DO*DN2*D*CON(156)
      YURI(101)=CCN(163)+CON(164)
      YURI(102)=DO*YURI(101)
      YURI(103)=YURI(99)+DN2*(D*CON(156)+CON(161))
      YURI(104)=CON(162)+DN2*CON(158)+DO2*CON(157)
      RETURN
      END
      SUBROUTINE INTEG
      COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175
     1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)
      COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2
     1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,K
     2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5,NSKIP,EPSI,IFAIL,TOTO,T
     3OTN,DEL,XMAS,KB4,B5,KB7
      DIMENSION RK(4,17)
      IFAIL=0
      L=KINT
      DO 59 J=1,NUMB
      TREG(L)=TREG(J+3)
      L=L+1
   59 CONTINUE
   26 KOUNT=0
      L=LINT
      DO 31 J=1,NUMB
      TREG(L)=TREG(J+3)
      L=L+1
   31 CONTINUE
      TREG(MINT)=TREG(2)
   49 IF(TREG(2)-5.0E-6)1,11,11
   11 IF(TREG(3)-1.0E-15) 116,1,1
    1 ASSIGN 18 TO K1
      TREG(NINT)=TREG(3)
   32 K=N2NT
      DO 33 J=1,NUMB
      TREG(K)=TREG(J+3)
      K=K+1
   33 CONTINUE
      TREG(I3NT)=TREG(2)
    2 DO 6 I=1,4
      CALL DAUX
      L=NUMB+4
      DO 3 J=1,NUMB
      RK(I,J)=TREG(L)*TREG(3)
      L=L+1
    3 CONTINUE
      IF(I-3) 4,7,9
    4 L=N2NT
      DO 5 J=1,NUMB
```

```
      IF(KEY(J)-1) 220,220,221
  220 TREG(J+3)=TREG(L)+(0.5*RK(I,J))
      IF(TREG(J+3)) 25,221,221
  221 L=L+1
    5 CONTINUE
      TREG(2)=(TREG(I3NT)+(0.5*TREG(3)))
      DO 23 K=1,NUMB
      IF(KEY(K)-2) 23,68,23
   23 CONTINUE
      GO TO 6
   68 CALL ALGA
  400 L=JAKE
      GO TO (15,15,73),L
   15 L=JAM
      GO TO (6,500),L
    7 L=N2NT
      DO 8 J=1,NUMB
      IF(KEY(J)-1) 222,222,223
  222 TREG(J+3)=TREG(L)+RK(I,J)
      IF(TREG(J+3)) 25,223,223
  223 L=L+1
    8 CONTINUE
      TREG(2)=TREG(I3NT)+TREG(3)
      DO 65 K=1,NUMB
      IF(KEY(K)-2) 65,48,65
   65 CONTINUE
      GO TO 6
   48 CALL ALGA
  403 L=JAKE
      GO TO (16,16,73),L
   16 L=JAM
      GO TO (6,500),L
    6 CONTINUE
    9 L=N2NT
      DO 10 J=1,NUMB
      TREG(J+3)=TREG(L)+((1.0/6.0)*(RK(1,J)+2.0*RK(2,J)+2.0*RK(3,J)+RK(4
     1,J)))
      IF(TREG(J+3)) 25,120,120
  120 L=L+1
   10 CONTINUE
      DO 110 K=1,NUMB
      IF(KEY(K)-2) 110,64,110
  110 CONTINUE
      GO TO 14
   64 CALL ALGA
  406 L=JAKE
      GO TO (17,17,73),L
   17 L=JAM
      GO TO (14,500),L
   14 GO TO K1,(18,19,20)
   18 K=I2NT
  408 DO 21 J=1,NUMB
      TREG(K)=TREG(J+3)
      K=K+1
   21 CONTINUE
      ASSIGN 19 TO K1
      GO TO 32
   19 K=K2NT
      L=LINT
  410 DO 22 J=1,NUMB
```

```
      TREG(K)=TREG(J+3)
      TREG(J+3)=TREG(L)
      K=K+1
      L=L+1
   22 CONTINUE
      TREG(2)=TREG(MINT)
      TREG(3)=2.0*TREG(NINT)
      ASSIGN 20 TO K1
      GO TO 32
   20 K=J2NT
  411 DO 36 J=1,NUMB
      TREG(K)=TREG(J+3)
      K=K+1
   36 CONTINUE
      L=K2NT
      DO 37 J=1,NUMB
      IF(KEY(J)-2) 102,24,24
  102 IF(TREG(J+3))  25,100,100
  100 IF(TREG(L)) 25,101,101
  101 IF((ABS(TREG(L)-TREG(J+3))/TREG(L))-EUBAR)  24,24,25
   24 TREG(J+3)=TREG(L)
      L=L+1
   37 CONTINUE
      GO TO 73
  500 DO 501 J=1,NUMB
      IF(KEY(J)-2) 501,502,501
  502 IF(LKEY(J)-1) 501,503,501
  501 CONTINUE
      GO TO 25
  503 KEY(J)=1
      TREG(3)=TREG(NINT)
      GO TO 504
   25 TREG(3)=TREG(NINT)/2.0
  504 K=LINT
      DO 47 I=1,NUMB
      TREG(I+3)=TREG(K)
      K=K+1
   47 CONTINUE
      TREG(2)=TREG(MINT)
      N=JACK
      GO TO (49,66),N
   66 KOUNT=KOUNT+1
      IFAIL=1
      IF(KOUNT-3) 49,12,12
   12 TREG(3)=TREG(NINT)/10.0
      GO TO 49
  116 JAKE=2
   73 GO TO (130,131),NSKIP
  130 IF(TREG(2)-1.0E-6) 132,132,133
  132 FIRST=TREG(3)
  133 NSKIP=2
  131 RETURN
      END
      SUBROUTINE ALGA
      COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175
     1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)
      COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2
     1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,K
     2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5,NSKIP,EPSI,IFAIL,TOTO,T
     3OTN,DEL,XMAS,KB4,B5,KB7
```

```
      DIMENSION Y(17),RAT(17)
      DO 1 J=1,NUMB
      Y(J)=TREG(J+3)
      RAT(J)=0.0
    1 CONTINUE
    2 KOUNT=0
    8 CALL ALGA2
      FORM(9)=FORM(9)-PNO
      IF(KB4 .EQ. 0) GO TO 3
  401 FORM(15)=FORM(15)-PO
    3 DO 9 J=1,NUMB
      IF(KEY(J)-2) 9,5,9
    5 Y(J)=FORM(J)/REMV(J)
    9 CONTINUE
    4 K=NUMB
      DO 200 J=1,K
      IF(KEY(J)-2) 200,100,200
  100 RAT(J)=(TREG(J+3)/Y(J))
  200 CONTINUE
      DO 47 J=1,K
      IF(KEY(J)-2) 47,45,47
   45 IF(RAT(J)-(1.0+ELBAR)) 46,70,70
   46 IF(RAT(J)-(1.0-ELBAR)) 70,47,47
   47 CONTINUE
      GO TO 80
   70 DO 71 J=1,K
      IF(KEY(J)-2) 71,110,71
  110 TREG(J+3)=(TREG(J+3)+Y(J))/2.0
   71 CONTINUE
      KOUNT=KOUNT+1
      IF(KOUNT-ITFR) 8,72,72
   72 DO 73 J=1,K
      IF(KEY(J)-1) 73,75,73
   73 CONTINUE
      TREG(3)=TREG(3)/2.0
      TREG(2)=TREG(2)-TREG(3)
      IF(FIRST-TREG(3)) 11,10,10
   10 JAKE=3
      GO TO 114
   11 L=LINT
      DO 74 J=1,K
      TREG(J+3)=TREG(L)
      L=L+1
   74 CONTINUE
      GO TO 2
   75 JAM=2
      GO TO 114
   80 DO 82 J=1,K
      IF(KEY(J)-2) 82,6,82
    6 TREG(J+3)=(TREG(J+3)+Y(J))/2.0
   82 CONTINUE
      JAM=1
  114 RETURN
      END
      SUBROUTINE DAUX
      COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175
     1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)
      COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2
     1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,K
     2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5,NSKIP,EPSI,IFAIL,TOTO,T
```

```
      30TN,DEL,XMAS,KB4,B5,KB7
      CALL SLOP
   19 L=NUMB+4
      DO 4 J=1,NUMB
      IF(KEY(J)-2) 1,2,2
    1 TREG(L)=FORM(J)-(REMV(J)*TREG(J+3))
      GO TO 3
    2 TREG(L)=0.0
    3 L=L+1
    4 CONTINUE
      IF(KEY(9)-2) 5,12,12
    5 TREG(NUMB+12)=TREG(NUMB+12)-PNO
   12 IF(KB4 .EQ. 0) GO TO 18
   15 IF(KEY(15)-2) 16,17,17
   16 TREG(NUMB+18)=TREG(NUMB+18)-PO
      GO TO 18
   17 TREG(NUMB+18)=0.0
   18 RETURN
      END
      SUBROUTINE SLOP
      COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175
     1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)
      COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2
     1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,K
     2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5,NSKIP,EPSI,IFAIL,TOTO,T
     30TN,DEL,XMAS,KB4,B5,KB7
      IF(KB4 .EQ. 0) GO TO 104
  103 DO=TREG(18)
  104 CALL BALAN
      DNOPL=TREG(16)
      IF(KEY(1)-2) 50,51,51
   50 FORM(1)=PNE+(TREG(6)*(YURI(1)+(TREG(13)*CON(14))))+(TREG(5)*(YURI(
     145)+(TREG(13)*CON(10))+(TREG(12)*CON(12))+(TREG(15)*CON(13))))+(TR
     2EG(8)*CON(3))+(TREG(7)*CON(4))
      REMV(1)=YURI(44)+(TREG(15)*YURI(5))+(TREG(14)*CON(18))+(TREG(9)*YU
     1RI(6))+(TREG(10)*YURI(7))+(TREG(11)*YURI(8))+(DNOPL*YURI(47))
     2+YURI(87)+(TREG(14)*YURI(88))
   51 IF(KEY(2)-2) 52,53,53
   52 FORM(2)=(TREG(4)*(YURI(3)+(TREG(15)*CON(20))))+(TREG(6)*YURI(39))
      REMV(2)=Y[illegible](46)+(TREG(13)*CON(10))+(TREG(15)*YURI(14))+(TREG(12)*
     1CON(12))+[illegible]REG(14)*CON(65))+(TREG(9)*(YURI(15)+(TREG(13)*CON(52)))
     2)+(TREG([illegible]*YURI(16))+(TREG(11)*YURI(17))+(DNOPL*YURI(18))
     3+TREG(12)[illegible]YURI(89)+YURI(90)
   53 IF(KEY(3)-2) 54,55,55
   54 FORM(3)=TREG(4)*(YURI(4)+(TREG(15)*CON(21)))+TREG(4)*YURI(87)
      REMV(3)=YURI(49)+(TREG(13)*CON(14))+(TREG(15)*CON(66))+(TREG(14)*C
     1ON(67))+(TREG(9)*YURI(19))+(TREG(10)*YURI(20))+(TREG(11)*YURI(21))
     2+(DNOPL*YURI(50))+TREG(13)*YURI(91)
   55 IF(KEY(4)-2) 56,57,57
   56 FORM(4)=(TREG(15)*(TREG(4)*CON(19)))+(TREG(5)*(YURI(11)+(TREG(15)*
     1CON(64))))+(TREG(15)*(TREG(6)*CON(66)))+(TREG(8)*TREG(15)*CON(68))
     2+TREG(5)*YURI(90)
      REMV(4)=YURI(54)+(TREG(9)*CON(51))+(TREG(10)*CON(46))+(DNOPL*YURI(
     113))+(TREG(14)*CON(111))+(TREG(11)*CON(142))+TREG(11)*CON(148)
   57 IF(KEY(5)-2) 58,59,59
   58 FORM(5)=(TREG(14)*(TREG(4)*CON(18)))+(TREG(14)*(TREG(5)*CON(65)))+
     1(TREG(6)*((TREG(14)*CON(67))+YURI(23)))+(TREG(7)*(YURI(12)+(TREG(1
     24)*CON(111))))+TREG(4)*TREG(14)*YURI(88)+TREG(6)*TREG(13)*YURI(91)
     3+TREG(5)*TREG(12)*YURI(89)
      REMV(5)=CON(3)+(TREG(9)*CON(49))+(TREG(10)*CON(50))+(TREG(15)*CON(
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  168))+(DNOPL*YURI(48))+(TREG(11)*CON(141))+TREG(11)*CON(147)
 59 IF(KEY(6)-2) 60,61,61
 60 FORM(6)=PO+(TREG(13)*(TREG(10)*CON(85)))+(TREG(11)*YURI(41))
    REMV(6)=YURI(56)+(TREG(13)*YURI(28))+(TREG(12)*YURI(29))+(TREG(4)*
   1YURI(6))+(TREG(5)*(YURI(15)+(TREG(13)*CON(52))))+(TREG(6)*YURI(19)
   2)+(TREG(7)*CON(51))+(TREG(8)*CON(49))+(TREG(14)*CON(76))+(TREG(17)
   3*CON(134))
 61 IF(KEY(7)-2) 62,63,63
 62 FORM(7)=PO2+(TREG(9)*(YURI(25)+(TREG(12)*CON(84))))+(TREG(11)*YURI
   1(42))
    REMV(7)=YURI(51)+(TREG(13)*YURI(26))+(TREG(12)*CON(72))+(TREG(14)*
   1CON(115))+(TREG(4)*YURI(7))+(TREG(5)*YURI(16))+(TREG(6)*YURI(20))+
   2(TREG(7)*CON(46))+(TREG(8)*CON(50))
 63 IF(KEY(8)-2) 64,65,65
 64 FORM(8)=PN2
    REMV(8)=YURI(55)+(TREG(13)*CON(74))+(TREG(12)*CON(75))+(TREG(4)*YU
   1RI(8))+(TREG(5)*YURI(17))+(TREG(6)*YURI(21))+YURI(53)+(TREG(8)*CON
   2(141))+(TREG(7)*CON(142))+TREG(8)*CON(147)+TREG(7)*CON(148)
 65 DO 26 J=6,8
    IF(LAM+5-J) 26,12,26
 12 FORM(J)=0.0
    REMV(J)=0.0
    KEY(J)=4
 26 CONTINUE
    IF(LAM-4) 28,27,28
 27 FORM(13)=0.0
    REMV(13)=0.0
    KEY(13)=4
    GO TO 67
 28 IF(KEY(13)-2) 66,67,67
 66 FORM(13)=PNO+(TREG(10)*((TREG(12)*CON(72))+YURI(36)+(TREG(13)*CON(
   187))+(TREG(14)*CON(115))))+(TREG(9)*((TREG(12)*CON(71))+(TREG(13)*
   2YURI(28))+YURI(27)))+(TREG(11)*((TREG(12)*CON(75))+YURI(67)))
    REMV(13)=(TREG(4)*YURI(47))+(TREG(5)*YURI(18))+(TREG(6)*YURI(50))+
   1(TREG(8)*YURI(48))+(TREG(7)*YURI(13))+YURI(65)
 67 IF(KEY(9)-2) 29,68,68
 29 FORM(9)=(TREG(5)*((TREG(13)*CON(10))+(DNOPL*CON(38))))+(
   1TREG(6)*((DNOPL*YURI(22))+(2.0*TREG(11)*CON(119))))+(TREG(7)*(YURI
   2(12)+(DNOPL*CON(47 ))))+(TREG(8)*(DNOPL*YURI(24)))+(TREG(4)*(DNOPL
   3*YURI(9)))+(TREG(10)*(YURI(36)+(TREG(13)*CON(85))))+(TREG(11)*YURI
   4(52))+(TREG(13)*(YURI(59)+(TREG(15)*CON(105))+(2.0*TREG(14)*CON(10
   58))))+(TREG(14)*(YURI(40)+CON(131))+TREG(17)*CON(132))+(TREG(8)*TR
   6EG(11)*CON(141))+YURI(92) + 2.0* TREG(17)*YURI(93)
    REMV(9)=(TREG(5)*CON(12))+(TREG(9)*YURI(29))+(TREG(10)*CON(72))+(T
   1REG(11)*CON(75))+(TREG(12)*YURI(32))+(TREG(13)*YURI(33))+YURI(37)+
   2CON(129)+TREG(5)*YURI(89) + YURI(98)+TREG(13)*YURI(96)+TREG(15)*CO
   3N(166)
 68 IF(KEY(10)-2) 69,70,70
 69 FORM(10)=(TREG(4)*((2.0*TREG(11)*CON(26))+(DNOPL*YURI(10))))+(TREG
   1(6)*((DNOPL*YURI(34))+(TREG(11)*YURI(61))))+(TREG(8)*(DNOPL*YURI(6
   22)))+(TREG(9)*(YURI(27)+(TREG(12)*CON(84))))+(TREG(11)*YURI(43))+(
   3TREG(7)*(DNOPL*CON(126)))+YURI(92)    + TREG(12)*YURI(95)    +(CON(
   4129)*TREG(12))+(CON(132)*TREG(17))
    REMV(10)=(TREG(5)*CON(10))+(TREG(6)*CON(14))+(TREG(11)*CON(74))+(T
   1REG(9)*YURI(28))+(TREG(13)*(YURI(63)+2.0*TREG(13)*CON(98)))+(TREG(
   212)*YURI(33))+(TREG(15)*CON(105))+(TREG(14)*YURI(35))+(TREG(10)*YU
   3RI(26))+YURI(77)+TREG(6)*YURI(91)+2.0*TREG(13)*CON(152)+YURI(97)+
   4TREG(12)*YURI(96)+TREG(14)*CON(165)
 70 IF(KEY(11)-2) 71,72,72
 71 FORM(11)=(TREG(8)*(CON(3)+(TREG(9)*CON(49)))+(TREG(10)*CON(50))+(DN
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     1OPL*CON(48))+(TREG(15)*CON(68)))))+(TREG(12)*(YURI(37)+(TREG(5)*CON
     2(12))+(TREG(12)*YURI(32)))))+(TREG(13)*(YURI(31)+(TREG(6)*CON(14)))
     3)+(TREG(6)*(YURI(23)+(DNOPL*CON(116))+(TREG(11)*CON(120)))))+(TREG(
     47)*(DNOPL*CON(127)))+(TREG(5)*TREG(16)*YURI(78))+TREG(11)*TREG(8)*
     5CON(147)+TREG(13)*YURI(97)+(TREG(12)*(YURI(94)+TREG(15)*CON(166)))
      REMV(11)=YURI(40)+(TREG(4)*CON(18))+(TREG(5)*CON(65))+(TREG(6)*CON
     1(67))+(TREG(9)*CON(76))+(TREG(10)*CON(115))+(TREG(13)*YURI(35))+CO
     2N(131)+(TREG(7)*CON(111))+TREG(4)*YURI(88)+TREG(13)*CON(165)
   72 IF(KEY(12)-2) 73,74,74
   73 FORM(12)=(TREG(7)*(CON(4)+(TREG(10)*CON(46))+(TREG(9)*CON(51))+(DN
     1OPL* CON(47))+(TREG(14)*CON(111)))))+(TREG(5)*YURI(38))+(TREG(6)*(Y
     2URI(57)+(TREG(9)*YURI(79))+(TREG(16)*CON(117)))))+(TREG(10)*((TREG(
     35)*YURI(80))+(TREG(14)*CON(115)))))+(TREG(8)*TREG(16)*CON(125))+YUR
     4I(58)+TREG(11)*TREG(7)*CON(148)+DO*YURI(99)
      REMV(12)=(TREG(4)*YURI(5))+(TREG(5)*YURI(14))+(TREG(6)*CON(66))+(T
     1REG(8)*CON(68))+(TREG(13)*CON(105))+YURI(60)+CON(130)
     2+TREG(12)*CON(166)
   74 IF(KEY(14)-2) 75,76,76
   75 FORM(14)=(TREG(5)*(YURI(66)+(TREG(11)*YURI(81)))))+(TREG(12)*TREG(1
     13)*CON(101))+YURI(69)+(TREG(11)*((TREG(6)*CON(124))+(TREG(8)*CON(1
     241))+(TREG(7)*CON(142)))))+YURI(100)+TREG(13)*(TREG(12)*YURI(96)+T
     3REG(14)*CON(165))
      REMV(14)=YURI(82)+TREG(9)*CON(134)+YURI(102)
   76 IF(KB4 .EQ. 0) GO TO 78
      IF(KEY(15)-2) 77,78,78
   77 FORM(15)=(TREG(5)*(CON(2)+(TREG(16)*CON(38))+(TREG(11)*CON(39))+(
     1TREG(10)*CON(40))+(2.0*TREG(9)*CON(41))+(TREG(15)*CON(64))+(TREG(
     2 14)*CON(65)))))+(TREG(6)*((TREG(9)*CON(42))+(TREG(16)*(CON(116)+
     3CON(118)))+(2.0*TREG(11)*CON(121)))))+(TREG(4)*((TREG(15)*CON(21))
     4+(2.0*TREG(10)*CON(28))+(TREG(16)*YURI(10))+(TREG(9)*YURI(6)))))+(T
     5REG(8)*(TREG(9)*CON(49)))+(TREG(7)*(TREG(9)*CON(51)))+(TREG(9)*(YU
     6RI(71)+(TREG(12)*CON(71))+(TREG(14)*CON(76)))))+(TREG(13)*((TREG(10
     7)*CON(87))+(TREG(12)*CON(109))+YURI(72)))+(TREG(12)*CON(129))+(TRE
     8G(15)*CON(130))+(TREG(14)*(CON(131)+TREG(13)*CON(165)))+(TREG(17)*
     9(CON(133)+TREG(9)*CON(134)))+TREG(6)*TREG(11)*CON(124)+YURI(73)
      REMV(15)=(TREG(5)*CON(8))+(TREG(6)*YURI(74))+(TREG(4)*(CON(16)+YUR
     1I(75)))+TREG(9)*YURI(76) +TREG(10)*CON(81)+TREG(11)*YURI(83)+TREG
     2(16)*CON(82)+TREG(13)*YURI(84)+TREG(12)*YURI(85)+TREG(15)*CON(104)
     3+TREG(14)*CON(106)+YURI(86)+YURI(103)+TREG(17)*YURI(101)+TREG(12)*
     4YURI(104)
   78 RETURN
      END
      SUBROUTINE ALGA2
      COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175
     1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)
      COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2
     1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,K
     2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5,NSKIP,EPSI,IFAIL,TOTO,T
     3OTN,DEL,XMAS,KB4,B5,KB7
      IF(KB4 .EQ. 0) GO TO 104
  103 DO=TREG(18)
  104 CALL BALAN
      DNOPL=TREG(16)
      IF(KEY(1)-2) 51,50,51
   50 FORM(1)=PNE+(TREG(6)*(YURI(1)+(TREG(13)*CON(14))))+(TREG(5)*(YURI(
     145)+(TREG(13)*CON(10))+(TREG(12)*CON(12))+(TREG(15)*CON(13))))+(TR
     2EG(8)*CON(3))+(TREG(7)*CON(4))
      REMV(1)=YURI(44)+(TREG(15)*YURI(5))+(TREG(14)*CON(18))+(TREG(9)*YU
     1RI(6))+(TREG(10)*YURI(7))+(TREG(11)*YURI(8))+(DNOPL*YURI(47))
     2+YURI(87)+(TREG(14)*YURI(88))
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51 IF(KEY(2)-2) 53,52,53
52 FORM(2)=(TREG(4)*(YURI(3)+(TREG(15)*CON(20))))+(TREG(6)*YURI(39))
   REMV(2)=YURI(46)+(TREG(13)*CON(10))+(TREG(15)*YURI(14))+(TREG(12)*
  1CON(12))+(TREG(14)*CON(65))+(TREG(9)*(YURI(15)+(TREG(13)*CON(52)))
  2)+(TREG(10)*YURI(16))+(TREG(11)*YURI(17))+(DNOPL*YURI(18))
  3+TREG(12)*YURI(89)+YURI(90)
53 IF(KEY(3)-2) 55,54,55
54 FORM(3)=TREG(4)*(YURI(4)+(TREG(15)*CON(21)))+TREG(4)*YURI(87)
   REMV(3)=YURI(49)+(TREG(13)*CON(14))+(TREG(15)*CON(66))+(TREG(14)*C
  1ON(67))+(TREG(9)*YURI(19))+(TREG(10)*YURI(20))+(TREG(11)*YURI(21))
  2+(DNOPL*YURI(50))+TREG(13)*YURI(91)
55 IF(KEY(4)-2) 57,56,57
56 FORM(4)=(TREG(15)*(TREG(4)*CON(19)))+(TREG(5)*(YURI(11)+(TREG(15)*
  1CON(64))))+(TREG(15)*(TREG(6)*CON(66)))+(TREG(8)*TREG(15)*CON(68))
  2+TREG(5)*YURI(90)
   REMV(4)=YURI(54)+(TREG(9)*CON(51))+(TREG(10)*CON(46))+(DNOPL*YURI(
  113))+(TREG(14)*CON(111))+(TREG(11)*CON(142))+TREG(11)*CON(148)
57 IF(KEY(5)-2) 59,58,59
58 FORM(5)=(TREG(14)*(TREG(4)*CON(18)))+(TREG(14)*(TREG(5)*CON(65)))+
  1(TREG(6)*((TREG(14)*CON(67))+YURI(23)))+(TREG(7)*(YURI(12)+(TREG(1
  24)*CON(111))))+TREG(4)*TREG(14)*YURI(88)+TREG(6)*TREG(13)*YURI(91)
  3+TREG(5)*TREG(12)*YURI(89)
   REMV(5)=CON(3)+(TREG(9)*CON(49))+(TREG(10)*CON(50))+(TREG(15)*CON(
  168))+(DNOPL*YURI(48))+(TREG(11)*CON(141))+TREG(11)*CON(147)
59 IF(KEY(6)-2) 61,60,61
60 FORM(6)=PO+(TREG(13)*(TREG(10)*CON(85)))+(TREG(11)*YURI(41))
   REMV(6)=YURI(56)+(TREG(13)*YURI(28))+(TREG(12)*YURI(29))+(TREG(4)*
  1YURI(6))+(TREG(5)*(YURI(15)+(TREG(13)*CON(52))))+(TREG(6)*YURI(19)
  2)+(TREG(7)*CON(51))+(TREG(8)*CON(49))+(TREG(14)*CON(76))+(TREG(17)
  3*CON(134))
61 IF(KEY(7)-2) 63,62,63
62 FORM(7)=PO2+(TREG(9)*(YURI(25)+(TREG(12)*CON(84))))+(TREG(11)*YURI
  1(42))
   REMV(7)=YURI(51)+(TREG(13)*YURI(26))+(TREG(12)*CON(72))+(TREG(14)*
  1CON(115))+(TREG(4)*YURI(7))+(TREG(5)*YURI(16))+(TREG(6)*YURI(20))+
  2(TREG(7)*CON(46))+(TREG(8)*CON(50))
63 IF(KEY(8)-2) 65,64,65
64 FORM(8)=PN2
   REMV(8)=YURI(55)+(TREG(13)*CON(74))+(TREG(12)*CON(75))+(TREG(4)*YU
  1RI(8))+(TREG(5)*YURI(17))+(TREG(6)*YURI(21))+YURI(53)+(TREG(8)*CON
  2(141))+(TREG(7)*CON(142))+TREG(8)*CON(147)+TREG(7)*CON(148)
65 IF(KEY(9)-2) 68,67,68
67 FORM(9)=(TREG(5)*((TREG(13)*CON(10))+(DNOPL*CON(38))))+(
  1TREG(6)*((DNOPL*YURI(22))+(2.0*TREG(11)*CON(119))))+(TREG(7)*(YURI
  2(12)+(DNOPL*CON(47 ))))+(TREG(8)*(DNOPL*YURI(24)))+(TREG(4)*(DNOPL
  3*YURI(9)))+(TREG(10)*(YURI(36)+(TREG(13)*CON(85))))+(TREG(11)*YURI
  4(52))+(TREG(13)*(YURI(59)+(TREG(15)*CON(105))+(2.0*TREG(14)*CON(10
  58))))+(TREG(14)*(YURI(40)+CON(131))+TREG(17)*CON(132))+(TREG(8)*TR
  6EG(11)*CON(141))+YURI(92) + 2.0* TREG(17)*YURI(93)
   REMV(9)=(TREG(5)*CON(12))+(TREG(9)*YURI(29))+(TREG(10)*CON(72))+(T
  1REG(11)*CON(75))+(TREG(12)*YURI(32))+(TREG(13)*YURI(33))+YURI(37)+
  2CON(129)+TREG(5)*YURI(89) + YURI(98)+TREG(13)*YURI(96)+TREG(15)*CO
  3N(166)
68 IF(KEY(10)-2) 70,69,70
69 FORM(10)=(TREG(4)*((2.0*TREG(11)*CON(26))+(DNOPL*YURI(10))))+(TREG
  1(6)*((DNOPL*YURI(34))+(TREG(11)*YURI(61))))+(TREG(8)*(DNOPL*YURI(6
  22)))+(TREG(9)*(YURI(27)+(TREG(12)*CON(84))))+(TREG(11)*YURI(43))+(
  3TREG(7)*(DNOPL*CON(126)))+YURI(92)    + TREG(12)*YURI(95)
  4+(CON(129)*TREG(12))+(CON(132)*TREG(17))
   REMV(10)=(TREG(5)*CON(10))+(TREG(6)*CON(14))+(TREG(11)*CON(74))+(T
```

```
     1REG(9)*YURI(28))+(TREG(13)*(YURI(63)+2.0*TREG(13)*CON(98)))+(TREG(ALG2
     212)*YURI(33))+(TREG(15)*CON(105))+(TREG(14)*YURI(35))+(TREG(10)*YUALG2
     3RI(26))+YURI(77)+TREG(6)*YURI(91)+2.0*TREG(13)*CON(152)+YURI(97)+ ALG2
     4TREG(12)*YURI(96)+TREG(14)*CON(165)                               ALG2
   70 IF(KEY(11)-2) 72,71,72                                           ALG2
   71 FORM(11)=(TREG(8)*(CON(3)+(TREG(9)*CON(49))+(TREG(10)*CON(50))+(DNALG2
     1OPL*CON(48))+(TREG(15)*CON(68))))+(TREG(12)*(YURI(37)+(TREG(5)*CONALG2
     2(12))+(TREG(12)*YURI(32))))+(TREG(13)*(YURI(31)+(TREG(6)*CON(14)))ALG2
     3)+(TREG(6)*(YURI(23)+(DNOPL*CON(116))+(TREG(11)*CON(120))))+(TREG(ALG2
     47:*(DNOPL*CON(127)))+(TREG(5)*TREG(16)*YURI(78))+TREG(11)*TREG(8)*ALG2
     5CON(147)+TREG(13)*YURI(97)+(TREG(12)*(YURI(94)+TREG(15)*CON(166)))ALG2
      REMV(11)=YURI(40)+(TREG(4)*CON(18))+(TREG(5)*CON(65))+(TREG(6)*CONALG2
     1(67))+(TREG(9)*CON(76))+(TREG(10)*CON(115))+(TREG(13)*YURI(35))+COALG2
     2N(131)+(TREG(7)*CON(111))+TREG(4)*YURI(88)+TREG(13)*CON(165)      ALG2
   72 IF(KEY(12)-2) 74,73,74                                           ALG2
   73 FORM(12)=(TREG(7)*(CON(4)+(TREG(10)*CON(46))+(TREG(9)*CON(51))+(DNALG2
     1OPL* CON(47))+(TREG(14)*CON(111))))+(TREG(5)*YURI(38))+(TREG(6)*(YALG2
     2URI(57)+(TREG(9)*YURI(79))+(TREG(16)*CON(117))))+(TREG(10)*((TREG(ALG2
     35)*YURI(80))+(TREG(14)*CON(115))))+(TREG(8)*TREG(16)*CON(125))+YURALG2
     4I(58)+TREG(11)*TREG(7)*CON(148)+DO*YURI(99)                        ALG2
      REMV(12)=(TREG(4)*YURI(5))+(TREG(5)*YURI(14))+(TREG(6)*CON(66))+(TALG2
     1REG(8)*CON(68))+(TREG(13)*CON(105))+YURI(60)+CON(130)             ALG2
     2+TREG(12)*CON(166)                                                ALG2
   74 IF(KEY(13)-2) 76,75,76                                           ALG2
   75 FORM(13)=PNO+(TREG(10)*((TREG(12)*CON(72))+YURI(36)+(TREG(13)*CON(ALG2
     187))+(TREG(14)*CON(115))))+(TREG(9)*((TREG(12)*CON(71))+(TREG(13)*ALG2
     2YURI(28))+YURI(27)))+(TREG(11)*((TREG(12)*CON(75))+YURI(67)))     ALG2
      REMV(13)=(TREG(4)*YURI(47))+(TREG(5)*YURI(18))+(TREG(6)*YURI(50))+ALG2
     1(TREG(8)*YURI(48))+(TREG(7)*YURI(13))+YURI(65)                    ALG2
   76 IF(KEY(14)-2) 78,77,78                                           ALG2
   77 FORM(14)=(TREG(5)*(YURI(66)+(TREG(11)*YURI(81))))+(TREG(12)*TREG(1ALG2
     13)*CON(101))+YURI(69)+(TREG(11)*((TREG(6)*CON(124))+(TREG(8)*CON(1ALG2
     241))+(TREG(7)*CON(142))))+YURI(100)+TREG(13)*(TREG(12)*YURI(96)+T ALG2
     3REG(14)*CON(165))                                                 ALG2
      REMV(14)=YURI(82)+TREG(9)*CON(134)+YURI(102)                      ALG2
   78 IF(KB4 .EQ. 0) GO TO 100                                         ALG2
  101 IF(KEY(15)-2) 100,79,100                                         ALG2
   79 FORM(15)=(TREG(5)*(CON(2)+(TREG(16)*CON(38))+(TREG(11)*CON(39))+( ALG2
     1TREG(10)*CON(40))+(2.0*TREG(9)*CON(41))+(TREG(15)*CON(64))+(TREG( ALG2
     2 14)*CON(65))))+(TREG(6)*((TREG(9)*CON(42))+(TREG(16)*(CON(116)+  ALG2
     3CON(118)))+(2.0*TREG(11)*CON(121))))+(TREG(4)*((TREG(15)*CON(21)) ALG2
     4+(2.0*TREG(10)*CON(28))+(TREG(16)*YURI(10))+(TREG(9)*YURI(6))))+(TALG2
     5REG(8)*(TREG(9)*CON(49)))+(TREG(7)*( TREG(9)*CON(51)))+(TREG(9)*(YUALG2
     6RI(71)+(TREG(12)*CON(71))+(TREG(14)*CON(76))))+(TREG(13)*((TREG(10ALG2
     7)*CON(87))+(TREG(12)*CON(109))+YURI(72)))+(TREG(12)*CON(129))+(TREALG2
     8G(15)*CON(130))+(TREG(14)*(CON(131)+TREG(13)*CON(165)))+(TREG(17)*ALG2
     9(CON(133)+TREG(9)*CON(134)))+TREG(6)*TREG(11)*CON(124)+YURI(73)   ALG2
      REMV(15)=(TREG(5)*CON(8))+(TREG(6)*YURI(74))+(TREG(4)*(CON(16)+YURALG2
     1I(75)))+TREG(9)*YURI(76) +TREG(10)*CON(81)+TREG(11)*YURI(83)+TREG ALG2
     2(16)*CON(82)+TREG(13)*YURI(84)+TREG( 12)*YURI(85)+TREG(15)*CON(104)ALG2
     3+TREG(14)*CON(106)+YURI(86)+YURI(103)+TREG(17)*YURI(101)+TREG(12)*ALG2
     4YURI(104)                                                         ALG2
  100 RETURN                                                           ALG2
      END                                                              ALG2
      SUBROUTINE BALAN                                                 BALAN
      COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175BALA
     1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)        BALA
      COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2BALA
     1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,KBALA
     2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5,NSKIP,EPSI,IFAIL,TOTO,TBALA
```

```
     3OTN,DEL,XMAS,KB4,B5,KB7                                           BALA
      EQUIVALENCE(DO,DO),(DO2,DZ2)                                      BALA
    1 SUM=TREG(4)+TREG(5)+TREG(6)+TREG(7)+TREG(8)                       BALA
      GO TO (215,216,218,219,222),LAM                                   BALA
  215 TREG(9)=SUM-TREG(10)-TREG(11)-TREG(16)                            BALA
      GO TO 222                                                         BALA
  216 TREG(10)=SUM-TREG(9)-TREG(11)-TREG(16)                            BALA
      GO TO 222                                                         BALA
  218 TREG(11)=SUM-TREG(9)-TREG(10)-TREG(16)                            BALA
      GO TO 222                                                         BALA
  219 TREG(16)=SUM-TREG(9)-TREG(10)-TREG(11)                            BALA
  222 IF(KB4 .EQ. 0) GO TO 6                                            BALA
    7 DO=TREG(18)                                                       BALA
    6 DZ2=((TOTO-TREG(5)-3.0*TREG(7)-TREG(9)-TREG(12)-3.0*TREG(15)-TREG(BALA
     116)-TREG(I7)-DO       )/2.0)-TREG(6)-TREG(8)-TREG(10)-TREG(14)    BALA
      DN2=((TOTN-TREG(8)-TREG(12)-TREG(13)-TREG(14)-TREG(16))/2.0)-TREG(BALA
     111)-TREG(17)                                                      BALA
      IF(DO2) 8,9,9                                                     BALA
    8 DZ2=0.0                                                           BALA
    9 IF(DN2) 10,11,11                                                  BALA
   10 DN2=0.0                                                           BALA
   11 CALL COEFF                                                        BALA
    5 RETURN                                                            BALA
      END                                                               BALA
      SUBROUTINE EQUIL                                                  EQIL
C PROGRAM TO DETERMINE THE EQUILIBRIUM STATUS OF SPECIES.               EQIL
      COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175EQIL
     1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)        EQIL
      COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2EQIL
     1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,KEQIL
     2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5, SKIP,EPSI,IFAIL,TOTO,TEQIL
     3OTN,DEL,XMAS,KB4,B5,KB7                                           EQIL
      CALL SLOP                                                         EQIL
      CALL ALGA2                                                        EQIL
      L=KINT                                                            EQIL
      DO 2 I=1,NUMB                                                     EQIL
      CRITN(I)=ABS((TREG(L)-TREG(I+3))/TREG(3))                         EQIL
      CRTNO(I)=REMV(I)*TREG(I+3)                                        EQIL
      L=L+1                                                             EQIL
    2 CONTINUE                                                          EQIL
      CRTNO(9)=CRTNO(9)+PNO                                             EQIL
      IF(KB4 .EQ. 0) GO TO 417                                          EQIL
  416 CRTNO(15)=CRTNO(15)+PO                                            EQIL
  417 DO 27 J=1,NUMB                                                    EQIL
      IF(CRITN(J)-1.0E-3) 85,85,80                                      EQIL
   85 IF(TREG(3)-XMAS) 30,30,82                                         EQIL
   82 IF(CRTNO(J)) 83,30,83                                             EQIL
   83 IF(ABS(1.0-(FORM(J)/CRTNO(J)))-DEL) 31,31,30                      EQIL
   80 IF(CRTNO(J)) 88,27,88                                             EQIL
   88 IF((CRITN(J)/CRTNO(J))-DEL) 31,30,30                              EQIL
   30 LOCK(J)=0                                                         EQIL
      GO TO 27                                                          EQIL
   31 LOCK(J)=LOCK(J)+1                                                 EQIL
   27 CONTINUE                                                          EQIL
      DO 118 J=1,NUMB                                                   EQIL
      IF(KEY(J)-3) 121,118,118                                          EQIL
  121 IF(LOCK(J)-3) 119,120,120                                         EQIL
  119 KEY(J)=1                                                          EQIL
      GO TO 118                                                         EQIL
  120 KEY(J)=2                                                          EQIL
```

```
118 CONTINUE                                                            EQIL
    RETURN                                                              EQIL
    END                                                                 EQIL
    SUBROUTINE DAUXT                                                    DXT
    COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175DXT
   1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)          DXT
    COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2DXT
   1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,KDXT
   2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5,NSKIP,EPSI,IFAIL,TOTO,TDXT
   3OTN,DEL,XMAS,KB4,B5,KB7                                             DXT
    IF(KB5 .EQ. 0) GO TO 29                                             DXT
 28 IF(TIME-TREG(2)) 29,30,30                                           DXT
 29 DNOPL=TREG(16)                                                      DXT
    R(1)=TREG(6)*CON(1)                                                 DXT
    R(2)=TREG(5)*CON(2)                                                 DXT
    R(3)=TREG(8)*CON(3)                                                 DXT
    R(4)=TREG(7)*CON(4)                                                 DXT
    R(5)=TREG(6)*DO2*CON(5)                                             DXT
    R(6)=TREG(6)*DN2*CON(6)                                             DXT
    R(7)=TREG(6)*DO*CON(7)                                              DXT
    R(8)=TREG(5)*DO*CON(8)                                              DXT
    R(9)=TREG(5)*DO2*CON(9)                                             DXT
    R(10)=TREG(5)*TREG(13)*CON(10)                                      DXT
    R(11)=TREG(5)*DN2*CON(11)                                           DXT
    R(12)=TREG(5)*TREG(12)*CON(12)                                      DXT
    R(13)=TREG(5)*TREG(15)*CON(13)                                      DXT
    R(14)=TREG(6)*TREG(13)*CON(14)                                      DXT
    R(15)=TREG(6)*DO*CON(15)                                            DXT
    R(16)=TREG(4)*DO*CON(16)                                            DXT
    R(17)=TREG(4)*DO2*CON(17)                                           DXT
    R(18)=TREG(4)*TREG(14)*CON(18)                                      DXT
    R(19)=TREG(4)*TREG(15)*CON(19)                                      DXT
    R(20)=TREG(4)*TREG(15)*CON(20)                                      DXT
    R(21)=TREG(4)*TREG(15)*CON(21)                                      DXT
    R(22)=TREG(4)*DO*DO2*CON(22)                                        DXT
    R(23)=TREG(4)*DO*DN2*CON(23)                                        DXT
    R(24)=TREG(4)*DO2*DO2*CON(24)                                       DXT
    R(25)=TREG(4)*DO2*DN2*CON(25)                                       DXT
    R(26)=TREG(4)*TREG(11)*CON(26)                                      DXT
    R(27)=TREG(4)*DNOPL*CON(27)                                         DXT
    R(28)=TREG(4)*TREG(10)*CON(28)                                      DXT
    R(29)=TREG(4)*D*TREG(9)*CON(29)                                     DXT
    R(30)=TREG(4)*D*TREG(10)*CON(30)                                    DXT
    R(31)=TREG(4)*D*TREG(11)*CON(31)                                    DXT
    R(32)=TREG(4)*D*DNOPL*CON(32)                                       DXT
    R(33)=TREG(4)*D*DNOPL*CON(33)                                       DXT
    R(34)=TREG(4)*TREG(9)*CON(34)                                       DXT
    R(35)=TREG(4)*TREG(10)*CON(35)                                      DXT
    R(36)=TREG(4)*TREG(11)*CON(36)                                      DXT
    R(37)=TREG(4)*DNOPL*CON(37)                                         DXT
    R(38)=TREG(5)*DNOPL*CON(38)                                         DXT
    R(39)=TREG(5)*TREG(11)*CON(39)                                      DXT
    R(40)=TREG(5)*TREG(10)*CON(40)                                      DXT
    R(41)=TREG(5)*TREG(9)*CON(41)                                       DXT
    R(42)=TREG(6)*TREG(9)*CON(42)                                       DXT
    R(43)=TREG(6)*TREG(10)*CON(43)                                      DXT
    R(44)=TREG(6)*TREG(11)*CON(44)                                      DXT
    R(45)=TREG(6)*DNOPL*CON(45)                                         DXT
    R(46)=TREG(7)*TREG(10)*CON(46)                                      DXT
    R(47)=TREG(7)*DNOPL*CON(47)                                         DXT
```

```
R(48)=TREG(8)*DNOPL*CON(48)
R(49)=TREG(8)*TREG(9)*CON(49)
R(50)=TREG(8)*TREG(10)*CON(50)
R(51)=TREG(7)*TREG(9)*CON(51)
R(52)=TREG(5)*TREG(9)*(TREG(13)*CON(52))
R(53)=TREG(5)*TREG(10)*(D*CON(53))
R(54)=TREG(5)*TREG(11)*(D*CON(54))
R(55)=TREG(5)*DNOPL*(D*CON(55))
R(56)=TREG(5)*TREG(9)*(DO2*CON(56))
R(57)=TREG(5)*TREG(9)*(DN2*CON(57))
R(58)=TREG(5)*TREG(9)*(DO*CON(58))
R(59)=TREG(6)*D*TREG(10)*CON(59)
R(60)=TREG(6)*D*TREG(11)*CON(60)
R(61)=TREG(6)*D*DNOPL*CON(61)
R(62)=TREG(6)*D*TREG(9)*CON(62)
R(63)=TREG(6)*DO*CON(63)
R(64)=TREG(5)*TREG(15)*CON(64)
R(65)=TREG(5)*TREG(14)*CON(65)
R(66)=TREG(6)*TREG(15)*CON(66)
R(67)=TREG(6)*TREG(14)*CON(67)
R(68)=TREG(8)*TREG(15)*CON(68)
R(69)=TREG(11)*DO*CON(69)
R(70)=TREG(9)*DO2*CON(70)
R(71)=TREG(9)*TREG(12)*CON(71)
R(72)=TREG(10)*TREG(12)*CON(72)
R(73)=TREG(11)*DO2*CON(73)
R(74)=TREG(11)*TREG(13)*CON(74)
R(75)=TREG(11)*TREG(12)*CON(75)
R(76)=TREG(9)*TREG(14)*CON(76)
R(77)=TREG(9)*DO*CON(77)
R(78)=TREG(9)*TREG(13)*CON(78)
R(79)=TREG(9)*DN2*CON(79)
R(80)=TREG(9)*TREG(12)*CON(80)
R(81)=TREG(10)*DO*CON(81)
R(82)=DNOPL*DO*CON(82)
R(83)=TREG(9)*DN2*CON(83)
R(85)=TREG(10)*TREG(13)*CON(85)
R(84)=TREG(9)*TREG(12)*CON(84)
R(86)=TREG(10)*DN2*CON(86)
R(87)=TREG(10)*TREG(13)*CON(87)
R(88)=TREG(11)*DO*CON(88)
R(89)=TREG(11)*DO2*CON(89)
R(90)=(TREG(9)*DO)*(D*CON(90))
R(91)=TREG(9)*TREG(13)*(D*CON(91))
R(92)=TREG(9)*DN2*(D*CON(92))
R(93)=(TREG(13)**2)*(D*CON(93))
R(94)=TREG(13)*DO*D*CON(94)
R(95)=TREG(12)*DO*D*CON(95)
R(96)=DO*DO2*D*CON(96)
R(97)=DN2*(TREG(13)**2)*CON(97)
R(98)=(TREG(13)**2)*CON(98)*TREG(13)
R(99)=TREG(13)*DO*CON(99)
R(100)=TREG(12)*DO*CON(100)
R(101)=TREG(12)*TREG(13)*CON(101)
R(102)=TREG(13)*DO2*CON(102)
R(103)=DO*DO2*CON(103)
R(104)=DO*TREG(15)*CON(104)
R(105)=TREG(13)*TREG(15)*CON(105)
R(106)=TREG(14)*DO*CON(106)
R(107)=TREG(14)*TREG(13)*CON(107)
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R(108)=TREG(14)*TREG(13)*CON(108)
R(109)=TREG(12)*TREG(13)*CON(109)
R(110)=CON(110)*TREG(13)*DO2
R(111)=TREG(7)*TREG(14)*CON(111)
R(112)=TREG(5)*DO2*CON(112)
R(113)=(TREG(6)*DO2)*(DN2*CON(113))
R(114)=TREG(7)*DN2*CON(114)
R(115)=TREG(10)*TREG(14)*CON(115)
R(116)=TREG(6)*DNOPL*CON(116)
R(117)=TREG(6)*DNOPL*CON(117)
R(118)=TREG(6)*DNOPL*CON(118)
R(119)=TREG(6)*TREG(11)*CON(119)
R(120)=TREG(6)*TREG(11)*CON(120)
R(121)=TREG(6)*TREG(11)*CON(121)
R(122)=TREG(8)*DNOPL*CON(122)
R(123)=TREG(8)*DNOPL*CON(123)
R(124)=TREG(11)*TREG(6)*CON(124)
R(125)=TREG(8)*DNOPL*CON(125)
R(126)=TREG(7)*DNOPL*CON(126)
R(127)=TREG(7)*DNOPL*CON(127)
R(128)=(TREG(12)**2)*DO2*CON(128)
R(129)=TREG(12)*CON(129)
R(130)=TREG(15)*CON(130)
R(131)=TREG(14)*CON(131)
R(132)=TREG(17)*CON(132)
R(133)=TREG(17)*CON(133)
R(134)=TREG(9)*TREG(17)*CON(134)
R(135)=TREG(11)*DN2*CON(135)
R(136)=DO*(CON(136)*DO2)*DO
R(137)=DO*(CON(137)*DO)*DO
R(138)=DO*(CON(138)*DN2)*DO
R(139)=DO*(CON(139)*DO)
R(140)=DO*(CON(140)*DN2)
R(141)=TREG(11)*TREG(8)*CON(141)
R(142)=TREG(11)*TREG(7)*CON(142)
R(143)=DO2*CON(143)
R(144)=TREG(4)*DO2*DO*CON(144)
R(145)=TREG(4)*TREG(14)*DO2*CON(145)
R(146)=TREG(4)*TREG(14)*DN2*CON(146)
R(147)=TREG(8)*TREG(11)*CON(147)
R(148)=TREG(7)*TREG(11)*CON(148)
R(149)=TREG(5)*TREG(12)*D*CON(149)
R(150)=TREG(6)*TREG(13)*D*CON(150)
R(151)=TREG(5)*DO2*DO2*CON(151)
R(152)=(TREG(13)**2)*CON(152)
R(153)=DO*DO2*DO2*CON(153)
R(154)=DO*DO2*DN2*CON(154)
R(155)=DO2*DO*DO*CON(155)
R(156)=DO*DN2*D*CON(156)
R(157)=DO2*DO*TREG(12)*CON(157)
R(158)=TREG(12)*DO*DN2*CON(158)
R(159)=TREG(13)*DO2*D*CON(159)
R(160)=TREG(12)*TREG(13)*D*CON(160)
R(161)=DO*DN2*CON(161)
R(162)=TREG(12)*DO*CON(162)
R(163)=TREG(17)*DO*CON(163)
R(164)=TREG(17)*DO*CON(164)
R(165)=TREG(13)*TREG(14)*CON(165)
R(166)=TREG(12)*TREG(15)*CON(166)
WRITE (3,1)
```

```
      WRITE (3,2)TREG(2)
      WRITE (3,3)
      WRITE (3,4)
      WRITE (3,5)(CON(J),R(J),J=1,4)
      WRITE (3,6)
      WRITE (3,4)
      WRITE (3,7)(CON(J),R(J),J=5,7)
      WRITE (3,8)
      WRITE (3,4)
      WRITE (3,9)(CON(J),R(J),J=8,15)
      WRITE (3,10)
      WRITE (3,4)
      WRITE (3,11)(CON(J),R(J),J=16,19)
      WRITE (3,12)
      WRITE (3,4)
      WRITE (3,13)(CON(J),R(J),J=20,21)
      WRITE (3,14)
      WRITE (3,4)
      WRITE(3,15)(CON(J),R(J),J=22,25),(CON(J),R(J),J=144,146)
      WRITE (3,16)
      WRITE (3,4)
      WRITE (3,17)(CON(J),R(J),J=26,28)
      WRITE (3,18)
      WRITE (3,4)
      WRITE (3,19)(CON(J),R(J),J=29,33)
      WRITE (3,20)
      WRITE (3,4)
      WRITE (3,21)(CON(J),R(J),J=34,37)
      WRITE (3,22)
      WRITE (3,4)
      WRITE (3,23)(CON(J),R(J),J=38,51)
      WRITE(3,231)(CON(J),R(J),J=147,148)
      WRITE (3,24)
      WRITE (3,4)
      WRITE (3,25)(CON(J),R(J),J=52,62)
      WRITE (3,26)
      WRITE (3,4)
      WRITE (3,27)(CON(J),R(J),J=63,76)
      WRITE (3,31)CON(111),R(111),CON(134),R(134)
      CALL DAUXT2
      TIME=TIME*10.0
   30 RETURN
    1 FORMAT(1H1,47X28H KINETICS OF THE REACTIONS. )
    2 FORMAT(1H0,47X7H TIME =1PE12.5,6H SEC. )
    3 FORMAT(19H0PHOTO DETACHMENT. )
    4 FORMAT(1H0,18X9HREACTIONS,13X8HCONSTANT,5X4HRATE,22X9HREACTIONS,13
     1X8HCONSTANT,5X4HRATE )
    5 FORMAT(6X9HO2-  + HV,7X10H= O2    + E,7X1P2E10.2,8X9HO-    + HV,7X10
     1H= O     + E,7X1P2E10.2/6X9HNO2- + HV,7X10H= NO2  + E,7X1P2E10.2,8X
     29HO3-  + HV,7X10H= O3    + E,7X1P2E10.2 )
    6 FORMAT(25H0COLLISIONAL DETACHMENT. )
    7 FORMAT(6X9HO2-   + O2,7X17H= O2    + O2  + E ,1P2E10.2,8X9HO2-   + N2
     1,7X17H= O2    + N2  + E ,1P2E10.2/6X8HO2-   + O,8X17H= O2    + O    +
     2E ,1P2E10.2 )
    8 FORMAT(25H0ASSOCIATIVE DETACHMENT. )
    9 FORMAT(6X8HO-    + O,8X10H= O2    + E,7X1P2E10.2,8X9HO-    + O2,7X10H
     1= O3    + E,7X1P2E10.2/6X8HO-    + N,8X10H= NO    + E,7X1P2E10.2,8X9H
     2O-    + N2,7X10H= N2O  + E,7X1P2E10.2/6X9HO-    + NO,7X10H= NO2  + E
     3,7X1P2E10.2,8X9HO-    + O3,7X17H= O2    + O2  + E ,1P2E10.2/6X8HO2-
     4 + N,8X10H= NO2  + E,7X1P2E10.2,8X8HO2-   + O,8X10H= O3    + E,7X1P2
```

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     5E10.2 )
  10 FORMAT(23HORADIATIVE ATTACHMENT. )
  11 FORMAT(6X8HO      + E,8X11H= O-    + HV,6X1P2E10.2,8X8HO2    + E,8X11H
     1= O2-   + HV,6X1P2E10.2/6X8HNO2   + E,8X11H= NO2- + HV,6X1P2E10.2,8X
     28HO3    + E,8X11H= O3-   + HV,6X1P2E10.2 )
  12 FORMAT(26HODISSOCIATIVE ATTACHMENT. )
  13 FORMAT(6X8HO3    + E,8X11H= O-    + O2,6X1P2E10.2,8X8HO3    + E,8X10H
     1= O2-   + O,7X1P2E10.2 )
  14 FORMAT(24HOTHREE BODY ATTACHMENT. )
  15 FORMAT(6X27HO     + O2   + E   = O-    + O2,6X1P2E10.2,8X27HO     + N2 
     1 + E   = O-    + N2,6X1P2E10.2/6X27HO2    + O2   + E   = O2-   + O2,6X1P
     22E10.2,8X27HO2    + N2   + E   = O2-   + N2,6X1P2E10.2/
     36X27HO2    + O    + E   = O2-   + O  ,6X1P2E10.2,8X27HNO2   + O2   + E   =
     4 NO2- + O2,6X1P2E10.2/6X27HNO2   + N2   + E   = NO2- + N2,6X1P2E10.2)
  16 FORMAT(29HODISSOCIATIVE RECOMBINATION. )
  17 FORMAT(6X8HN2+   + E,8X10H= N     + N,7X1P2E10.2,8X8HNO+   + E,8X10H=
     1 N     + O,7X1P2E10.2/6X8HO2+   + E,8X10H= O     + O,7X1P2E10.2 )
  18 FORMAT(27HOTHREE BODY RECOMBINATION. )
  19 FORMAT(6X26HO+    + E    + M   = O     + M,7X1P2E10.2,8X26HO2+   + E   
     1+ M   = O2    + M,7X1P2E10.2/6X26HN2+   + E    + M   = N2    + M,7X1P2E1
     20.2,8X26HNO+   + E    + M   = NO    + M,7X1P2E10.2/6X33HNO+   + E    + M
     3  = N     + O    + M ,1P2E10.2 )
  20 FORMAT(26HIRADIATIVE RECOMBINATION. )
  21 FORMAT(6X8HO+    + E,8X11H= O     + HV,6X1P2E10.2,8X8HO2+   + E,8X11H
     1= O2    + HV,6X1P2E10.2/6X8HN2+   + E,8X11H= N2    + HV,6X1P2E10.2,8X
     28HNO+   + E,8X11H= NO    + HV,6X1P2E10.2 )
  22 FORMAT(24HOMUTUAL NEUTRALIZATION. )
  23 FORMAT(6X10HO-    + NO+,6X11H= O     + NO,6X1P2E10.2,8X10HO-    + N2+
     1,6X11H= O     + N2,6X1P2E10.2/6X10HO-    + O2+,6X11H= O     + O2,6X1P
     22E10.2,8X9HO-    + O+,7X10H= O     + O,7X1P2E10.2/6X9HO2-   + O+,7X11
     3H= O     + O2,6X1P2E10.2,8X10HO2-   + O2+,6X11H= O2    + O2,6X1P2E10.
     42/6X10HO2-   + N2+,6X11H= O2    + N2,6X1P2E10.2,8X10HO2-   + NO+,6X11
     5H= O2    + NO,6X1P2E10.2/6X10HO3-   + O2+,6X11H= O2    + O3,6X1P2E10.
     62,8X10HO3-   + NO+,6X11H= O3    + NO,6X1P2E10.2/6X10HNO2- + NO+,6X11
     7H= NO2   + NO,6X1P2E10.2,8X9HNO2- + O+,7X10H= NO2   + O,7X1P2E10.2/6
     8X10HNO2- + O2+,6X11H= NO2   + O2,6X1P2E10.2,8X9HO3-   + O+,7X10H= O3
     9    + O,7X1P2E10.2 )
  24 FORMAT(35HOTHREE BODY ION ION RECOMBINATION. )
  25 FORMAT(6X33HO-    + O+   + N   = O2    + N        ,1P2E10.2,8X33HO-    +
     1 O2+ + M   = O3    + M        ,1P2E10.2/6X33HO-    + N2+ + M   = N2O   +
     2 M        ,1P2E10.2,8X33HO-    + NO+ + M   = NO2   + M        ,1P2E10.2
     3/6X33HO-    + O+   + O2 = O2    + O2        ,1P2E10.2,8X33HO-    + O+   +
     4 N2 = O2    + N2        ,1P2E10.2/6X33HO-    + O+   + O   = O2    + O   
     5    ,1P2E10.2,8X33HO2-   + O2+ + M   = O2    + O2    + M ,1P2E10.2/6X33H
     6O2-   + N2+ + M   = O2    + N2    + M ,1P2E10.2,8X33HO2-   + NO+ + M   = 
     7O2    + NO    + M ,1P2E10.2/6X33HO2-   + O+   + M   = O3    + M        ,1P
     82E10.2 )
  26 FORMAT(18HOCHARGE TRANSFER. )
  27 FORMAT(6X8HO2-   + O,8X11H= O-    + O2,6X1P2E10.2,8X9HO-    + O3,7X10
     1H= O3-   + O,7X1P2E10.2/6X10HO-    + NO2,6X10H= NO2- + O,7X1P2E10.2,
     28X9HO2-   + O3,7X11H= O3-   + O2,6X1P2E10.2/6X10HO2-   + NO2,6X11H= N
     3O2- + O2,6X1P2E10.2,8X9HNO2- + O3,7X12H= O3-   + NO2,5X1P2E10.2/6X8
     4HN2+   + O,8X11H= O+    + N2,6X1P2E10.2,8X9HO+    + O2,7X10H= O2+   + 
     5O,7X1P2E10.2/6X9HO+    + NO,7X10H= NO+   + O,7X1P2E10.2,8X9HO2+   + N
     6O,7X11H= NO+   + O2,6X1P2E10.2/6X9HN2+   + O2,7X11H= O2+   + N2,6X1P2
     7E10.2,8X8HN2+   + N,8X11H= N+    + N2,6X1P2E10.2/6X9HN2+   + NO,7X11H
     8= NO+   + N2,6X1P2E10.2,8X10HO+    + NO2,6X10H= NO2+ + O,7X1P2E10.2)
  31 FORMAT(6X10HO3-   + NO2,6X11H= NO2- + O3,6X1P2E10.2,8X10HO+    + N2O
     1,6X10H= N2O+ + O,7X1P2E10.2 )
 231 FORMAT(6X27HNO2- + N2+       = NO2   + N2,6X1P2E10.2,8X27HO3-   + N2+
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1       = N2   + 03,6X1P2E10.2 )
 END
 SUBROUTINE DAUXT2
 COMMONTREG(150),YURI(125),KEY(15),FORM(15),REMV(15),R(175),CON(175
1),COB(175),LKEY(15),BEGIN(15),LOCK(15),CRITN(15),CRTNO(15)
 COMMON NUMB,EUBAR,ELBAR,LINT,D,DO2,DO,DN2,T,DNO,PNE,PNO,PO2,PO,PN2
1,TOTAL,JACK,JAKE,JAM,PTNO,PTO2,PTN2,PTO,ITER,I2NT,K2NT,J2NT,N2NT,K
2INT,MINT,NINT,I3NT,FIRST,PROD,LAM,TIME,KB5,NSKIP,EPSI,IFAIL,TOTO,T
3OTN,DEL,XMAS,KB4,B5,KB7
 WRITE (3,2)
 WRITE (3,1)
 WRITE (3,3)(CON(J),R(J),J=77,82),CON(135),R(135),CON(112),R(112)
 WRITE (3,4)
 WRITE (3,1)
 WRITE (3,5) (CON(J),R(J),J=83,89),CON(115),R(115)
 WRITE (3,6)
 WRITE (3,1)
 WRITE (3,7)(CON(J),R(J),J=90,92),(CON(J),R(J), J=149,151)
 WRITE (3,8)
 WRITE (3,1)
 WRITE (3,9)(CON(J),R(J),J=93,98),CON(128),R(128),(CON(J),R(J),J=13
16,138)
 WRITE (3,91) (CON(J),R(J),J=153,160)
 WRITE (3,10)
 WRITE (3,1)
 WRITE(3,11)(CON(J),R(J),J=99,103),(CON(J),R(J),J=139,140),CON(152)
1,R(152)
 WRITE (3,12)
 WRITE (3,1)
 WRITE (3,13)(CON(J),R(J),J=104,110),(CON(J),R(J),J=161,166)
 WRITE (3,14)
 WRITE (3,1)
 WRITE (3,15)(CON(J),R(J),J=112,115)
 WRITE (3,16)
 WRITE (3,1)
 WRITE (3,17)(CON(J),R(J),J=116,127),(CON(J),R(J),J=141,142)
 WRITE (3,20)
 WRITE (3,1)
 WRITE (3,21)(CON(J),R(J),J=129,133),CON(143),R(143)
 WRITE (3,18)TOTAL
 WRITE (3,1)
 WRITE (3,19)PTNO,PNO,PTO2,PO2,PTO,PO,PTN2,PN2
 WRITE (3,22)(J,R(J),J=1,165)
 J=166
 WRITE(3,23)  J,R(J)
 RETURN
1 FORMAT(1HO,18X9HREACTIONS,13X8HCONSTANT,5X4HRATE,22X9HREACTIONS,13
 1X8HCONSTANT,5X4HRATE )
2 FORMAT(35HOION NEUTRAL ASSOCIATION TWO-BODY. )
3 FORMAT(6X8HO+    + 0,8X11H= 02+  + HV,6X1P2E10.2,8X8HO+    + N,8X11H
 1= NO+  + HV,6X1P2E10.2/6X9HO+    + N2,7X11H= N2O+ + HV,6X1P2E10.2,8
 2X9HO+    + NO,7X11H= NO2+ + HV,6X1P2E10.2/6X8HO2+  + 0,8X11H= 03+
 3+ HV,6X1P2E10.2,8X8HNO+  + 0,8X11H= NO2+ + HV,6X1P2E10.2/6X9HN2+
 4+ N2,7X11H= N4+  + HV,6X1P2E10.2,8X27HO-   + 02        = 03-  + HV,
 5 X1P2E10.2 )
4 FORMAT(40HOCHARGED REARRANGEMENT - POSITIVE IONS. )
5 FORMAT(6X9HO+    + N2,7X10H= NO+  + N,7X1P2E10.2,8X9HO+    + NO,7X10
 1H= 02+  + N,7X1P2E10.2/6X8HO2+  + N,8X11H= O+   + NO,6X1P2E10.2,8X
 29HO2+  + N2,7X11H= NO+  + NO,6X1P2E10.2/6X8HO2+  + N,8X10H= NO+  +
 3 0,7X1P2E10.2,8X8HN2+  + 0,8X10H= NO+  + N,7X1P2E10.2/6X9HN2+  + 0
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 42,7X11H= NO+   + NO,6X1P2E10.2,8X27HO2+   + NO2        = NO+   + O3,6X1DXT2
 5P2E10.2)                                                              DXT2
6 FORMAT(39H1ION NEUTRAL ASSOCIATION - THREE BODY. )                   DXT2
7 FORMAT(6X26HO+    + O    + M   = O2+   + M,7X1P2E10.2,8X26HO+    + N  DXT2
 1+ M   = NO+   + M,7X1P2E10.2/6X26HO+    + N2   + M   = N2O+ + M,7X1P2E1DXT2
 20.2,8X27HO-    + NO   + M   = NO2- + M ,6X1P2E10.2/6X27HO2-   + N    + DXT2
 3M   = NO2- + M ,6X1P2E10.2,8X27HO-    + O2   + O2 = O3-   + O2,6X1P2E1DXT2
 40.2 )                                                                 DXT2
8 FORMAT(32HOTHREE BODY ATOM RECOMBINATION. )                          DXT2
9 FORMAT(6X26HN     + N    + M   = N2    + M,7X1P2E10.2,8X26HN     + O  DXT2
 1+ M   = NO    + M,7X1P2E10.2/6X26HO     + NO   + M   = NO2   + M,7X1P2E1DXT2
 20.2,8X26HO     + O2   + M   = O3    + M, 7X1P2E10.2/6X27HN     + N    + NDXT2
 32 = N2    + N2,6X1P2E10.2,8X26HN     + N    + N   = N2    + N,7X1P2E10.DXT2
 42/6X28HNO    + O2   + NO = NO2   + NO2,5X1P2E10.2,8X27HO     + O    + ODXT2
 52 = O2    + O2,6X1P2E10.2/6X26HO     + O    + O   = O2    + O,7X1P2E10.DXT2
 62,8X27HO     + O    + N2 = O2    + N2,6X1P2E10.2 )                    DXT2
91 FORMAT(6X27HO    + O2   + O2 = O3    + O2,6X1P2E10.2,8X27HO     + O2 DXT2
 1 + N2 = O3    + N2,6X1P2E10.2/6X27HO     + O2   + O   = O3    + O ,6X1PDXT2
 22E10.2,8X27HO     + N2   + M   = N2O   + M ,6X1P2E10.2/6X27HO     + NO DXT2
 3 + O2 = NO2   + O2,6X1P2E10.2,8X27HO     + NO   + N2 = NO2   + N2,6X1PDXT2
 42E10.2/6X27HN     + O2   + M   = NO2   + M ,6X1P2E10.2,8X27HN     + NO DXT2
 5 + M   = N2O   + M ,6X1P2E10.2)                                       DXT2
10 FORMAT(30HOTWO-BODY ATOM RECOMBINATION. )                           DXT2
11 FORMAT(6X8HN     + O,8X11H= NO    + HV,6X1P2E10.2,8X8HNO    + O,8X11HDXT2
 1= NO2   + HV,6X1P2E10.2/6X8HNO    + N,8X11H= N2O   + HV,6X1P2E10.2,8XDXT2
 29HN     + O2,7X11H= NO2   + HV,6X1P2E10.2/6X9HO     + O2,7X11H= O3    DXT2
 3+ HV,6X1P2E10.2,8X8HO     + O,8X11H= O2    + HV,6X1P2E10.2/6X9HO      DXT2
 4+ N2,7X11H= N2O   + HV,6X1P2E10.2,8X27HN     + N          = N2    + HV,DXT2
 56X1P2E10.2)                                                           DXT2
12 FORMAT(23HONEUTRAL REARRANGEMENT.)                                  DXT2
13 FORMAT(6X9HO     + O3,7X11H= O2    + O2,6X1P2E10.2,8X9HN     + O3,7X1DXT2
 11H= NO    + O2,6X1P2E10.2/6X8HNO2   + O,8X11H= NO    + O2,6X1P2E10.2,DXT2
 28X8HNO2   + N,8X11H= N2    + O2,6X1P2E10.2/6X8HNO2   + N,8X11H= NO    DXT2
 3+ NO,6X1P2E10.2,8X8HNO    + N,8X10H= N2    + O,7X1P2E10.2/6X9HN      +DXT2
 4 O2,7X10H= NO    + O,7X1P2E10.2,8X27HO     + N2         = NO    + N ,6XDXT2
 51P2E10.2/6X9HO     + NO,7X11H= O2    + N ,6X1P2E10.2,8X10HO     + N2ODXT2
 6,6X11H= NO    + NO,6X1P2E10.2/6X27HO     + N2O        = O2    + N2,6X1PDXT2
 72E10.2,8X27HN     + NO2        = N2O   + 3 ,6X1P2E10.2/6X27HNO    + O3 DXT2
 8          = NO2   + O2,6X1P2E10.2)                                    DXT2
14 FORMAT(25HOION ATOM REARRANGEMENT. )                                DXT2
15 FORMAT(6X9HO-    + O2,7X11H= O3-   + HV, 6X1P2E10.2,8X28HO2-   + O2  DXT2
 1+ N2 = NO2- + NO2,5X1P2E10.2/6X9HO3-   + N2,7X11H= NO2- + NO,6X1P2EDXT2
 210.2,8X10HO2+   + NO2,6X11H= NO+   + O3,6X1P2E10.2 )                  DXT2
16 FORMAT(25HOION ION NEUTRALIZATION. )                                DXT2
17 FORMAT(6X10HO2-   + NO+,6X10H= NO2   + O,7X1P2E10.2,8X10HO2-   + NO+,DXT2
 16X10H= O3    + N,7X1P2E10.2/6X10HO2-   + NO+,6X17H= O2    + N    + O ,DXT2
 21P2E10.2,8X10HO2-   + N2+,6X11H= NO    + NO,6X1P2E10.2/6X10HO2-   + NDXT2
 32+,6X10H= NO2   + N,7X1P2E10.2,8X10HO2-   + N2+,6X11H= 2N    + 2O,6X1DXT2
 4P2E10.2/6X10HNO2- + NO+,6X10H= NO3   + N,7X1P2E10.2,8X10HNO2- + NO+DXT2
 5,6X17H= NO    + O2   + N ,1P2E10.2/6X10HO2-   + N2+,6X11H= N2O   + O ,DXT2
 66X1P2E10.2,8X10HNO2- + NO+,6X11H= O3    + N2,6X1P2E10.2/6X10HNO+   +DXT2
 7 O3-,6X17H= O2    + O2   + N ,1P2E10.2,8X10HNO+   + O3-,6X11H= NO2   +DXT2
 8 O2,6X1P2E10.2/6X10HNO2- + N2+,6X11H= N2O   + NO,6X1P2E10.2,8X10HO3DXT2
 9-   + N2+,6X11H= N2O   + O2,6X1P2E10.2 )                              DXT2
18 FORMAT(18HOSOURCE FUNCTION =1P1E12.5,20H   ION PAIRS/CC/SEC. )      DXT2
19 FORMAT(6X9HNO    + HV,7X10H= NO+   + E,7X1P2E10.2,8X9HO2     + HV,7X10DXT2
 1H= O2+   + E,7X1P2E10.2/6X9HO     + HV,7X10H= O+    + E,7X1P2E10.2,8XDXT2
 29HN2    + HV,7X10H= N2+   + E,7X1P2E10.2////)                         DXT2
20 FORMAT(21H1PHOTO-DISSOCIATION. )                                    DXT2
21 FORMAT(6X9HNO    + HV,7X10H= N     + O,7X1P2E10.2,8X9HO3     + HV,7X10DXT2
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     1H= O2    + O,7X1P2E10.2/6X9HNO2   + HV,7X10H= NO     + O,7X1P2E10.2,8X
     29HN2O   + HV,7X11H= N      + NO,6X1P2E10.2/6X9HN2O   + HV,7X10H= N2
     3+ O,7X1P2E10.2,8X9HO2    + HV,7X10H= O     + O,7X1P2E10.2 )
  22 FORMAT(5(2X2HR(,I3,2H)=1PE14.7))
  23 FORMAT(2X2HR(,I3,2H)=1PE14.7)
  24 FORMAT(1H1)
     END
E
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13. ABSTRACT

One of the Keneshea computer codes has been adapted for use on the Ballistic Research Laboratories Electronic Scientific Computer at Aberdeen Proving Ground. Using this modified code, reaction rate equations have been solved for the following 15 species: e, NO_2^-, O^-, O_2^-, O_3^-, N_2^+, NO^+, O^+, O_2^+, N, NO, N_2O, NO_2, O, and O_3. The calculations were made for a 4:1 mixture of N_2 and O_2 at 1 torr total pressure and 300°K. Rate constants as given by Keneshea and Fowler (Research Report AFCRL-66-741, October 1966) were used. Initial electron production rates of 1.61×10^6, 1.61×10^7, 1.61×10^8, and 1.61×10^9 cm^{-3} sec^{-1} were used, where a rate of 1.61×10^9 cm^{-3} sec^{-1} corresponds to an irradiating electron beam current density of 100 microampere per square meter impinging on the cavity of the G. C. Dewey experimental system (Technical Report ECOM-01354-F, September 1966). The solutions are presented as number densities versus time after the start of the irradiating electron beam. A description of the modified code is presented.

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14. KEY WORDS	LINK A		LINK B		LINK C	
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