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by

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CHEMISTRY COMPUTATIONS FOR IRRADIATED HOT AIR

by

C. Dexter Sutherland and John Zinn

ABSTRACT

This report describes a computational model of chemical kinetics in air at temperatures between 300 and 4000 K, with and without imposed fluxes of ionizing radiation and uv radiation, at pressures up to 10 atmospheres. Included are 1360 chemical reactions, involving 71 H, C, N, and O-containing chemical species. The reaction set is complete in the sense of including a reverse reaction for every reaction and including the dominant destruction reactions for each species produced. Photochemical reaction rates are computed in terms of a prescribed intensity and spectral distribution of radiant flux. Reactions of the metastable species $O(^1D)$, $N(^2D)$, $O_2(^1\Delta_g)$, and $O_2(^1\Sigma_g^+)$ are included explicitly, but all other quantum state populations are assumed to be in thermodynamic equilibrium.

Results of several sets of model computations are described. These include: (1) computations of rates of equilibration of systems subjected to abrupt temperature changes at a pressure of 1 atmosphere; (2) computations of relaxation of systems subjected to impulsive sources of ionizing radiation at $P = 1$ atmosphere and 0.01 atm, with and without superimposed sources of optical-uv radiation; and (3) computations of the approach to steady state in systems subjected to steady sources of ionizing radiation, for pressures between 10^{-3} atm and 10 atm.

For computing concentrations of electrons, ions, NO, NO_2 , O, N, and O_3 , we have constructed an abbreviated lumped-parameter reaction set with 31 reactions, designed to be incorporated in a fluid-dynamics code. Rate coefficients have been calibrated against results from the 1360-reaction code for temperatures between 300 and 4000 K and pressures between 10^{-3} and 10 atm.

I. INTRODUCTION

This report describes a set of computations of chemical kinetics in hot and/or irradiated air. The temperature range is 300 to 4000 K, and we include effects of ionizing radiation and optical-ultraviolet radiation.

The chemical reaction set and computer code are continually being changed, and this report describes the status in July

1975. Relative to a year ago we have made a number of improvements, which include:

- A. Expansion of the chemical species list to include most mono- and di-hydrated ions, together with some N_2 , O_2 , NO, and CO_2 -complexed ions.
- B. Inclusion of the metastable species $O(^1D)$, $N(^2D)$, $O_2(^1\Delta_g)$, and $O_2(^1\Sigma_g^+)$.
- C. Systematic elimination of dead-end reaction paths, and completion of reaction subsets.

- D. Inclusion of a reverse reaction for every reaction.
- E. Elaboration of the treatment of photochemical reactions to reflect the explicit dependence of each reaction rate on intensity and spectral composition of the photon flux.

Each of the above items, A through E, are described more fully in Section II. A complete listing of the chemical reactions is included in Section II-G.

Our facility to make changes in the chemistry is enhanced by an "equation-writer" code, which generates FORTRAN source code for extensive subroutines required for the solution of the differential equations. Further details are given in Section III.

Specific computations and results are described in Section IV. The problem parameters are ones that would be applicable to nuclear fireball phenomena in the troposphere and stratosphere. However, they are intentionally general, and do not refer to specific weapon outputs or nuclear test data. Data comparisons will be considered in a later report.

Lumped-parameter rate equations and fitted rate coefficients for computation of electron and ion concentrations are described in Section V.

II. CHEMICAL REACTIONS AND RATES

A. Chemical Species

The chemical system in these computations is assumed to include the neutral, positive, and negative ionic species listed in Table I. All are composed of the elements H, C, N, and O, and they are a subset of the longer list of species considered in our recently published equilibrium report.¹

B. Metastable States

It is obviously impractical to consider all quantum levels of each chemical species individually. In general we have made the assumption that the quantum state populations for each species are in thermodynamic equilibrium, and specified simply by a temperature T . We have, however, made four

TABLE I

LIST OF CHEMICAL SPECIES INCLUDED IN THE COMPUTATIONS

Atoms:

H, N, O, $O(^1D)$, $N(^2D)$

Molecules and Radicals:

H_2 , N_2 , O_2 , OH, NO, CO, $O_2(^1\Delta_g)$, $O_2(^1\Sigma_g^+)$,

O_3 , H_2O , HO_2 , CO_2 , NO_2 , N_2O ,

H_2O_2 , NO_3 , HNO_2 , HNO_3 , $(H_2O)_2$

Positive Ions:^a

H^+ , N^+ , O^+ ,

N_2^+ , O_2^+ , OH^+ , NO^+ , CO^+ ,

N_3^+ , H_2O^+ , NO_2^+ , N_2O^+ , CO_2^+ ,

N_4^+ , O_4^+ , H_3O^+ , WO_2^+ , WNO^+ ,

OHH_3O^+ , WH_3O^+ , W_2NO^+ , $W_2H_3O^+$,

W_3NO^+ , $W_3H_3O^+$

Negative Species:

e^- , O^- ,

O_2^- , NO^- , OH^- ,

O_3^- , NO_2^- ,

O_4^- , NO_3^- , $OONO^-$, CO_3^- , WO^- ,

CO_4^- , WO_2^- , WNO^- , WOH^- , WO_3^- , WNO_2^- ,

WCO_3^- , WNO_3^- , WO_4^- , $W_2O_2^-$, WCO_4^-

^aNote: Throughout this report, "W" will mean H_2O . Also, "M" will mean the total neutral number density.

exceptions: namely, the two metastable atomic states $O(^1D)$ and $N(^2D)$, and the molecular O_2 states $^1\Delta_g$ and $^1\Sigma_g^+$. Exceptional circumstances with respect to these species are (1) the computations involve strong sources of ionizing radiation which lead to rapid production of the metastable atoms $O(^1D)$ and $N(^2D)$ and metastable O_2 molecules; the metastable O_2 is also produced in reactions of $O(^1D)$ with O_2 and in the photolysis of ozone, (2) the rates of many reactions involving these states have been measured, and (3) the concentrations of

these metastable species can be orders of magnitude larger than equilibrium concentrations, while usually, at the same time, very small compared to total O, N, or O₂ concentrations.

Because the concentrations of O(¹D), N(²D), O₂(¹Δ_g), and O₂(¹Σ_g⁺) are small compared to the total concentrations of O, N, or O₂, respectively, reactions involving the metastable species as *reactants* can simply be added to the set *in addition to* the corresponding normal O, N, or O₂ reactions. On the other hand, when the metastable species appear as *products*, the state-specific reaction will usually *replace*, rather than supplement, the normal reaction. (For example, the reaction O₂⁺ + e → O + O(¹D) replaces O₂⁺ + e → O + O, whereas O(¹D) + O₃ → O₂ + O₂ is included *in addition to* the nonspecific reaction O + O₃ → O₂ + O₂).

C. Elimination of Dead-End Paths and Completion of Reaction Subsets

Our basic starting set of chemical reactions can be identified as approximately the set listed in Chapter 24 of the DNA Reaction Rate Handbook.² Most of the subsets of reactions in that list are, however, incomplete--that is, only a few reactions of each type are included. For example, only a few of the many possible exothermic ion charge transfer reactions are given. Some entire classes of (endothermic) reactions are neglected (for example, the set of collisional ionization reactions).

The reaction set, unmodified, leads to a number of dead-end paths. For instance, a few positive ion hydration reactions are given, whereas dissociative recombination reactions for the hydrated ions are not given. In such cases recombination rates may be suppressed artificially by inclusion of the hydration reactions.

Obviously, rates for all of the reactions of every type have not been measured. Omitting a reaction from the set is, however, tantamount to assuming that its rate is zero, which is usually *incorrect*. In

many cases we can guess values of rate constants that are more realistic than the alternative zeros. Reaction subsets that we have expanded with such guesses include:

1. Three-Body Ion-Electron Recombination (A⁺ + e + M → A + M): General expressions used for estimating rate coefficients in this category are from the DNA Reaction Rate Handbook.² When the neutral product, A, is not a stable molecule, it is assumed to break up into two or more stable fragments (see item 11 below).

2. Collisional Ionization (A + M → A⁺ + e + M): These are the reverse counterparts of the 3-body recombination reactions (II-C-1 above), and are treated accordingly, as described in Section II-D below.

3. Dissociative Recombination (AB⁺ + e → A + B): Unknown rate coefficients in this category are set equal to 2. × 10⁻⁷ cm³/s for simple positive ions and 1. × 10⁻⁶ cm³/s for complex ions. Breakup of the neutralized ion is assumed to proceed as far as is necessary to produce stable fragments.

4. Associative Ionization (A + B → AB⁺ + e): Reverse of category 3 above. All rate coefficients computed accordingly, as described in Section II-D.

5. Mutual Neutralization (A⁺ + B⁻ → A + B and A⁺ + B⁻ + M → A + B + M): General expressions used for estimating rate coefficients in this category are from the DNA Reaction Rate Handbook.² If either of the neutral products A or B is unstable, it is assumed to break up into stable fragments.

6. Three-Body Attachment (A + e + M → A⁻ + M): In this category we have estimated four rate coefficients, namely for A = O, O₃, NO₃, and OH. For A = O the rate coefficient was obtained from that of the reverse (detachment) reaction, together with the equilibrium constant (Section II-D). For the other three cases the rate coefficients were guessed to be 1. × 10⁻³⁰ cm⁶/s.

7. Collisional Detachment (A⁻ + M → A + e + M): Several reactions in this category are reverse counterparts of 3-body attachment reactions with known rates, and

they are treated accordingly in the next section (II-D). The rate coefficients obtained in this way have activation energies equal to the calculated heats of reaction, and pre-exponential factors within a factor of 3 of $6 \times 10^{-11} (T/300)^{+1.4}$. Therefore, for other collisional detachment reactions, if other information is not available, we assume rate coefficients of $6 \times 10^{-11} (T/300)^{+1.4} \exp(-\Delta H/RT) \text{ cm}^3/\text{s}$. When the simple product molecule A is unstable, it is assumed to break up into stable products, and ΔH , the heat of reaction, is calculated accordingly.

8. Ion Charge Transfer ($A^+ + B \rightarrow A + B^+$ and $A^- + B \rightarrow A + B^-$): Unknown rate coefficients are estimated to be $3. \times 10^{-10} \text{ cm}^3/\text{s}$ for exothermic charge transfer reactions. Rate coefficients for endothermic charge transfers are computed with equilibrium constants (Section II-D), since each is the reverse of a corresponding exothermic charge transfer.

9. Three-Body Ion Hydration ($A^+ + H_2O + M \rightarrow WA^+ + M$ and $A^- + H_2O + M \rightarrow WA^- + M$): The third-order rate constant for hydration of H^+ was assumed to be $1 \times 10^{-27} \text{ cm}^6/\text{s}$. (However, see Par. II-F-3 below.) Rate constants of hydration of O_4^+ , NO^+ , NO_3^+ , OH^+ , CO_2^+ , and CO_4^+ were all assumed to be $1. \times 10^{-28} \text{ cm}^6/\text{s}$.

10. Special Reactions of Hydrated Ions: An alleged important mechanism for production of NO_2 in the presence of strong ionization sources involves the associative detachment reaction

It is also found, however, that O_2^- tends to hydrate quickly to WO_2^- and $W_2O_2^-$, thus avoiding the above reaction. Although rate measurement results are not available, it seems likely that the reactions

and

should proceed at rates similar to that of the $N + O_2^-$ reaction. We have assumed that this is the case, and set the latter two rate coefficients equal to $1 \times 10^{-10} \text{ cm}^3/\text{s}$. It is comforting to find that these reactions do not make an appreciable difference in the computed results. That is, we do not find the reactions to be important.

11. Other Details: In some instances rate data are given for a few reactions of transient species such as, for example, $O_2^+ \cdot N_2$. Inclusion of any such chemical species without providing a suitably complete set of reactions for its production and destruction can lead to erroneous results. As an alternative to including the reactions, we may omit the species altogether. Known species for which we have exercised this option include $O_2^+ \cdot N_2$, $O_2^- \cdot N_2$, $O_4^+ \cdot N_2$, $O_2^+ \cdot N_4$, O_6^+ , $O(^1S)$, and obviously many others. In omitting such species we assume, implicitly, that their reactions do not lead to any important alternative paths for production or destruction of important species.

For a large number of reactions the reaction products are uncertain. In all such cases we assume that the products are those that lead to the maximum value of $-\Delta F$ (negative free-energy change) for the reaction.

D. Equilibrium Pairing of Forward and Reverse Reactions

A requirement closely related to the requirement for complete subsets of reactions is that for each reaction we must include a reverse. The rate constants for corresponding forward and reverse reactions are related through the equilibrium constant, i.e.,

$$k_r = k_f/K_{eq} \quad (1)$$

Reactions which are highly exothermic tend, at normal temperatures, to be unidirectional--that is, the reverse (endothermic) reactions are negligibly slow and frequently have immeasurably low rate constants. However, as the temperature is raised, the endothermic reactions become more important, and must be taken into account.

If a chemical system is in thermodynamic equilibrium, then the reaction kinetic equations, if they are correct, must show that the rates of change of all species concentrations are zero. This is a simple and instructive test to perform, provided one has a way of computing the states of equilibrium. We have constructed a code to compute chemical equilibria, as described in the equilibrium report.¹

Because published rate coefficients are usually not available for the endothermic reactions, they must be computed, using the computed equilibrium constants and the rate coefficients of their exothermic reverse counterparts. Formulae and the necessary data for computing equilibrium constants are given in the equilibrium report.¹ We have generated reverse reaction parameters for every forward reaction included in the kinetics code, with the few exceptions to be enumerated below. The resulting list of reactions and rate parameters is tabulated in Section II-G.

With this set of reactions we have performed the equilibrium test. That is, we use the equilibrium set of concentrations for initial conditions, and find that, in the absence of sources or sinks, the kinetics code results show all concentrations remaining *almost* constant. The test is passed satisfactorily over a range of temperatures between 300 and 4000 K. Some examples of these computations are included in Section IV, with some additional discussion.

For reasons of computer cost economy, we have not insisted that the reaction set be *absolutely* complete in the forward-reverse sense. We have omitted some endothermic reactions of the following special types:

1. Associative Ionization ($A + B \rightarrow AB^+ + e$): In this category we have omitted all but the three reactions

2. All Reactions of the Type $A + B \rightarrow A^+ + B^-$: (i.e., reverses of ion-ion recombination).

The omissions are justified by the fact that the system passes the equilibrium test in spite of them. It can also be argued that there are faster indirect paths to produce the same results. For instance, the result $A + B \rightarrow AB^+ + e$ is also produced by $A + B + M \rightarrow AB + M$ followed by $AB + M \rightarrow AB^+ + e + M$, or by $A + M \rightarrow A^+ + e + M$ followed by $A^+ + B + M \rightarrow AB^+ + M$.

E. Photochemical Reactions

We shall consider photochemical reactions of the general types:

and

where " $h\nu$ " shall mean a photon, and " A^* " means an excited quantum state. The rate expression for disappearance of a reactant A by photochemical reaction i can be written as $(d[A]/dt)_i = -J_i[A]$, where $[A]$ means the concentration of A, and J_i is the photochemical rate coefficient (units of s^{-1}). Suppose that the photochemical cross section of A for the specified reaction i is $\sigma_i(\lambda)$ at wavelength λ , and we describe the local radiation flux in terms of a function N_λ , defined as the number of photons per cm^2 per unit wavelength. Then the quasi-first order photochemical rate coefficient is

$$J_i = c \int_0^\infty N_\lambda \sigma_i d\lambda \quad (s^{-1}) \quad (2)$$

where c is the speed of light.

For all of the computations in this report we shall assume that the spectral distribution of N_λ is that of a Planckian of temperature T_s truncated at a short-wavelength cutoff λ_m ($\lambda_m \geq 0$). The strength of the photon source is specified by a scale factor f , between 0 and 1. Then

$$N_\lambda = \begin{cases} 8\pi f / \lambda^4 [\exp(hc/\lambda kT_s) - 1] & \text{for } \lambda > \lambda_m \\ 0 & \text{for } \lambda < \lambda_m \end{cases} \quad (3)$$

For a large number of photochemical reactions the cross-sections $\sigma_i(\lambda)$ are known, and the J_i can be evaluated via Eq. (2) if the source parameters f , T_s , and λ_m are specified. (Note: We assume that the σ_i are independent of temperature.)

For photoexcitation of bound levels the cross-section data will in effect be expressed in terms of the Einstein A_{nm} coefficients (s^{-1}). In such cases the operation of combining Eqs. (2) and (3) gives

$$J_i = f A_{nm} g_n / g_m \left(e^{hc/\lambda kT_s} - 1 \right) \quad (4)$$

where λ is the central wavelength of the line or band and g_n and g_m are statistical weight factors.

There are, of course, many reactions for which the photochemical cross sections are not known. We have simply omitted most such reactions. However, we have made an exception in the case of negative ion photo-detachment reactions where, in the absence of better information, we assume that the cross sections are $6 \times 10^{-18} \text{ cm}^2$ for photons of wavelength shorter than a threshold, λ_c , and 0 for $\lambda > \lambda_c$. λ_c is set equal to $hc/(EA)$, where EA is the electron affinity of the negative ion, derivable from its heat of formation.¹

Returning to the matter of the photon flux, Eq. (3) is intended to approximate the photon density from a hot body such as the

sun or a nuclear fireball, subtending a solid angle of $4\pi f$ sr, and transmitted through an absorber, such as O_2 , which has a distinct short-wavelength cutoff. The local spectral intensities of radiation in a real physical system would usually be influenced by the spatial distribution of concentrations of photoabsorbing species, which themselves depend on the spectral intensities. Therefore, for accurate computation of the radiation field and photo reaction rates, a coupled chemistry and radiation transport computation would be required. Such a complexity is beyond the scope of this report, and we assume simply that the radiation field can be specified as a Planckian, with or without the dilution factor f and with or without the short-wavelength cutoff.

Since we do not consider photoabsorption processes in detail nor keep track of detailed quantum state populations, we also do not attempt to keep track of photons emitted through radiative recombination, radiative attachment, or bound-bound transitions.

F. Miscellaneous Special Rate Adjustments

1. Adjustments for Certain Endothermic Reactions:

For an endothermic reaction one is entitled to expect that the activation energy will be at least as large as the positive heat of reaction. However, our set contains four reactions for which the published rate coefficients violate this rule, if one accepts the heat of formation values given in Ref. 1. For these reactions we have therefore adjusted the published activation energies upward to equal the heats of reaction and adjusted the pre-exponential factors to give the published reaction rates at 298 K. That is, $C = \Delta H/R$ and $A = k(298 \text{ K}) \exp(\Delta H/298 \text{ R})$, where we use the DNA Rate Handbook notation² [see Eq. (5), Section G].

2. Two-Step Processes via Reactive Intermediates:

The oxidation of NO_2 by O atoms was described by Bérces and Förgeteg³ as proceeding through the excited intermediate NO_3^* :

Since we wish to avoid including NO_3^* in our list of species (for the reasons given in Section C-11), we have substituted the single reaction

with $k = k_2 k_f / k_r = 1.5 \times 10^{-31} \text{ cm}^6/\text{s}$. This expression for k is consistent with the Bércecs and Förgeteg mechanism only in cases where $k_r \gg k_2[\text{M}]$. A more accurate expression would be $k = k_2 k_f / (k_r + k_2[\text{M}])$.

In another case we have worked the same logic in reverse. Instead of the classic third-order reaction for oxidation of NO, viz.,

we have substituted the sequence

If this is the true sequence, then the first reaction would have been rate-controlling for the formation of NO_2 under the conditions of measurement of k . We therefore set $k_1 = k = 6.6 \times 10^{-39} \exp(+526/T) \text{ cm}^6/\text{s}$.

3. Three-Body Ion-Neutral Association Reactions: Two positive ion-neutral association reactions, namely

and

are known to be third order at low pressures

(below 1 torr) and second order at higher pressures.⁴ In the absence of any information to the contrary, we assume that the same is true for all other three-body positive ion-neutral association reactions. These reactions are all listed as third order in Table II; however, in the computations we scale down the third-order rate coefficients by the factor $\text{Min}\{1, 1 \times 10^{17}/[\text{M}]\}$. Thus the reaction rates become second order for moderator densities above $1 \times 10^{17} \text{ cm}^{-3}$. The rate coefficients for the corresponding reverse reactions are modified accordingly, so the limiting equilibrium behavior is preserved.

For lack of any data for guidance, we have not made any analogous adjustments to the rates of negative ion-neutral association reactions. The correction factor, or lack of it, constitutes a large potential source of error for pressures above about 10 torr. At normal atmospheric density the factor is about 0.004.

G. Listing of the Chemical Reactions

Table II is a computer listing of the chemical reactions considered in these calculations, grouped according to reaction types. The first column in the table is a reaction catalog number. The next three columns give reactants. The next five (following the $\Rightarrow$) give the products. [Note the obvious fact that there are no sub- or superscripts, so that "H2O" is intended to mean H_2O , and so on. Also "O(1D)" refers to $\text{O}(^1\text{D})$, "N(2D)" means $\text{N}(^2\text{D})$, "O2(DL)" means $\text{O}_2(^1\Delta_g)$, and "O2(SG)" means $\text{O}_2(^1\Sigma_g^+)$.] The next three columns give the parameters A, B, and C for rate constants expressed in the form

$$k(T) = A(T/300)^B e^{-C/T} \quad (5)$$

(except for photochemical reactions and ion-ion mutual neutralization, see below). The last column contains the bibliography reference numbers for the reaction rate or cross-section data.

For photochemical reactions the A, B, and C columns contain computed values of the

J_i for source temperatures T_s of 5000, 7500, and 10 000 K, respectively, with $\lambda_m \equiv 0$ and $f \equiv 1$ [see Eqs. (2), (3)].

For ion-ion mutual neutralization reactions, where we have used the general rate coefficient formulae from the DNA Handbook,² the effective two-body rate coefficients

are assumed to be of the form

$$k = A(T/300)^B + C(T/300)^{B-2}[M] \quad (6)$$

For these reactions column C of the listing is used for the coefficient of the three-body term [Eq. (6)]. (These reactions have zero activation energy.)

TABLE II
LISTING OF REACTIONS

NO.				A	B	C	REFERENCE
CATEGORY 1. RADIATIVE RECOMBINATION							
2521. E	+ O ⁺	= O		3.5E-12	-1.70	0	5
2523. E	+ N ⁺	= N		3.5E-12	-1.70	0	5
2525. E	+ H ⁺	= H		3.5E-12	-1.70	0	5
2527. E	+ O ₂ ⁺	= O ₂		4.0E-12	-1.70	0	5
2529. E	+ N ₂ ⁺	= N ₂		4.0E-12	-1.70	0	5
2531. E	+ NO ⁺	= NO		4.0E-12	-1.70	0	5
CATEGORY 3. THREE-BODY RECOMBINATION							
17. E	+ N ⁺	+ M	= N	6.0E-27	-2.50	0	5
19. E	+ E	+ N ⁺	= E	7.0E-20	-4.50	0	5
21. E	+ N ₂ ⁺	+ M	= N ₂	6.0E-27	-2.50	0	5
23. E	+ E	+ N ₂ ⁺	= E	7.0E-20	-4.50	0	5
151. E	+ O ⁺	+ M	= O	6.0E-27	-2.50	0	5
153. E	+ E	+ O ⁺	= E	7.0E-20	-4.50	0	5
155. E	+ O ₂ ⁺	+ M	= O ₂	6.0E-27	-2.50	0	5
157. E	+ E	+ O ₂ ⁺	= E	7.0E-20	-4.50	0	5
373. E	+ NO ⁺	+ M	= NO	6.0E-27	-2.50	0	5
375. E	+ NO ₂ ⁺	+ M	= NO ₂	6.0E-27	-2.50	0	5
377. E	+ N ₂ O ⁺	+ M	= N ₂ O	6.0E-27	-2.50	0	5
379. E	+ E	+ NO ⁺	= E	7.0E-20	-4.50	0	5
381. E	+ E	+ NO ₂ ⁺	= E	7.0E-20	-4.50	0	5
383. E	+ E	+ N ₂ O ⁺	= E	7.0E-20	-4.50	0	5
767. E	+ CO ⁺	+ M	= CO	6.0E-27	-2.50	0	5
769. E	+ CO ₂ ⁺	+ M	= CO ₂	6.0E-27	-2.50	0	5
771. E	+ E	+ CO ⁺	= E	7.0E-20	-4.50	0	5
773. E	+ E	+ CO ₂ ⁺	= E	7.0E-20	-4.50	0	5
1001. E	+ H ⁺	+ M	= H	6.0E-27	-2.50	0	5
1003. E	+ OH ⁺	+ M	= OH	6.0E-27	-2.50	0	5
1005. E	+ H ₂ O ⁺	+ M	= H ₂ O	6.0E-27	-2.50	0	5
1007. E	+ E	+ H ⁺	= E	7.0E-20	-4.50	0	5
1009. E	+ E	+ OH ⁺	= E	7.0E-20	-4.50	0	5
1011. E	+ E	+ H ₂ O ⁺	= E	7.0E-20	-4.50	0	5
1301. E	+ O ₄ ⁺	+ M	= O ₂	6.0E-27	-2.50	0	5
1303. E	+ H ₃ O ⁺	+ M	= H	6.0E-27	-2.50	0	5
1305. E	+ OH ₂ O ⁺	+ M	= H ₂ O	5.0E-26	-2.50	0	5
1307. E	+ H ₃ O ⁺	+ M	= H ₂ O	5.0E-26	-2.50	0	5
1309. E	+ H ₃ O ⁺	+ M	= H ₂ O	5.0E-26	-2.50	0	5
1311. E	+ H ₃ O ⁺	+ M	= H ₂ O	5.0E-26	-2.50	0	5
1313. E	+ H ₂ O ⁺	+ M	= H ₂ O	5.0E-26	-2.50	0	5
1315. E	+ E	+ H ₃ O ⁺	= E	7.0E-20	-4.50	0	5
1317. E	+ E	+ OH ₂ O ⁺	= E	7.0E-20	-4.50	0	5
1319. E	+ E	+ H ₃ O ⁺	= E	7.0E-20	-4.50	0	5
1321. E	+ E	+ H ₃ O ⁺	= E	7.0E-20	-4.50	0	5
1323. E	+ E	+ H ₃ O ⁺	= E	7.0E-20	-4.50	0	5
1325. E	+ E	+ H ₂ O ⁺	= E	7.0E-20	-4.50	0	5
1401. E	+ N ₃ ⁺	+ M	= N	6.0E-27	-2.50	0	5
1403. E	+ N ₄ ⁺	+ M	= N ₂	6.0E-27	-2.50	0	5
1405. E	+ HNO ⁺	+ M	= H ₂ O	5.0E-26	-2.50	0	5
1407. E	+ HNO ⁺	+ M	= H ₂ O	5.0E-26	-2.50	0	5
1409. E	+ HNO ⁺	+ M	= H ₂ O	5.0E-26	-2.50	0	5
1411. E	+ E	+ OH ⁺	= E	7.0E-20	-4.50	0	5
1413. E	+ E	+ N ₃ ⁺	= E	7.0E-20	-4.50	0	5
1415. E	+ E	+ N ₄ ⁺	= E	7.0E-20	-4.50	0	5

TABLE II (cont)

NO.								A	B	C	REFERENCE
CATEGORY 3. THREE-BODY RECOMBINATION											
1417. E	• E	• HNO•	• E	• NO	• H2O			3.0E-19	-4.50	0	5
1419. E	• E	• H2NO•	• E	• NO	• H2O	• H2O		3.0E-19	-4.50	0	5
1421. E	• E	• H3NO•	• E	• NO	• H2O	• H2O	• H2O	3.0E-19	-4.50	0	5
CATEGORY 53. COLLISIONAL IONIZATION											
18. N	• M		• E	• N+	• M			2.5E-07	-1.86	168669	PAR. 11-D
20. E	• N		• E	• E	• N+			2.9E+00	-2.86	168669	PAR. 11-D
22. N2	• M		• E	• N2+	• M			2.9E-07	-1.94	168669	PAR. 11-D
24. E	• N2		• E	• E	• N2+			3.4E+00	-2.94	168669	PAR. 11-D
152. O	• M		• E	• O+	• M			8.9E-09	-1.10	158030	PAR. 11-D
154. E	• O		• E	• E	• O+			1.0E+00	-3.10	158030	PAR. 11-D
156. O2	• M		• E	• O2+	• M			1.4E-07	-1.95	139987	PAR. 11-D
158. E	• O2		• E	• E	• O2+			1.6E+00	-2.96	139987	PAR. 11-D
374. NO	• M		• E	• NO+	• M			4.1E-09	-1.16	107952	PAR. 11-D
376. N2	• M		• E	• N2+	• M			7.6E-06	-1.00	113535	PAR. 11-D
378. N2O	• M		• E	• N2O+	• M			5.2E-07	-1.62	149635	PAR. 11-D
380. E	• NO		• E	• E	• NO+			4.6E-01	-3.16	107952	PAR. 11-D
382. E	• N2		• E	• E	• N2+			8.6E-01	-3.00	113535	PAR. 11-D
384. E	• N2O		• E	• E	• N2O+			6.1E+00	-2.62	149635	PAR. 11-D
788. CO	• M		• E	• CO+	• M			3.0E-07	-1.00	162043	PAR. 11-D
770. CO2	• M		• E	• CO2+	• M			3.0E-07	-1.00	159757	PAR. 11-D
772. E	• CO		• E	• E	• CO+			3.9E+00	-3.00	162043	PAR. 11-D
774. E	• CO2		• E	• E	• CO2+			3.9E+00	-3.00	159757	PAR. 11-D
1002. H	• M		• E	• H+	• M			7.9E-09	-1.00	157815	PAR. 11-D
1004. OH	• M		• E	• OH+	• M			1.6E-07	-1.09	152961	PAR. 11-D
1006. H2O	• M		• E	• H2O+	• M			3.0E-07	-1.00	149441	PAR. 11-D
1008. E	• H		• E	• E	• H+			8.6E-01	-3.00	157815	PAR. 11-D
1010. E	• OH		• E	• E	• OH+			1.9E+00	-3.08	152961	PAR. 11-D
1012. E	• H2O		• E	• E	• H2O+			3.9E+00	-3.00	149441	PAR. 11-D
1302. O2	• O2	• M	• E	• O4+	• M			4.7E-33	-2.05	134895	PAR. 11-D
1304. H	• H2O	• M	• E	• H3O+	• M			8.9E-32	-1.89	74715	PAR. 11-D
1306. H2O	• H2O	• M	• E	• OH+H3O+	• M			9.7E-31	-1.71	120526	PAR. 11-D
1314. H2O	• H2O	• M	• E	• H2O2+	• M			6.9E-30	-1.46	129885	PAR. 11-D
1316. E	• H2O	• M	• E	• E	• H3O+			1.0E-24	-3.88	74715	PAR. 11-D
1318. E	• H2O	• H2O	• E	• E	• OH+H3O+			5.6E-24	-2.71	120526	PAR. 11-D
1326. E	• O2	• H2O	• E	• E	• H2O2+			3.9E-23	-2.46	129885	PAR. 11-D
1402. N	• N2	• M	• E	• N3+	• M			2.0E-32	-1.82	133597	PAR. 11-D
1404. N2	• N2	• M	• E	• NH+	• M			4.0E-32	-1.73	173514	PAR. 11-D
1406. H2O	• NO	• M	• E	• HNO+	• M			1.9E-30	-1.46	97449	PAR. 11-D
1412. E	• O2	• O2	• E	• E	• O4+			5.9E-26	-4.05	134895	PAR. 11-D
1414. E	• N2	• N	• E	• E	• N3+			2.3E-25	-3.82	133597	PAR. 11-D
1416. E	• N2	• N2	• E	• E	• NH+			4.7E-25	-3.73	173514	PAR. 11-D
1418. E	• NO	• H2O	• E	• E	• HNO+			8.6E-24	-2.46	97449	PAR. 11-D
CATEGORY 4. DISSOCIATIVE RECOMBINATION											
1. E	• N2+	• N	• N	• N(2D)				1.6E-07	-1.39	0	5
7. E	• N3+	• N	• N	• N2				7.0E-07	-1.00	0	5
13. E	• N4+	• N2	• N2	• N2				2.0E-06	-1.00	0	5
119. E	• O2+	• O	• O	• O(1D)				2.1E-07	-1.63	0	5
159. E	• O4+	• O2	• O2	• O2				2.0E-06	-1.00	0	5
297. E	• NO+	• O	• O	• N(2D)				4.0E-07	-1.80	0	5

TABLE II (cont)

NO.				A	B	C	REFERENCE
CATEGORY 4. DISSOCIATIVE RECOMBINATION							
299. E	+ NO ₂ ⁺	= O	+ NO	3.0E-07	-.50	0	5
365. E	+ H ₂ O ⁺	= O	+ N ₂	2.0E-07	0.00	0	PAR. 11-C-3
775. E	+ CO ₂ ⁺	= C	+ CO	2.0E-07	0.00	0	PAR. 11-C-3
859. E	+ HNO ⁺	= NO	+ H ₂ O	1.0E-06	-.20	0	5
861. E	+ H ₂ NO ⁺	= NO	+ H ₂ O + H ₂ O	2.0E-06	-.20	0	5
863. E	+ H ₃ NO ⁺	= NO	+ H ₂ O + H ₂ O	3.0E-06	-.20	0	5
1013. E	+ OH ⁺	= O	+ H	2.0E-07	0.00	0	PAR. 11-C-3
1015. E	+ H ₂ O ⁺	= O	+ H ₂	2.0E-07	0.00	0	PAR. 11-C-3
1017. E	+ H ₃ O ⁺	= H	+ H ₂ O	1.3E-06	-.20	0	5
1019. E	+ OH-H ₃ O ⁺	= H ₂ O	+ H + OH	3.0E-06	-1.00	0	5
1021. E	+ H-H ₃ O ⁺	= H	+ H ₂ O + H ₂ O	2.6E-06	-.20	0	5
1023. E	+ H ₂ -H ₃ O ⁺	= H	+ H ₂ O + H ₂ O + H ₂ O	5.1E-06	-.20	0	5
1025. E	+ NO ₂ ⁺	= O ₂	+ H ₂ O	1.5E-06	-.20	0	5
1327. E	+ H ₃ -H ₃ O ⁺	= H	+ H ₂ O + H ₂ O + H ₂ O + H ₂ O	6.1E-06	-.20	0	5
CATEGORY 5A. ASSOCIATIVE IONIZATION							
2. N	+ N(2D)	= E	+ N ₂ ⁺	6.5E-13	.75	39683	PAR. 11-D
120. O	+ O(1D)	= E	+ O ₂ ⁺	1.2E-12	.95	57800	PAR. 11-D
298. O	+ N(2D)	= E	+ NO ⁺	7.6E-13	.17	4162	PAR. 11-D
CATEGORY 5. MUTUAL NEUTRALIZATION							
121. O-	+ O ₂ ⁺	= O	+ O ₂	9.6E-08	-.50	3.0E-25	5
123. O ₂ -	+ O ₂ ⁺	= O ₂	+ O ₂	4.2E-07	-.50	3.0E-25	5
125. O-	+ O ⁺	= O	+ O	2.7E-07	-.50	3.0E-25	5
127. O ₂ -	+ O ⁺	= O	+ O ₂	4.0E-07	-.50	3.0E-25	5
143. O ₄ -	+ O ₂ ⁺	= O ₂	+ O ₂ + O ₂	4.0E-07	-.50	3.0E-25	5
161. O-	+ O ₄ ⁺	= O ₃	+ O ₂	4.0E-07	-.50	3.0E-25	5
163. O ₂ -	+ O ₄ ⁺	= O ₂	+ O ₂ + O ₂	4.0E-07	-.50	3.0E-25	5
165. O ₃ -	+ O ⁺	= O ₂	+ O ₂	4.0E-07	-.50	3.0E-25	5
167. O ₃ -	+ O ₄ ⁺	= O ₃	+ O ₂ + O ₂	4.0E-07	-.50	3.0E-25	5
169. O ₄ -	+ O ⁺	= O ₃	+ O ₂	4.0E-07	-.50	3.0E-25	5
171. O ₄ -	+ O ₄ ⁺	= O ₂	+ O ₂ + O ₂ + O ₂	4.0E-07	-.50	3.0E-25	5
301. O ₂ -	+ N ⁺	= N	+ O ₂	4.0E-07	-.50	3.0E-25	5
303. O ₂ -	+ N ₂ ⁺	= O ₂	+ N ₂	1.6E-07	-.50	3.0E-25	5
307. O ₂ -	+ NO ⁺	= NO	+ O ₂	4.0E-07	-.50	3.0E-25	5
309. O ₂ -	+ NO ₂ ⁺	= NO ₂	+ O ₂	4.0E-07	-.50	3.0E-25	5
313. O ₃ -	+ O ₂ ⁺	= O	+ O ₂ + O ₂	4.0E-07	-.50	3.0E-25	5
315. O ₃ -	+ NO ⁺	= O	+ NO + O ₂	4.0E-07	-.50	3.0E-25	5
319. NO ₂ -	+ N ⁺	= NO	+ NO	4.0E-07	-.50	3.0E-25	5
321. NO ₂ -	+ O ₂ ⁺	= NO ₂	+ O ₂	4.1E-07	-.50	3.0E-25	5
323. NO ₂ -	+ NO ⁺	= NO	+ NO ₂	3.5E-07	-.50	3.0E-25	5
325. NO ₃ -	+ N ⁺	= NO	+ NO ₂	4.0E-07	-.50	3.0E-25	5
327. NO ₃ -	+ N ₃ ⁺	= NO	+ NO ₂ + N ₂	4.0E-07	-.50	3.0E-25	5
329. NO ₃ -	+ N ₂ ⁺	= NO ₂	+ H ₂ O	4.0E-07	-.50	3.0E-25	5
331. NO ₃ -	+ O ⁺	= NO ₂	+ O ₂	4.0E-07	-.50	3.0E-25	5
333. NO ₃ -	+ N ₄ ⁺	= NO ₂	+ H ₂ O + N ₂	4.0E-07	-.50	3.0E-25	5
335. NO ₃ -	+ O ₂ ⁺	= NO ₂	+ O + O ₂	1.3E-07	-.50	3.0E-25	5
337. NO ₃ -	+ NO ⁺	= NO ₂	+ NO ₂	4.0E-07	-.50	3.0E-25	5
339. NO ₃ -	+ N ₂ O ⁺	= NO	+ NO + NO ₂	4.0E-07	-.50	3.0E-25	5
341. NO ₃ -	+ NO ₂ ⁺	= NO	+ NO ₂ + O ₂	4.0E-07	-.50	3.0E-25	5
357. O ₄ -	+ NO ₂ ⁺	= NO ₂	+ O ₂ + O ₂	4.0E-07	-.50	3.0E-25	5

TABLE II (cont)

NO.				A	B	C	REFERENCE
CATEGORY 5. MUTUAL NEUTRALIZATION							
359. O ₄ -	+ NO ₂	= NO	+ O ₂	4.0E-07	- .50	3.0E-25	5
361. NO ₃ -	+ O ₄	= O ₃	+ NO ₂	4.0E-07	- .50	3.0E-25	5
363. NO ₂ -	+ O ₄	= NO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
387. O-	+ N ₂	= O	+ N ₂	2.6E-07	- .50	3.0E-25	5
389. O-	+ N ₂	= O	+ N ₂	4.0E-07	- .50	3.0E-25	5
391. O-	+ N ₂	= NO	+ N ₂	4.0E-07	- .50	3.0E-25	5
393. O-	+ N ₂	= NO	+ N ₂	4.0E-07	- .50	3.0E-25	5
395. O-	+ NO ₂	= NO	+ O ₂	4.0E-07	- .50	3.0E-25	5
397. O-	+ NO ₂	= NO	+ O ₂	4.0E-07	- .50	3.0E-25	5
399. O-	+ NO ₂	= NO	+ O ₂	4.0E-07	- .50	3.0E-25	5
401. O ₂ -	+ N ₂	= NO ₂	+ N ₂	4.0E-07	- .50	3.0E-25	5
403. O ₂ -	+ N ₂	= NO ₂	+ N ₂	4.0E-07	- .50	3.0E-25	5
405. O ₂ -	+ N ₂	= NO ₂	+ N ₂	4.0E-07	- .50	3.0E-25	5
407. O ₃ -	+ N ₂	= NO	+ O ₂	4.0E-07	- .50	3.0E-25	5
409. O ₃ -	+ N ₂	= NO	+ O ₂	4.0E-07	- .50	3.0E-25	5
411. O ₃ -	+ N ₂	= NO ₃	+ O ₂	4.0E-07	- .50	3.0E-25	5
413. O ₃ -	+ N ₂	= NO ₃	+ O ₂	4.0E-07	- .50	3.0E-25	5
415. O ₃ -	+ NO ₂	= NO ₃	+ O ₂	4.0E-07	- .50	3.0E-25	5
417. O ₃ -	+ NO ₂	= NO ₃	+ O ₂	4.0E-07	- .50	3.0E-25	5
419. O ₄ -	+ N ₂	= NO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
421. O ₄ -	+ N ₂	= NO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
423. O ₄ -	+ N ₂	= NO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
425. O ₄ -	+ N ₂	= NO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
427. O ₄ -	+ NO ₂	= NO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
429. O ₄ -	+ O ₂	= NO	+ O ₂	4.0E-07	- .50	3.0E-25	5
431. NO-	+ O ₂	= NO	+ O ₂	4.0E-07	- .50	3.0E-25	5
433. NO-	+ O ₄	= NO ₃	+ O ₂	4.0E-07	- .50	3.0E-25	5
435. NO-	+ N ₂	= O	+ N ₂	4.0E-07	- .50	3.0E-25	5
437. NO-	+ N ₂	= NO	+ N ₂	4.0E-07	- .50	3.0E-25	5
439. NO-	+ N ₂	= NO	+ N ₂	4.0E-07	- .50	3.0E-25	5
441. NO-	+ N ₂	= NO	+ N ₂	4.0E-07	- .50	3.0E-25	5
443. NO-	+ NO ₂	= NO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
445. NO-	+ NO ₂	= NO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
447. NO-	+ NO ₂	= NO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
449. NO ₂ -	+ O ₂	= NO	+ O ₂	4.0E-07	- .50	3.0E-25	5
451. NO ₂ -	+ N ₂	= NO ₂	+ N ₂	4.0E-07	- .50	3.0E-25	5
453. NO ₂ -	+ N ₂	= NO ₂	+ N ₂	4.0E-07	- .50	3.0E-25	5
455. NO ₂ -	+ N ₂	= NO ₂	+ N ₂	4.0E-07	- .50	3.0E-25	5
457. NO ₂ -	+ NO ₂	= NO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
459. NO ₂ -	+ NO ₂	= NO ₃	+ N ₂	4.0E-07	- .50	3.0E-25	5
719. CO ₃ -	+ NO ₂	= O	+ CO ₂	4.0E-07	- .50	3.0E-25	5
721. CO ₃ -	+ NO ₂	= O	+ CO ₂	4.0E-07	- .50	3.0E-25	5
723. CO ₃ -	+ NO ₂	= O	+ CO ₂	4.0E-07	- .50	3.0E-25	5
743. CO ₄ -	+ NO ₂	= NO ₂	+ CO ₂	4.0E-07	- .50	3.0E-25	5
745. CO ₄ -	+ NO ₂	= NO	+ CO ₂	4.0E-07	- .50	3.0E-25	5
747. CO ₄ -	+ O ₂	= CO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
749. CO ₃ -	+ O ₄	= O ₃	+ CO ₂	4.0E-07	- .50	3.0E-25	5
751. CO ₄ -	+ O ₄	= O ₃	+ CO ₂	4.0E-07	- .50	3.0E-25	5
777. O-	+ CO ₂	= O	+ CO ₂	4.0E-07	- .50	3.0E-25	5
779. O-	+ CO ₂	= O	+ CO ₂	4.0E-07	- .50	3.0E-25	5
781. O ₂ -	+ CO ₂	= O	+ CO ₂	4.0E-07	- .50	3.0E-25	5
783. O ₂ -	+ CO ₂	= O ₂	+ CO ₂	4.0E-07	- .50	3.0E-25	5
785. O ₃ -	+ CO ₂	= CO ₂	+ O ₂	4.0E-07	- .50	3.0E-25	5
787. O ₃ -	+ CO ₂	= O ₃	+ CO ₂	4.0E-07	- .50	3.0E-25	5
789. O ₄ -	+ CO ₂	= O	+ CO ₂	4.0E-07	- .50	3.0E-25	5

TABLE II (cont)

NO.						A	B	C	REFERENCE
CATEGORY 5. MUTUAL NEUTRALIZATION									
791.	O4-	+ CO2+	= CO2	+ O2		4.0E-07	- .50	3.0E-25	5
793.	NO-	+ CO+	= NO	+ CO		4.0E-07	- .50	3.0E-25	5
795.	NO-	+ CO2+	= NO	+ CO2		4.0E-07	- .50	3.0E-25	5
797.	NO3-	+ CO+	= NO2	+ CO2		4.0E-07	- .50	3.0E-25	5
799.	NO3-	+ CO2+	= NO3	+ CO2		4.0E-07	- .50	3.0E-25	5
865.	CO3-	+ H2NO+	= CO2	+ O	+ NO	5.0E-07	- .50	3.0E-25	5
867.	NO3-	+ H2NO+	= NO2	+ NO2	+ H2O	5.0E-07	- .50	3.0E-25	5
869.	NO2-	+ H2NO+	= NO2	+ NO	+ H2O	5.0E-07	- .50	3.0E-25	5
871.	CO4-	+ H2NO+	= CO2	+ O2	+ NO	5.0E-07	- .50	3.0E-25	5
873.	O2-	+ H2NO+	= O2	+ NO	+ H2O	5.0E-07	- .50	3.0E-25	5
875.	CO3-	+ H2NO+	= NO2	+ CO2	+ O	5.0E-07	- .50	3.0E-25	5
877.	NO3-	+ H2NO+	= NO2	+ H2O	+ H2O	5.0E-07	- .50	3.0E-25	5
879.	NO2-	+ H2NO+	= NO	+ NO2	+ H2O	5.0E-07	- .50	3.0E-25	5
881.	CO4-	+ H2NO+	= NO	+ CO2	+ O2	5.0E-07	- .50	3.0E-25	5
883.	O2-	+ H2NO+	= NO	+ O2	+ H2O	5.0E-07	- .50	3.0E-25	5
885.	CO3-	+ H2NO+	= NO	+ CO2	+ H2O	5.0E-07	- .50	3.0E-25	5
887.	NO3-	+ H2NO+	= NO2	+ NO2	+ H2O	5.0E-07	- .50	3.0E-25	5
889.	NO2-	+ H2NO+	= NO	+ NO2	+ H2O	5.0E-07	- .50	3.0E-25	5
891.	CO4-	+ H2NO+	= NO	+ CO2	+ O2	5.0E-07	- .50	3.0E-25	5
893.	O2-	+ H2NO+	= NO	+ O2	+ H2O	5.0E-07	- .50	3.0E-25	5
901.	CO3-	+ H2O2+	= H2O	+ O2	+ CO2	5.0E-07	- .50	3.0E-25	5
903.	NO3-	+ H2O2+	= O3	+ NO2	+ H2O	5.0E-07	- .50	3.0E-25	5
905.	NO2-	+ H2O2+	= NO2	+ O2	+ H2O	5.0E-07	- .50	3.0E-25	5
907.	CO4-	+ H2O2+	= O2	+ H2O	+ CO2	5.0E-07	- .50	3.0E-25	5
911.	CO3-	+ OH+O2+	= CO2	+ H2O2	+ H2O	5.0E-07	- .50	3.0E-25	5
913.	NO3-	+ OH+O2+	= NO2	+ H2O2	+ H2O	5.0E-07	- .50	3.0E-25	5
915.	NO2-	+ OH+O2+	= NO2	+ H2O	+ H2O	5.0E-07	- .50	3.0E-25	5
917.	CO4-	+ OH+O2+	= CO2	+ O2	+ H2O	5.0E-07	- .50	3.0E-25	5
923.	CO3-	+ H3O+	= CO2	+ OH	+ H2O	4.0E-07	- .50	3.0E-25	5
925.	NO3-	+ H3O+	= NO2	+ OH	+ H2O	4.0E-07	- .50	3.0E-25	5
927.	NO2-	+ H3O+	= NO2	+ H	+ H2O	4.0E-07	- .50	3.0E-25	5
929.	CO4-	+ H3O+	= H2O2	+ H2O	+ CO2	4.0E-07	- .50	3.0E-25	5
931.	CO3-	+ H+O2+	= CO2	+ OH	+ H2O	5.0E-07	- .50	3.0E-25	5
933.	NO3-	+ H+O2+	= NO2	+ OH	+ H2O	5.0E-07	- .50	3.0E-25	5
935.	NO2-	+ H+O2+	= NO2	+ H	+ H2O	5.0E-07	- .50	3.0E-25	5
937.	CO4-	+ H+O2+	= H2O2	+ CO2	+ H2O	5.0E-07	- .50	3.0E-25	5
939.	CO3-	+ H2+O2+	= CO2	+ OH	+ H2O	5.0E-07	- .50	3.0E-25	5
941.	NO3-	+ H2+O2+	= NO2	+ OH	+ H2O	5.0E-07	- .50	3.0E-25	5
943.	NO2-	+ H2+O2+	= NO2	+ H	+ H2O	5.0E-07	- .50	3.0E-25	5
945.	CO4-	+ H2+O2+	= H2O2	+ CO2	+ H2O	5.0E-07	- .50	3.0E-25	5
1027.	O-	+ H+	= O	+ H		4.0E-07	- .50	3.0E-25	5
1029.	O-	+ OH+	= H	+ O2		4.0E-07	- .50	3.0E-25	5
1031.	O-	+ H2O+	= O	+ H2O		4.0E-07	- .50	3.0E-25	5
1033.	O-	+ H3O+	= OH	+ H2O		4.0E-07	- .50	3.0E-25	5
1035.	O-	+ OH+O2+	= H2O2	+ H2O		5.0E-07	- .50	3.0E-25	5
1037.	O-	+ H+O2+	= OH	+ H2O		5.0E-07	- .50	3.0E-25	5
1039.	O-	+ H2+O2+	= OH	+ H2O	+ H2O	5.0E-07	- .50	3.0E-25	5
1041.	O-	+ H2O2+	= O3	+ H2O		5.0E-07	- .50	3.0E-25	5
1043.	O-	+ H2NO+	= NO2	+ H2O		5.0E-07	- .50	3.0E-25	5
1045.	O-	+ H2NO2+	= NO2	+ H2O	+ H2O	5.0E-07	- .50	3.0E-25	5
1047.	O2-	+ H+	= O2	+ H		4.0E-07	- .50	3.0E-25	5
1049.	O2-	+ OH+	= O2	+ OH		4.0E-07	- .50	3.0E-25	5
1051.	O2-	+ H2O+	= O2	+ H2O		4.0E-07	- .50	3.0E-25	5
1053.	O2-	+ H3O+	= H2O2	+ H2O		4.0E-07	- .50	3.0E-25	5
1055.	O2-	+ OH+O2+	= O2	+ H2O	+ H2O	5.0E-07	- .50	3.0E-25	5

TABLE II (cont)

NO.					A	B	C	REFERENCE
CATEGORY 5. MUTUAL NEUTRALIZATION								
1057.	02-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1059.	02-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1061.	02-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1063.	03-	+ H+	= OH	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1065.	03-	+ OH+	= H ₂ O	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1067.	03-	+ H ₂ O+	= OH	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1069.	03-	+ H ₂ O+	= OH	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1071.	03-	+ OH+H ₂ O+	= H ₂ O	+ OH	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1073.	03-	+ H ₂ O+	= OH	+ OH	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1075.	03-	+ H ₂ O+	= OH	+ OH	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1077.	03-	+ H ₂ O+	= OH	+ OH	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1079.	03-	+ H ₂ O+	= OH	+ OH	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1081.	03-	+ H ₂ O+	= OH	+ OH	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1083.	04-	+ H+	= H ₂ O	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1085.	04-	+ OH+	= H ₂ O	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1087.	04-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1089.	04-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1091.	04-	+ OH+H ₂ O+	= H ₂ O	+ OH	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1093.	04-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1095.	04-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1097.	04-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1099.	04-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1101.	04-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1103.	NO-	+ H+	= H ₂ O	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1105.	NO-	+ OH+	= H ₂ O	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1107.	NO-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1109.	NO-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1111.	NO-	+ OH+H ₂ O+	= H ₂ O	+ OH	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1113.	NO-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1115.	NO-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1117.	NO-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1119.	NO-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1121.	NO-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1123.	NO-	+ H+	= H ₂ O	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1125.	NO-	+ OH+	= H ₂ O	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1127.	NO-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1133.	NO3-	+ H+	= H ₂ O	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1135.	NO3-	+ OH+	= H ₂ O	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1137.	NO3-	+ H ₂ O+	= H ₂ O	+ H ₂ O	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1139.	OH+	+ O+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1141.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1143.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1145.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1147.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1149.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1151.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1153.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1155.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1157.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1159.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1161.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1163.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1165.	OH+	+ OH+	= H	+ OH	+ H ₂ O	4.0E-07	-.50 3.0E-25	5
1167.	OH+	+ OH+	= H	+ OH	+ H ₂ O	5.0E-07	-.50 3.0E-25	5
1169.	OH+	+ OH+	= H	+ OH	+ H ₂ O	5.0E-07	-.50 3.0E-25	5

TABLE II (cont)

NO.						A	B	C	REFERENCE
CATEGORY 5. MUTUAL NEUTRALIZATION									
1171.	OH-	+ H2H3O+	= H2O	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1173.	OH-	+ H2O2+	= OH	+ O2	+ H2O	5.0E-07	-.50	3.0E-25	5
1175.	OH-	+ HNO+	= HNO2	+ H2O		5.0E-07	-.50	3.0E-25	5
1177.	OH-	+ H2NO+	= HNO2	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1179.	OH-	+ CO+	= H	+ CO2		4.0E-07	-.50	3.0E-25	5
1181.	OH-	+ CO2+	= OH	+ CO2		4.0E-07	-.50	3.0E-25	5
1183.	CO3--	+ H+	= CO2	+ OH		4.0E-07	-.50	3.0E-25	5
1185.	CO3--	+ OH+	= H	+ CO2	+ O2	4.0E-07	-.50	3.0E-25	5
1187.	CO3--	+ H2O+	= O	+ H2O	+ CO2	4.0E-07	-.50	3.0E-25	5
1189.	CO4--	+ H+	= H2O2	+ CO2		4.0E-07	-.50	3.0E-25	5
1191.	CO4--	+ OH+	= CO2	+ O2	+ OH	4.0E-07	-.50	3.0E-25	5
1193.	CO4--	+ H2O+	= CO2	+ O2	+ H2O	4.0E-07	-.50	3.0E-25	5
1231.	H2O2-	+ O+	= O3	+ H2O		5.0E-07	-.50	3.0E-25	5
1233.	H2O2-	+ O2+	= H2O	+ O2	+ O2	5.0E-07	-.50	3.0E-25	5
1235.	H2O2-	+ N+	= NO2	+ H2O		5.0E-07	-.50	3.0E-25	5
1237.	H2O2-	+ N2+	= H2O	+ O2	+ N2	5.0E-07	-.50	3.0E-25	5
1239.	H2O2-	+ NO+	= NO3	+ H2O		5.0E-07	-.50	3.0E-25	5
1241.	H2O2-	+ NO2+	= H2O	+ O2	+ NO2	5.0E-07	-.50	3.0E-25	5
1243.	H2O2-	+ N2O+	= H2O	+ O2	+ N2O	5.0E-07	-.50	3.0E-25	5
1245.	H2O2-	+ H+	= H2O2	+ H2O		5.0E-07	-.50	3.0E-25	5
1247.	H2O2-	+ OH+	= H2O	+ O2	+ OH	5.0E-07	-.50	3.0E-25	5
1249.	H2O2-	+ H2O+	= H2O	+ O2	+ H2O	5.0E-07	-.50	3.0E-25	5
1251.	H2O2-	+ H3O+	= H2O2	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1253.	H2O2-	+ OH+H3O+	= H2O	+ O2	+ H2O	5.0E-07	-.50	3.0E-25	5
1255.	H2O2-	+ H+H3O+	= H2O2	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1257.	H2O2-	+ H2O2+	= H2O	+ O2	+ H2O	5.0E-07	-.50	3.0E-25	5
1259.	H2O2-	+ HNO+	= NO3	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1261.	H2O2-	+ CO+	= O	+ CO2	+ H2O	5.0E-07	-.50	3.0E-25	5
1263.	H2O2-	+ CO2+	= H2O	+ O2	+ CO2	5.0E-07	-.50	3.0E-25	5
1265.	H2O2-	+ O+	= H2O	+ O2	+ O2	5.0E-07	-.50	3.0E-25	5
1267.	H2O2-	+ N3+	= NO2	+ H2O	+ N2	5.0E-07	-.50	3.0E-25	5
1269.	H2O2-	+ N+	= H2O	+ O2	+ N2	5.0E-07	-.50	3.0E-25	5
1271.	H2O2-	+ H2H3O+	= H2O2	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1273.	H2O2-	+ H2NO+	= NO3	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1299.	H2O2-	+ H2H3O+	= H2O2	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1331.	H2O2-	+ O+	= O3	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1333.	H2O2-	+ O2+	= H2O	+ H2O	+ O2	5.0E-07	-.50	3.0E-25	5
1335.	H2O2-	+ O+	= H2O	+ H2O	+ O2	5.0E-07	-.50	3.0E-25	5
1337.	H2O2-	+ H+	= H2O2	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1339.	H2O2-	+ OH+	= H2O	+ H2O	+ O2	5.0E-07	-.50	3.0E-25	5
1341.	H2O2-	+ H2O+	= H2O	+ H2O	+ O2	5.0E-07	-.50	3.0E-25	5
1343.	H2O2-	+ H3O+	= H2O2	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1345.	H2O2-	+ OH+H3O+	= H2O	+ H2O	+ O2	5.0E-07	-.50	3.0E-25	5
1347.	H2O2-	+ H+H3O+	= H2O2	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1349.	H2O2-	+ H2H3O+	= H2O2	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1351.	H2O2-	+ H2H3O+	= H2O2	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1353.	H2O2-	+ H2O2+	= H2O	+ H2O	+ O2	5.0E-07	-.50	3.0E-25	5
1355.	H2O-	+ O+	= O2	+ H2O		5.0E-07	-.50	3.0E-25	5
1357.	H2O-	+ O2+	= O3	+ H2O		5.0E-07	-.50	3.0E-25	5
1359.	H2O-	+ O+	= O3	+ O2	+ H2O	5.0E-07	-.50	3.0E-25	5
1361.	H2O-	+ H+	= OH	+ H2O		5.0E-07	-.50	3.0E-25	5
1363.	H2O-	+ OH+	= H2O2	+ H2O		5.0E-07	-.50	3.0E-25	5
1365.	H2O-	+ H2O+	= O	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1367.	H2O-	+ H3O+	= OH	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5
1369.	H2O-	+ OH+H3O+	= O	+ H2O	+ H2O	5.0E-07	-.50	3.0E-25	5

[illegible]15

TABLE II (cont)

NO.	CATEGORY 5. MUTUAL NEUTRALIZATION										A	B	C	REFERENCE	
	NO.	NO.	NO.	NO.	NO.	NO.	NO.	NO.	NO.	NO.					
1551.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1553.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1555.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1556.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1557.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1558.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1559.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1561.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1561.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1563.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1565.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1567.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1569.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1571.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1573.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1575.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1577.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1579.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1751.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1753.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1755.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1757.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1759.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1761.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1763.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1765.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1767.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1769.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1771.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1773.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1775.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1777.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1779.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1781.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1783.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1785.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1787.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1789.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1791.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1793.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1795.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1797.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1799.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1801.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1803.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1805.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1807.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1809.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1811.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1813.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1815.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1817.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1819.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1821.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1823.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1825.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1827.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1829.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1831.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1833.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1835.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1837.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1839.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1841.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1843.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1845.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1847.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
1849.	O-	49-00+	04	00	00	00	00	00	00	00	5.0E-07	50	50	50	50
 

TABLE II (cont)

NO.	CATEGORY 5. MUTUAL NEUTRALIZATION					A	B	C	REFERENCE
2071.	HO-	* O+	* HO	* O	* HO	5.0E-07	1.0E-07	1.0E-07	5
2073.	HO-	* O2+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2075.	HO-	* O4+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2077.	HO-	* N+	* O	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2079.	HO-	* N2+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2081.	HO-	* N3+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2083.	HO-	* N4+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2085.	HO-	* NO+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2087.	HO-	* N22+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2089.	HO-	* N2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2091.	HO-	* H+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2093.	HO-	* H2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2097.	HO-	* H2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2099.	HO-	* CO+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2101.	HO-	* CO2+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2103.	HO-	* O4H2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2105.	HO-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2107.	HO-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2109.	HO-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2111.	HO-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2113.	HO-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2115.	HO-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2117.	HO-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2121.	HO2-	* O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2123.	HO2-	* O2+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2125.	HO2-	* O4+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2127.	HO2-	* N+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2129.	HO2-	* N2+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2131.	HO2-	* N3+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2133.	HO2-	* N4+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2135.	HO2-	* NO+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2137.	HO2-	* N2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2139.	HO2-	* N2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2141.	HO2-	* H+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2143.	HO2-	* H2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2145.	HO2-	* H2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2147.	HO2-	* H2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2149.	HO2-	* CO+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2151.	HO2-	* CO2+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2153.	HO2-	* O4H2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2155.	HO2-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2157.	HO2-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2159.	HO2-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2161.	HO2-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2163.	HO2-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2165.	HO2-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2167.	HO2-	* H2O2O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2171.	HO-	* O+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2173.	HO-	* O2+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2175.	HO-	* O4+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2177.	HO-	* N+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2179.	HO-	* N2+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2181.	HO-	* N3+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5
2183.	HO-	* N4+	* HO	* HO	* HO	5.0E-07	1.0E-07	1.0E-07	5

TABLE II (cont)

NO.						A	B	C	REFERENCE
CATEGORY 5. MUTUAL NEUTRALIZATION									
2187.	HO+	+ NO ₂	+ O ₂	+ NO ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2189.	HO+	+ H ₂ O	+ O ₂	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2191.	HO+	+ H	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2193.	HO+	+ OH	+ O ₂	+ OH	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2195.	HO+	+ H ₂ O	+ O ₂	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2197.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2199.	HO+	+ CO ₂	+ O ₂	+ CO ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2201.	HO+	+ CO ₂	+ O ₂	+ CO ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2203.	HO+	+ OH+O ₂	+ O ₂	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2205.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2207.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2209.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2211.	HO+	+ H ₂ O	+ O ₂	+ O ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2213.	HO+	+ H ₂ O	+ NO ₃	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2215.	HO+	+ H ₂ O	+ NO ₃	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2217.	HO+	+ H ₂ O	+ NO ₃	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2221.	HO+	+ O	+ H	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2223.	HO+	+ O ₂	+ O ₂	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2225.	HO+	+ O ₂	+ O ₂	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2227.	HO+	+ N	+ H	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2229.	HO+	+ N ₂	+ N ₂	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2231.	HO+	+ N ₂	+ H	+ N ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2233.	HO+	+ N ₂	+ N ₂	+ N ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2235.	HO+	+ NO	+ NO	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2237.	HO+	+ NO ₂	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2239.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2241.	HO+	+ H	+ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2243.	HO+	+ O ₂	+ O ₂	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2245.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2247.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2249.	HO+	+ CO ₂	+ H	+ CO ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2251.	HO+	+ CO ₂	+ OH	+ CO ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2253.	HO+	+ OH+O ₂	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2255.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2257.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2259.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2261.	HO+	+ H ₂ O	+ O ₂	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2263.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2265.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2267.	HO+	+ H ₂ O	+ H ₂ O	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2271.	HO ₂	+ O	+ CO ₂	+ O ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2273.	HO ₂	+ O ₂	+ CO ₂	+ O ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2275.	HO ₂	+ O ₂	+ CO ₂	+ O ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2277.	HO ₂	+ N	+ CO ₂	+ NO	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2279.	HO ₂	+ N ₂	+ CO ₂	+ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2281.	HO ₂	+ N ₂	+ CO ₂	+ N ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2283.	HO ₂	+ N ₂	+ CO ₂	+ N ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2285.	HO ₂	+ NO	+ CO ₂	+ NO ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2287.	HO ₂	+ NO ₂	+ CO ₂	+ NO ₃	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2289.	HO ₂	+ H ₂ O	+ CO ₂	+ O ₂	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2291.	HO ₂	+ H	+ CO ₂	+ OH	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2293.	HO ₂	+ O ₂	+ CO ₂	+ H	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2295.	HO ₂	+ H ₂ O	+ CO ₂	+ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2297.	HO ₂	+ H ₂ O	+ CO ₂	+ OH	+ H ₂ O	5.0E-07	-50	3.0E-28	5
2299.	HO ₂	+ CO	+ CO ₂	+ H ₂ O	+ H ₂ O	5.0E-07	-50	3.0E-28	5

TABLE II (cont)

[illegible]

TABLE II (cont)

NO.				A	B	C	REFERENCE
CATEGORY 5. MUTUAL NEUTRALIZATION							
2495. OONO-	+ HONO+	= NO2	+ NO2	+ H2O	+ H2O	5.0E-07	- .50 3.0E-25 5
2497. OONO-	+ HONO+	= NO2	+ NO2	+ H2O	+ H2O	5.0E-07	- .50 3.0E-25 5
2093. HNO-	+ OH+	= NO	+ OH	+ H2O	+ H2O	5.0E-07	- .50 3.0E-25 5
CATEGORY 7. RADIATIVE ATTACHMENT							
173. E	+ O	= O-				1.3E-15	0.00 0 5
175. E	+ O2	= O2-				2.0E-19	0.00 0 5
177. E	+ O3	= O3-				1.0E-17	0.00 0 5
463. E	+ NO2	= NO2-				1.0E-17	0.00 0 5
1195. E	+ OH	= OH-				2.5E-15	- .25 0 5
CATEGORY 8. PHOTODETACHMENT							
601. O-		= E	+ O			1.5E+05	8.9E+05 2.0E+06 18
602. O2-		= E	+ O2			6.0E+04	3.1E+05 9.0E+05 18
603. O3-		= E	+ O3			7.0E+04	6.3E+05 2.1E+06 PAR. 11-E
604. O4-		= E	+ O2	+ O2		1.0E+05	9.4E+05 2.7E+06 8
605. NO2-		= E	+ NO2			8.1E+03	6.3E+04 2.9E+05 18
607. NO3-		= E	+ NO3			5.0E+02	7.0E+04 6.1E+05 PAR. 11-E
608. OH-		= E	+ OH			1.3E+05	1.1E+06 3.0E+06 18
609. CO3-		= E	+ O	+ CO2		1.0E+03	9.0E+04 7.3E+05 PAR. 11-E
610. CO4-		= E	+ O2	+ CO2		2.0E+05	1.0E+06 2.7E+06 PAR. 11-E
611. H2O-		= E	+ O2	+ H2O		2.0E+05	1.0E+06 2.7E+06 PAR. 11-E
612. H2O2-		= E	+ O2	+ H2O	+ H2O	1.1E+05	7.0E+05 2.3E+06 PAR. 11-E
613. HO-		= E	+ O	+ H2O		3.4E+04	4.0E+05 1.0E+06 PAR. 11-E
614. HO3-		= E	+ O3	+ H2O		1.1E+04	2.0E+05 1.3E+06 PAR. 11-E
615. HNO2-		= E	+ NO2	+ H2O		2.0E+03	1.5E+05 9.4E+05 PAR. 11-E
616. HNO4-		= E	+ O2	+ O2	+ H2O	8.1E+04	6.7E+05 2.3E+06 PAR. 11-E
617. HNO-		= E	+ NO	+ H2O		2.9E+05	1.2E+06 3.0E+06 PAR. 11-E
618. HNO3-		= E	+ NO3	+ H2O		2.1E+01	1.7E+04 2.0E+05 PAR. 11-E
619. HOH+		= E	+ OH	+ H2O		8.4E+04	6.0E+05 2.3E+06 PAR. 11-E
620. HCO3-		= E	+ O	+ CO2	+ H2O	4.0E+01	2.5E+04 3.4E+05 PAR. 11-E
621. HCO4-		= E	+ O2	+ CO2	+ H2O	5.7E+04	5.7E+05 2.0E+06 PAR. 11-E
CATEGORY 26. NEUTRAL PHOTODISSOCIATION							
850. O2		= O	+ O			3.0E-02	9.0E+00 1.4E+02 5
851. O3		= O	+ O2			3.0E+01	3.2E+02 1.1E+03 13
852. NO2		= O	+ NO			5.0E+02	7.0E+03 3.1E+04 14
854. H2O		= H	+ OH			3.3E+00	1.0E+03 2.0E+04 5
855. CO2		= CO	+ O			1.0E-01	5.0E+01 1.5E+03 5
856. O2		= O	+ O(1D)			2.3E+00	1.2E+03 2.9E+04 5
857. O3		= O2(OL)	+ O(1D)			1.2E+03	4.9E+04 3.4E+05 13
858. H2O		= O(1D)	+ H2			4.0E-01	7.7E+01 1.0E+03 14
859. HNO3		= OH	+ NO2			3.3E+01	3.0E+03 4.3E+04 14
860. NO2		= O(1D)	+ NO			2.7E+01	6.0E+03 1.0E+05 14
861. NO3		= NO	+ O2			6.3E+03	3.3E+04 7.0E+04 14
862. H2O2		= OH	+ O			5.0E+01	4.4E+03 4.0E+04 9
863. HNO2		= OH	+ NO			4.3E+01	6.4E+02 2.5E+03 14
865. H2O2		= OH	+ OH			2.7E+01	1.0E+03 1.4E+04 7
853. NO		= N	+ O			2.0E+00	3.3E+02 4.3E+03 19

TABLE II (cont)

NO.	A	B	C	REFERENCE
CATEGORY 22. NEGATIVE-ION PHOTODISSOCIATION				
675. CO3-	9.6E+03	9.6E+04	3.3E+05	17
CATEGORY 31. ELECTRONIC STATE PHOTOEXCITATION				
680. O	7.6E-05	3.4E-04	7.6E-04	6
681. O2	1.9E-05	4.7E-05	7.6E-05	5
682. O2	1.4E-03	5.0E-03	1.0E-02	5
CATEGORY 9. THREE-BODY ATTACHMENT				
107. E	4.6E-31	0.00	0	5
131. E	6.6E-29	-1.53	9023	PAR. 11-D
179. E	1.0E-30	0.00	0	PAR. 11-C-6
367. E	8.0E-31	0.00	0	5
465. E	1.5E-30	0.00	0	5
466. E	1.0E-30	0.00	0	PAR. 11-C-6
1197. E	1.0E-30	0.00	0	PAR. 11-C-6
2426. E	1.6E-29	-1.38	6602	PAR. 11-D
CATEGORY 10. COLLISIONAL DETACHMENT				
108. O2-	7.6E-12	1.38	4582	PAR. 11-D
132. O3-	2.3E-09	0.00	28000	5
180. O4-	1.3E-11	1.50	24024	PAR. 11-D
381. O4-	6.0E-11	1.40	11885	PAR. 11-D
468. NO2-	2.1E-11	1.54	278	PAR. 11-D
467. NO3-	6.2E-11	1.37	27821	PAR. 11-D
1198. O4-	5.0E-11	1.50	42880	PAR. 11-D
1503. NO-	8.2E-11	1.60	21234	PAR. 11-D
1503. NO2-	6.0E-11	1.40	25312	PAR. 11-C-7
1507. NO3-	6.0E-11	1.40	14240	PAR. 11-C-7
1511. NO2-	6.0E-11	1.40	31520	PAR. 11-C-7
1733. CO3-	6.0E-11	1.40	34815	PAR. 11-C-7
2001. NO-	6.0E-11	1.40	22884	PAR. 11-C-7
2003. NO2-	6.0E-11	1.40	40270	PAR. 11-C-7
2007. NO4-	6.0E-11	1.40	14253	PAR. 11-C-7
2009. NO3-	6.0E-11	1.40	21084	PAR. 11-C-7
2011. NO4-	6.0E-11	1.40	5739	PAR. 11-C-7
2427. O2-	6.0E-11	1.40	48178	PAR. 11-C-7
	6.0E-11	1.40	32532	PAR. 11-C-7
	6.0E-11	1.40	45049	PAR. 11-C-7
	6.0E-11	1.40	21424	PAR. 11-C-7
	2.0E-10	0.00	0	5
CATEGORY 11. DISSOCIATIVE ATTACHMENT				
112. E	1.7E-11	1.50	13200	5
114. E	3.1E-05	-1.05	42382	PAR. 11-D
133. E	9.0E-12	1.50	0	5
184. E	2.0E-31	-1.05	23143	PAR. 11-D
212. E	2.0E-04	-1.13	47310	PAR. 11-D

TABLE II (cont)

NO.				A	B	C	REFERENCE
CATEGORY 11. DISSOCIATIVE ATTACHMENT							
282. E	+ NO	= O-	+ N	8.1E-06	-1.17	58533	PAR. 11-D
284. E	+ NO2	= O-	+ NO	1.7E-04	-1.73	19184	PAR. 11-D
754. E	+ CO2	= O-	+ CO	2.1E-03	-1.63	46306	PAR. 11-D
832. E	+ NO2	= O2-	+ H	1.4E-05	-1.79	18123	PAR. 11-D
844. E	+ H2O	= O-	+ H2	1.3E-05	-1.86	41443	PAR. 11-D
846. E	+ H2O2	= O2-	+ H2	3.9E-05	-1.97	10621	PAR. 11-D
976. E	+ H2O2	= OH-	+ O	9.4E-06	-1.02	10289	PAR. 11-D
2430. E	+ O3	= O-	+ O2(DL)	1.6E-04	-1.50	6820	PAR. 11-D
2512. E	+ NO2 + H2O	= NO2-	+ N	1.4E-28	-1.70	38063	PAR. 11-D
CATEGORY 12. ASSOCIATIVE DETACHMENT							
111. O2-	+ O	= E	+ O3	1.3E-17	2.85	5889	PAR. 11-D
113. O-	+ O	= E	+ O2	2.0E-10	0.00	0	5
134. O-	+ O2	= E	+ O3	1.4E-17	3.00	4774	PAR. 11-D
183. O3-	+ O	= E	+ O2 + O2	1.0E-11	0.00	0	5
211. O2-	+ N	= E	+ NO2	5.0E-10	0.00	0	5
281. O-	+ N	= E	+ NO	2.0E-10	0.00	0	5
283. O-	+ NO	= E	+ NO2	2.2E-10	-1.56	0	5
753. O-	+ CO	= E	+ COE	6.0E-10	-1.32	0	5
871. O2-	+ H	= E	+ H2O2	1.0E-09	0.00	0	33
843. O-	+ H2	= E	+ H2O	6.9E-10	-1.19	0	5
845. O2-	+ H2	= E	+ H2O2	1.0E-09	0.00	0	33
975. OH-	+ O	= E	+ H2O2	2.0E-10	0.00	0	5
2429. O-	+ O2(DL)	= E	+ O3	3.0E-10	0.00	0	5
2511. NO2-	+ N	= E	+ NO2 + H2O	1.0E-10	0.00	0	PAR. 11-C-10
2513. H2O2-	+ N	= E	+ NO2 + H2O + H2O	1.0E-10	0.00	0	PAR. 11-C-10
CATEGORY 13. POSITIVE-ION CHARGE TRANSFER							
115. O+	+ O2	= O2+	+ O	2.0E-11	-1.40	0	5
116. O2+	+ O	= O+	+ O2	1.3E-11	-1.55	18043	PAR. 11-D
249. N+	+ NO	= NO+	+ N	8.0E-10	0.00	0	5
250. NO+	+ N	= N+	+ NO	4.8E-09	.30	61116	PAR. 11-D
251. N+	+ N2O	= N2O+	+ N	5.0E-10	0.00	0	33
252. N2O+	+ N	= N+	+ N2O	2.4E-10	-1.24	19033	PAR. 11-D
255. N2+	+ O2	= O2+	+ N2	5.0E-10	-1.80	0	5
256. O2+	+ N2	= N2+	+ O2	1.1E-09	-1.79	40821	PAR. 11-D
259. N2+	+ NO	= NO+	+ N2	3.3E-10	0.00	0	5
260. NO+	+ N2	= N2+	+ NO	2.4E-09	.21	73256	PAR. 11-D
269. NO2+	+ NO	= NO+	+ NO2	2.9E-10	0.00	0	5
270. NO+	+ NO2	= NO2+	+ NO	5.4E-10	.16	5983	PAR. 11-D
273. O+	+ NO	= NO+	+ O	1.3E-12	0.00	0	5
274. NO+	+ O	= O+	+ NO	2.7E-12	.05	50478	PAR. 11-D
279. O2+	+ NO	= NO+	+ O2	6.3E-10	0.00	0	5
280. NO+	+ O2	= O2+	+ NO	2.1E-09	.20	32435	PAR. 11-D
345. N+	+ O2	= O2+	+ N	2.8E-10	0.00	0	5
346. O2+	+ N	= N+	+ O2	5.1E-10	.09	28681	PAR. 11-D
349. N+	+ O2	= O2+	+ N2 + N2	3.0E-10	0.00	0	PAR. 11-C-8
350. O2+	+ N2	= N+	+ O2	8.8E-35	-1.78	33527	PAR. 11-D
469. O+	+ NO2	= NO2+	+ O	1.6E-09	0.00	0	5
470. NO2+	+ O	= O+	+ NO2	1.8E-09	-1.10	44494	PAR. 11-D
471. O+	+ N2O	= N2O+	+ O	2.2E-10	0.00	0	5

TABLE II (cont)

NO.			A	B	C	REFERENCE
CATEGORY 13. POSITIVE-ION CHARGE TRANSFER						
472. N_2O^+	+ O	= O+	3.6E-11	-.48	8395	PAR. 11-D
473. N^+	+ O	= O+	1.0E-12	0.00	0	5
474. O^+	+ N	= N+	2.9E-12	.24	10538	PAR. 11-D
475. N_2^+	+ O	= O+	6.6E-11	0.00	1945	5
476. O^+	+ N ₂	= N ₂ +	2.3E-10	.16	24724	PAR. 11-D
761. CO^+	+ CO	= CO+	9.0E-10	0.00	0	5
762. CO^+	+ N	= N+	7.9E-10	.14	6025	PAR. 11-D
763. N^+	+ CO ₂	= CO ₂ +	1.3E-09	0.00	0	5
764. CO_2^+	+ N	= N+	1.1E-09	.14	8911	PAR. 11-D
765. N_2^+	+ CO ₂	= CO ₂ +	9.0E-10	0.00	0	5
766. CO_2^+	+ N ₂	= N ₂ +	8.7E-10	.06	21051	PAR. 11-D
955. O_2^+	+ O ₂	= O ₂ +	2.0E-10	0.00	0	5
956. O_2^+	+ OH	= OH+	2.4E-10	-.12	12974	PAR. 11-D
959. H_2O^+	+ O ₂	= O ₂ +	2.0E-10	0.00	0	5
960. O_2^+	+ H ₂ O	= H ₂ O+	4.4E-10	-.04	6454	PAR. 11-D
961. H^+	+ H ₂ O	= H ₂ O+	3.0E-10	0.00	0	PAR. 11-C-8
962. H_2O^+	+ N ₂	= N ₂ +	4.0E-35	-.73	27173	PAR. 11-D
963. N_2^+	+ H ₂ O	= H ₂ O+	6.1E-10	0.00	0	31
964. H_2O^+	+ N ₂	= N ₂ +	6.0E-10	.06	34367	PAR. 11-D
965. H^+	+ O ₂	= O ₂ +	5.0E-10	0.00	0	33
966. O_2^+	+ H	= H+	2.6E-10	-.04	17828	PAR. 11-D
1199. O^+	+ H	= H+	6.6E-10	0.00	0	5
1200. H^+	+ O	= O+	7.7E-10	-.10	215	PAR. 11-D
1201. O^+	+ H ₂ O	= H ₂ O+	2.3E-09	0.00	0	5
1202. H_2O^+	+ O	= O+	6.6E-10	-.10	11569	PAR. 11-D
1203. N^+	+ H ₂ O	= H ₂ O+	2.6E-09	0.00	0	5
1204. H_2O^+	+ N	= N+	2.2E-09	.14	22227	PAR. 11-D
1207. H^+	+ NO	= NO+	1.9E-09	0.00	0	5
1208. NO^+	+ H	= H+	3.5E-09	.16	50263	PAR. 11-D
1279. H^+	+ H ₂ O	= H ₂ O+	3.0E-10	0.00	0	PAR. 11-C-8
1280. H_2O^+	+ H	= H+	7.5E-11	-0.00	11374	PAR. 11-D
1513. OH^+	+ H ₂ O	= H ₂ O+	3.0E-10	0.00	0	PAR. 11-C-8
1514. H_2O^+	+ OH	= OH+	1.6E-10	-.08	6520	PAR. 11-D
1515. O^+	+ OH	= OH+	3.0E-10	0.00	0	PAR. 11-C-8
1516. OH^+	+ O	= O+	1.6E-10	-.03	5068	PAR. 11-D
1517. H^+	+ OH	= OH+	3.0E-10	0.00	0	PAR. 11-C-8
1518. OH^+	+ H	= H+	1.4E-10	.08	4854	PAR. 11-D
1637. $\text{OH}^+\text{H}_2\text{O}^+$	+ NO	= NO+	3.0E-10	0.00	0	PAR. 11-C-8
1639. $\text{OH}^+\text{H}_2\text{O}^+$	+ NO ₂	= NO ₂ +	3.0E-10	0.00	0	PAR. 11-C-8
1641. H_2O_2^+	+ NO ₂	= NO ₂ +	3.0E-10	0.00	0	PAR. 11-C-8
1643. N_2^+	+ NO	= NO+	3.0E-10	0.00	0	PAR. 11-C-8
1645. N_2^+	+ NO ₂	= NO ₂ +	3.0E-10	0.00	0	PAR. 11-C-8
1647. O_2^+	+ NO ₂	= NO ₂ +	3.0E-10	0.00	0	PAR. 11-C-8
1649. O_2^+	+ NO ₂	= NO ₂ +	6.6E-10	0.00	0	5
1650. NO_2^+	+ O ₂	= O ₂ +	1.2E-09	.04	26452	PAR. 11-D
1651. H_2O^+	+ NO	= NO+	3.0E-10	0.00	0	PAR. 11-C-8
1652. NO^+	+ H ₂ O	= H ₂ O+	2.2E-09	.16	36889	PAR. 11-D
1653. H_2O^+	+ NO ₂	= NO ₂ +	3.0E-10	0.00	0	PAR. 11-C-8
1654. NO_2^+	+ H ₂ O	= H ₂ O+	1.2E-09	0.00	32906	PAR. 11-D
1655. N_2O^+	+ NO	= NO+	3.0E-10	0.00	0	PAR. 11-C-8
1656. NO^+	+ N ₂ O	= N ₂ O+	3.9E-09	.94	42083	PAR. 11-D
1657. N_2O^+	+ NO ₂	= NO ₂ +	3.0E-10	0.00	0	PAR. 11-C-8
1658. NO_2^+	+ N ₂ O	= N ₂ O+	2.1E-09	.38	36100	PAR. 11-D
1659. N_2O^+	+ O ₂	= O ₂ +	3.0E-10	0.00	0	PAR. 11-C-8
1660. O_2^+	+ N ₂ O	= N ₂ O+	1.2E-09	.34	9548	PAR. 11-D

TABLE II (cont.)

NO.	CATEGORY 13. POSITIVE-ION CHARGE TRANSFER				A	B	C	REFERENCE
1661.	NEO*	+ NEO	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1662.	NEO*	+ NEO	+ NE		5.3E-10	0.38	3194	PAR. 11-D
1663.	NO*	+ NO	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1664.	OH*	+ OH	+ NE		1.2E-09	0.08	48409	PAR. 11-D
1665.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1666.	NO*	+ NO	+ NE		6.4E-10	-0.08	39426	PAR. 11-D
1667.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1668.	NEO*	+ NEO	+ NE		9.2E-11	-0.46	3326	PAR. 11-D
1669.	NEO*	+ NEO	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1670.	NEO*	+ NEO	+ NE		3.0E-10	0.00	44280	PAR. 11-D
1671.	H*	+ H	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1672.	NEO*	+ NEO	+ NE		4.3E-11	-0.38	8180	PAR. 11-D
1673.	NEO*	+ NEO	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1674.	OH*	+ OH	+ NE		9.0E-10	0.14	55133	PAR. 11-D
1675.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1676.	N*	+ N	+ NE		4.6E-10	-0.21	15707	PAR. 11-D
1677.	H*	+ H	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1678.	N*	+ N	+ NE		9.5E-10	0.14	10853	PAR. 11-D
1679.	NO*	+ NO	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1680.	NO*	+ NO	+ NE		3.0E-34	-0.58	86052	PAR. 11-D
1681.	NO*	+ NO	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1682.	NO*	+ NO	+ NE		1.6E-34	-0.73	60078	PAR. 11-D
1683.	NEO*	+ NEO	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1684.	OH*	+ OH	+ NE		2.3E-35	-1.11	23879	PAR. 11-D
1685.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1686.	OH*	+ OH	+ NE		7.5E-35	-0.66	20652	PAR. 11-D
1687.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1688.	OH*	+ OH	+ NE		1.4E-34	-0.63	19694	PAR. 11-D
1689.	OH*	+ OH	+ NE		1.6E-34	-0.73	15759	PAR. 11-D
1690.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1691.	OH*	+ OH	+ NE		4.0E-35	-0.87	4946	PAR. 11-D
1692.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1693.	NEO*	+ NEO	+ NE		1.2E-09	0.06	67273	PAR. 11-D
1694.	NEO*	+ NEO	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1695.	NEO*	+ NEO	+ NE		1.7E-10	-0.32	31173	PAR. 11-D
1696.	NEO*	+ NEO	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1697.	OH*	+ OH	+ NE		5.4E-10	0.13	27847	PAR. 11-D
1698.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1699.	OH*	+ OH	+ NE		1.2E-09	0.06	28394	PAR. 11-D
1700.	OH*	+ OH	+ NE		1.4E-10	0.00	0	PAR. 11-C-8
1701.	OH*	+ OH	+ NE		4.0E-10	0.10	4614	PAR. 11-D
1702.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1703.	OH*	+ OH	+ NE		2.4E-09	0.16	55091	PAR. 11-D
1704.	OH*	+ OH	+ NE		1.0E-10	0.00	0	PAR. 11-D
1705.	OH*	+ OH	+ NE		3.5E-10	0.10	1728	PAR. 11-D
1706.	OH*	+ OH	+ NE		5.0E-11	0.04	0	PAR. 11-D
1707.	OH*	+ OH	+ NE		1.1E-10	0.00	0	PAR. 11-D
1708.	OH*	+ OH	+ NE		1.2E-10	0.00	0	PAR. 11-D
1709.	OH*	+ OH	+ NE		9.5E-10	0.16	52205	PAR. 11-D
1710.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1711.	OH*	+ OH	+ NE		1.2E-09	-0.00	46222	PAR. 11-D
1712.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8
1713.	OH*	+ OH	+ NE		3.0E-10	-0.00	13316	PAR. 11-D
1714.	OH*	+ OH	+ NE		3.0E-10	0.00	0	PAR. 11-C-8

TABLE II (cont)

NO.				A	B	C	REFERENCE
CATEGORY 13. POSITIVE-ION CHARGE TRANSFER							
1822.	NEO+ + CO2	= CO2+ + NEO		1.7E-10	-.38	10122	PAR. 11-D
1823.	CO2+ + OH	= OH+ + CO2		3.0E-10	0.00	0	PAR. 11-C-B
1824.	OH+ + CO2	= CO2+ + OH		5.6E-10	.08	6795	PAR. 11-D
1825.	CO2+ + H	= H+ + CO2		3.0E-10	0.00	0	PAR. 11-C-B
1826.	H+ + CO2	= CO2+ + H		1.2E-09	0.00	1942	PAR. 11-D
1827.	CO+ + NO2	= NO2+ + CO		3.0E-10	0.00	0	PAR. 11-C-B
1828.	NO2+ + CO	= CO+ + NO2		1.2E-09	0.00	49108	PAR. 11-D
1829.	CO+ + O2	= O2+ + CO		3.0E-10	0.00	0	PAR. 11-C-B
1830.	O2+ + CO	= CO+ + O2		6.6E-10	-.04	22856	PAR. 11-D
1831.	CO+ + H2O	= H2O+ + CO		3.0E-10	0.00	0	PAR. 11-C-B
1832.	H2O+ + CO	= CO+ + H2O		3.0E-10	0.00	16202	PAR. 11-D
1833.	CO+ + NEO	= NEO+ + CO		3.0E-10	0.00	0	PAR. 11-C-B
1834.	NEO+ + CO	= CO+ + NEO		1.7E-10	-.38	13008	PAR. 11-D
1835.	CO+ + OH	= OH+ + CO		3.0E-10	0.00	0	PAR. 11-C-B
1836.	OH+ + CO	= CO+ + OH		5.6E-10	.08	9692	PAR. 11-D
1837.	CO+ + H	= H+ + CO		3.0E-10	0.00	0	PAR. 11-C-B
1838.	H+ + CO	= CO+ + H		1.2E-09	0.00	4828	PAR. 11-D
1839.	CO+ + CO2	= CO2+ + CO		3.0E-10	0.00	0	PAR. 11-C-B
1840.	CO2+ + CO	= CO+ + CO2		3.0E-10	0.00	2886	PAR. 11-D
1841.	NH+ + CO2	= CO2+ + NH	+ NE	3.0E-10	0.00	0	PAR. 11-C-B
1842.	CO2+ + NE	= NE+ + CO2	+ NE	4.0E-35	-.73	13895	PAR. 11-D
1843.	NH+ + CO	= CO+ + NH	+ NE	3.0E-10	0.00	0	PAR. 11-C-B
1844.	CO+ + NE	= NE+ + CO		4.0E-35	-.73	10970	PAR. 11-D
1845.	NE+ + CO	= CO+ + NE		3.0E-10	0.00	0	PAR. 11-C-B
1846.	CO+ + NE	= NE+ + CO		2.9E-10	.05	18165	PAR. 11-D
CATEGORY 14. POSITIVE ION-ATOM INTERCHANGE							
9.	NG+ + N	= N2+ + NG		2.0E-10	0.00	0	32
10.	NE+ + N2	= N3+ + NE		7.4E-11	-.46	65035	PAR. 11-D
15.	NH+ + N	= N3+ + NH		5.0E-11	0.00	0	32
16.	NG+ + N2	= N4+ + NG		1.0E-10	.09	40017	PAR. 11-D
117.	O+ + O3	= O2+ + O2		1.0E-10	0.00	0	33
118.	O2+ + O2	= O+ + O3		1.0E-11	.29	65209	PAR. 11-D
149.	O4+ + O	= O2+ + O3		3.0E-10	0.00	0	5
150.	O2+ + O3	= O4+ + O		2.2E-10	-.105	7081	PAR. 11-D
205.	O2+ + N	= NO+ + O		1.8E-10	0.00	0	5
206.	NO+ + O	= O2+ + N		1.8E-10	.10	48576	PAR. 11-D
223.	N2+ + O	= NO+ + N		7.0E-11	0.00	0	5
224.	NO+ + N	= N2+ + O		1.3E-10	.17	35521	PAR. 11-D
245.	N+ + O2	= NO+ + O		2.8E-10	0.00	0	5
246.	NO+ + O	= N+ + O2		4.9E-10	.19	77257	PAR. 11-D
247.	N+ + O3	= NO+ + O2		5.0E-10	0.00	0	33
248.	NO+ + O2	= N+ + O3		2.0E-10	.63	124424	PAR. 11-D
253.	N+ + NO2	= NO+ + NO		5.0E-10	0.00	0	33
254.	NO+ + NO	= N+ + NO2		1.8E-10	.30	100485	PAR. 11-D
257.	NE+ + O3	= O2+ + O	+ NE	1.0E-10	0.00	0	33
258.	O2+ + O	= NE+ + O3		9.8E-36	-.02	28618	PAR. 11-D
271.	O+ + NE	= NO+ + N		2.8E-12	.50	500	23
272.	NO+ + N	= O+ + NE		1.4E-12	.50	13242	PAR. 11-D
275.	O+ + NEO	= NO+ + NO		2.3E-10	0.00	0	5
276.	NO+ + NO	= O+ + NEO		5.4E-12	.29	68949	PAR. 11-D
277.	O+ + NO2	= NO+ + O2		5.0E-10	0.00	0	33
278.	NO+ + O2	= O+ + NO2		2.1E-10	.17	73686	PAR. 11-D

TABLE II (cont)

NO.				A	B	C	REFERENCE
CATEGORY 14. POSITIVE ION-ATOM INTERCHANGE							
347. NO ⁺	+ H ₂ O	= NO ₂ ⁺	+ N ₂	5.0E-11	0.00	0	33
348. NO ₂ ⁺	+ H ₂	= NO ⁺	+ H ₂ O	2.2E-11	.12	10774	PAR. 11-D
351. N ₃ ⁺	+ O ₂	= NO ⁺	+ O	1.0E-10	0.00	0	5
352. NO ⁺	+ O	= N ₃ ⁺	+ O ₂	1.3E-35	-.77	42186	PAR. 11-D
477. O ₂ ⁺	+ N ₂	= NO ⁺	+ NO	1.0E-16	0.00	0	5
478. NO ⁺	+ NO	= O ₂ ⁺	+ N ₂	2.3E-17	.04	10841	PAR. 11-D
481. NO ⁺	+ O ₃	= NO ₂ ⁺	+ O ₂	1.0E-14	0.00	0	5
482. NO ₂ ⁺	+ O ₂	= NO ⁺	+ O ₃	6.9E-15	.17	17975	PAR. 11-D
507. N ₂ ⁺	+ O ₂	= NO ⁺	+ NO	1.0E-17	0.00	0	5
509. NO ⁺	+ NO	= N ₂ ⁺	+ O ₂	4.9E-18	.06	51662	PAR. 11-D
735. O ⁺	+ CO ₂	= O ₂ ⁺	+ CO	1.1E-09	0.00	0	5
736. O ₂ ⁺	+ CO	= O ⁺	+ CO ₂	2.9E-11	.10	14130	PAR. 11-D
857. H ₃ NO ⁺	+ H ₂ O	= H ₂ NO ⁺	+ HNO ₂	2.9E-06	0.00	3146	5, PAR. 11-F-1
888. H ₂ NO ⁺	+ HNO ₂	= H ₃ NO ⁺	+ H ₂ O	1.1E-08	-2.60	0	PAR. 11-D
885. O ⁺	+ H ₂ O	= H ₂ O ⁺	+ O ₂	1.5E-09	0.00	0	5
886. H ₂ O ⁺	+ O ₂	= O ⁺	+ H ₂ O	9.2E-12	-1.59	4930	PAR. 11-D
897. H ₂ O ⁺	+ H ₂ O	= H ₃ O ⁺	+ OH	2.9E-04	0.00	4253	5, PAR. 11-F-1
898. H ₃ O ⁺	+ OH	= H ₂ O ⁺	+ H ₂ O	1.6E-27	.95	0	PAR. 11-D
899. H ₂ O ⁺	+ H ₂ O	= OH ₂ O ⁺	+ O ₂	1.0E-09	0.00	0	5
900. OH ₂ O ⁺	+ O ₂	= H ₂ O ⁺	+ H ₂ O	6.4E-09	.24	9359	PAR. 11-D
909. OH ₂ O ⁺	+ H ₂ O	= H ₃ O ⁺	+ OH	1.4E-09	0.00	0	5
910. H ₃ O ⁺	+ OH	= OH ₂ O ⁺	+ H ₂ O	2.1E-11	-1.46	4503	PAR. 11-D
949. H ₂ O ⁺	+ H ₂ O	= H ₃ O ⁺	+ OH	1.8E-09	0.00	0	5
950. H ₃ O ⁺	+ OH	= H ₂ O ⁺	+ H ₂ O	3.8E-09	.02	12303	PAR. 11-D
951. O ⁺	+ H ₂ O	= H ₃ O ⁺	+ O	1.5E-09	0.00	0	25
952. H ₃ O ⁺	+ O	= O ⁺	+ H ₂ O	7.7E-09	.32	27284	PAR. 11-D
953. H ₂ O ⁺	+ H ₂	= H ₃ O ⁺	+ H	1.4E-09	0.00	0	24
954. H ₃ O ⁺	+ H	= H ₂ O ⁺	+ H ₂	6.0E-09	.39	19761	PAR. 11-D
957. O ⁺	+ H ₂	= H ₂ O ⁺	+ H	1.5E-09	0.00	0	24
958. H ₂ O ⁺	+ H	= O ⁺	+ H ₂	1.7E-09	.29	13979	PAR. 11-D
957. H ⁺	+ O ₂	= O ⁺	+ OH	5.0E-10	0.00	8622	33, PAR. 11-F-1
968. O ⁺	+ OH	= H ⁺	+ O ₂	2.7E-11	.13	0	PAR. 11-D
1209. H ₂ O ⁺	+ NO	= NO ⁺	+ H ₂ O	1.0E-10	0.00	0	5
1210. NO ⁺	+ H ₂ O	= H ₂ O ⁺	+ NO	1.9E-33	.70	22333	PAR. 11-D
1227. O ⁺	+ H ₂	= O ⁺	+ H	2.0E-09	0.00	0	5
1228. O ⁺	+ H	= O ⁺	+ H ₂	4.9E-10	-.03	4057	PAR. 11-D
1639. NO ⁺	+ H ₂ O	= OH ₂ O ⁺	+ NO	8.8E-34	.45	12974	PAR. 11-D
1640. NO ₂ ⁺	+ H ₂ O	= OH ₂ O ⁺	+ NO ₂	4.8E-34	.29	8991	PAR. 11-D
1642. NO ₂ ⁺	+ H ₂ O	= H ₂ O ⁺	+ NO ₂	3.1E-33	.94	16349	PAR. 11-D
1644. NO ⁺	+ N ₂	= N ₃ ⁺	+ NO	1.5E-34	-.66	26045	PAR. 11-D
1646. NO ₂ ⁺	+ N ₂	= N ₃ ⁺	+ NO ₂	7.6E-35	-.82	20062	PAR. 11-D
1648. NO ₂ ⁺	+ O ₂	= O ₄ ⁺	+ NO ₂	1.9E-35	-1.05	21330	PAR. 11-D
1901. O ⁺	+ NO	= NO ⁺	+ O ₂	5.0E-10	0.00	0	5
1902. NO ⁺	+ O ₂	= O ⁺	+ NO	5.8E-35	-.89	27313	PAR. 11-D
2419. N ₂ ⁺	+ O	= NO ⁺	+ N(2D)	7.0E-11	0.00	0	5
2420. NO ⁺	+ N(2D)	= N ₂ ⁺	+ O	5.3E-11	.16	7642	PAR. 11-D
CATEGORY 15. NEGATIVE-ION CHARGE TRANSFER							
109. O ₂ ⁻	+ O	= O ⁻	+ O ₂	3.0E-10	0.00	0	PAR. 11-C-8
110. O ⁻	+ O ₂	= O ₂ ⁻	+ O	6.2E-10	.15	11985	PAR. 11-D
135. O ⁻	+ O ₃	= O ₃ ⁻	+ O	5.3E-10	0.00	0	5
136. O ₃ ⁻	+ O	= O ⁻	+ O ₃	1.9E-10	-.03	7046	PAR. 11-D
137. O ₂ ⁻	+ O ₃	= O ₃ ⁻	+ O ₂	4.0E-10	0.00	0	5

TABLE II (cont)

NO.					A	B	C	REFERENCE
CATEGORY 15. NEGATIVE-ION CHARGE TRANSFER								
138. O3-	+ O2		= O2-	+ O3	3.0E-10	.12	19032	PAR. 11-D
141. O4-	+ O3		= O3-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
142. O3-	+ O2	+ O2	= O4-	+ O3	5.2E-35	-1.05	12198	PAR. 11-D
287. O-	+ NO2		= NO2-	+ O	1.2E-09	0.00	0	5
288. NO2-	+ O		= O-	+ NO2	1.4E-09	-.17	10644	PAR. 11-D
288. O2-	+ NO2		= NO2-	+ O2	8.0E-10	0.00	0	5
290. NO2-	+ O2		= O2-	+ NO2	2.0E-09	-.02	22629	PAR. 11-D
343. O3-	+ NO2		= NO2-	+ O3	2.6E-10	0.00	0	5
344. NO2-	+ O3		= O3-	+ NO2	9.2E-10	-.13	3588	PAR. 11-D
365. O4-	+ NO2		= NO2-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
365. NO2-	+ O2	+ O2	= O4-	+ NO2	1.7E-35	-1.18	15795	PAR. 11-D
369. NO-	+ O2		= O2-	+ NO	5.0E-10	0.00	0	5
370. O2-	+ NO		= NO-	+ O2	3.3E-10	-.16	4714	PAR. 11-D
729. CO4-	+ NO2		= NO2-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
730. NO2-	+ O2	+ CO2	= CO4-	+ NO2	9.6E-34	-1.26	13362	PAR. 11-D
1211. OH-	+ NO2		= NO2-	+ OH	1.0E-09	0.00	0	5
1212. NO2-	+ OH		= OH-	+ NO2	5.1E-10	-.23	6387	PAR. 11-D
1519. O2-	+ OH		= OH-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
1520. OH-	+ O2		= O2-	+ OH	1.4E-09	.22	16242	PAR. 11-D
1521. O4-	+ OH		= OH-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
1522. OH-	+ O2	+ O2	= O4-	+ OH	3.4E-35	-.95	9408	PAR. 11-D
1523. NO2-	+ O		= O-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
1524. O-	+ O2	+ H2O	= NO2-	+ O	2.1E-33	.57	2738	PAR. 11-D
1525. NO2-	+ OH		= OH-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
1526. OH-	+ O2	+ H2O	= NO2-	+ OH	5.0E-33	.64	8894	PAR. 11-D
1527. NO2-	+ O3		= O3-	+ O2	3.0E-10	0.00	0	5
1528. O3-	+ O2	+ H2O	= NO2-	+ O3	7.7E-34	.94	9784	PAR. 11-D
1529. O-	+ OH		= OH-	+ O	3.0E-10	0.00	0	PAR. 11-C-8
1530. OH-	+ O		= O-	+ OH	7.0E-10	.07	4236	PAR. 11-D
1533. H2O2-	+ O3		= O3-	+ O2	3.4E-10	0.00	0	5
1535. OH-	+ O3		= O3-	+ OH	3.0E-10	0.00	0	PAR. 11-C-8
1536. O3-	+ OH		= OH-	+ O3	4.6E-11	-.10	2790	PAR. 11-D
1847. CO4-	+ OH		= OH-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
1848. OH-	+ O2	+ CO2	= CO4-	+ OH	1.9E-33	-1.02	8975	PAR. 11-D
1849. CO4-	+ O3		= O3-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
1850. O3-	+ O2	+ CO2	= CO4-	+ O3	2.9E-34	-1.12	9785	PAR. 11-D
1851. CO4-	+ NO3		= NO3-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
1852. NO3-	+ O2	+ CO2	= CO4-	+ NO3	1.2E-33	-1.12	28531	PAR. 11-D
1903. NO-	+ O		= O-	+ NO	3.0E-10	0.00	0	PAR. 11-C-8
1904. O-	+ NO		= NO-	+ O	4.0E-10	-.00	18889	PAR. 11-D
1905. NO-	+ OH		= OH-	+ NO	3.0E-10	0.00	0	PAR. 11-C-8
1906. OH-	+ NO		= NO-	+ OH	9.4E-10	.06	20925	PAR. 11-D
1907. NO-	+ O3		= O3-	+ NO	3.0E-10	0.00	0	PAR. 11-C-8
1908. O3-	+ NO		= NO-	+ O3	1.9E-10	-.04	23745	PAR. 11-D
1909. NO-	+ NO2		= NO2-	+ NO	3.0E-10	0.00	0	PAR. 11-C-8
1910. NO2-	+ NO		= NO-	+ NO2	4.6E-10	-.17	27343	PAR. 11-D
1911. NO-	+ NO3		= NO3-	+ NO	3.0E-10	0.00	0	PAR. 11-C-8
1912. NO3-	+ NO		= NO-	+ NO3	5.6E-10	-.04	42611	PAR. 11-D
1913. O2-	+ NO3		= NO3-	+ O2	5.0E-10	0.00	0	5
1914. NO3-	+ O2		= O2-	+ NO3	1.9E-09	.12	37898	PAR. 11-D
1915. O4-	+ O		= O-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
1916. O-	+ O2	+ O2	= O4-	+ O	1.9E-35	-1.02	5152	PAR. 11-D
1917. OH-	+ NO3		= NO3-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8
1918. NO3-	+ O2	+ O2	= OH-	+ NO3	2.1E-35	-1.05	31094	PAR. 11-D
1919. NO2-	+ NO2		= NO2-	+ O2	3.0E-10	0.00	0	PAR. 11-C-8

TABLE II (cont)

TABLE II (cont)

NO	4	8	C	REFERENCE
CATEGORY 18. NEGATIVE ION-ATOM INTERACTION				
371	• • • • •	• • • • •	0	5
372	• • • • •	• • • • •	1672	PAR. 11-0
443	• • • • •	• • • • •	0	5
709	• • • • •	• • • • •	3788	PAR. 11-0
710	• • • • •	• • • • •	0	5
711	• • • • •	• • • • •	4043	PAR. 11-0
712	• • • • •	• • • • •	0	5
713	• • • • •	• • • • •	24082	PAR. 11-0
714	• • • • •	• • • • •	0	5
715	• • • • •	• • • • •	23512	PAR. 11-0
716	• • • • •	• • • • •	0	5
717	• • • • •	• • • • •	27321	PAR. 11-0
718	• • • • •	• • • • •	3350	33
719	• • • • •	• • • • •	6038	PAR. 11-0
720	• • • • •	• • • • •	0	5
721	• • • • •	• • • • •	2433	PAR. 11-0
722	• • • • •	• • • • •	0	5
723	• • • • •	• • • • •	21700	PAR. 11-0
724	• • • • •	• • • • •	0	33
725	• • • • •	• • • • •	13808	PAR. 11-0
726	• • • • •	• • • • •	0	33
727	• • • • •	• • • • •	60882	PAR. 11-0
1275	• • • • •	• • • • •	0	5
1276	• • • • •	• • • • •	2414	PAR. 11-0
1277	• • • • •	• • • • •	0	5
1278	• • • • •	• • • • •	30888	PAR. 11-0
1279	• • • • •	• • • • •	0	5
1280	• • • • •	• • • • •	28011	PAR. 11-0
1281	• • • • •	• • • • •	0	5
1282	• • • • •	• • • • •	19	PAR. 11-0
1283	• • • • •	• • • • •	0	PAR. 11-C-0
1284	• • • • •	• • • • •	2619	PAR. 11-0
1285	• • • • •	• • • • •	0	5
1286	• • • • •	• • • • •	21719	PAR. 11-0
1287	• • • • •	• • • • •	0	5
1288	• • • • •	• • • • •	4616	PAR. 11-0
CATEGORY 19. THREE-BODY POSITIVE-ION-NEUTRAL ASSOCIATION				
5	• • • • •	• • • • •	1.0E-29	-1.00 0 5, PAR. 11-F-3
11	• • • • •	• • • • •	5.0E-29	-1.00 0 5, PAR. 11-F-3
25	• • • • •	• • • • •	1.0E-29	-1.00 0 2, PAR. 11-F-3
27	• • • • •	• • • • •	1.0E-29	-1.00 0 2, PAR. 11-F-3
147	• • • • •	• • • • •	2.0E-30	-1.00 0 5, PAR. 11-F-3
148	• • • • •	• • • • •	5.4E-29	-1.00 0 5, PAR. 11-F-3
149	• • • • •	• • • • •	1.0E-29	-1.00 0 2, PAR. 11-F-3
150	• • • • •	• • • • •	5.0E-29	-1.00 0 2, PAR. 11-F-3
151	• • • • •	• • • • •	1.0E-29	-1.00 0 2, PAR. 11-F-3
152	• • • • •	• • • • •	1.0E-29	-1.00 0 5, PAR. 11-F-3
153	• • • • •	• • • • •	1.1E-27	-1.00 0 5, PAR. 11-F-3
154	• • • • •	• • • • •	1.0E-27	-1.00 0 5, PAR. 11-F-3
155	• • • • •	• • • • •	2.3E-27	-1.00 0 5, PAR. 11-F-3
156	• • • • •	• • • • •	3.7E-27	-1.00 0 5, PAR. 11-F-3
157	• • • • •	• • • • •	5.4E-25	-1.70 0 PAR. 11-C-9, 11-F-3

TABLE II (cont)

A				A	B	C	REFERENCE
CATEGORY 19. THREE-BODY POSITIVE-ION-NEUTRAL ASSOCIATION							
1213. O ²⁺	• H ₂ O	• M	• H ₂ O ⁺	• M	1.9E-26	-1.00	0 5, PAR. 11-F-3
1277. H ⁺	• H ₂ O	• M	• H ₃ O ⁺	• M	1.0E-27	0.00	0 PAR. 11-C-9, 11-F-3
1539. H ₂ CO ⁺	• H ₂ O	• M	• H ₃ CO ⁺	• M	2.4E-27	-1.00	0 5, PAR. 11-F-3
CATEGORY 20. POSITIVE-ION COLLISIONAL DISSOCIATION							
6. N ₂ ⁺	• M		• N ⁺	• N ₂	• M	2.2E-04	-0.4 35071 PAR. 11-D, 11-F-3
12. N ₂ ⁺	• M		• N ₂ ⁺	• N ₂	• M	3.5E-04	-0.22 7195 PAR. 11-D, 11-F-3
26. N ₂ ⁺	• M		• N ⁺	• N	• M	4.0E-05	-0.50 101106 PAR. 11-D, 11-F-3
28. N ₂ ⁺	• M		• N ₂ ⁺	• N	• M	1.9E-04	-0.13 47211 PAR. 11-D, 11-F-3
148. O ⁺	• M		• O ₂ ⁺	• O ₂	• M	7.0E-05	.08 5122 PAR. 11-D, 11-F-3
485. NO ⁺	• M	• M	• O ⁺	• N ₂	• M	3.0E-29	-1.00 12742 PAR. 11-D, 11-F-3
490. NO ⁺	• M		• N ⁺	• O	• M	9.5E-05	-0.34 136527 PAR. 11-D, 11-F-3
492. NO ₂ ⁺	• M		• NO ⁺	• O	• M	7.0E-04	-0.80 30178 PAR. 11-D, 11-F-3
494. NO ⁺	• M		• NO ⁺	• N	• M	9.5E-05	-1.40 15057 PAR. 11-D, 11-F-3
852. H ₂ O ⁺	• M		• NO ⁺	• H ₂ O	• M	3.4E-05	-1.70 10103 PAR. 11-D, 11-F-3
854. H ₂ O ⁺	• M		• H ₂ O ⁺	• H ₂ O	• M	3.1E-01	.54 11220 PAR. 11-D, 11-F-3
856. H ₂ O ⁺	• M		• H ₂ O ⁺	• H ₂ O	• M	6.8E-01	.54 8953 PAR. 11-D, 11-F-3
920. H ₂ CO ⁺	• M		• H ₂ CO ⁺	• H ₂ O	• M	5.9E-01	.54 11220 PAR. 11-D, 11-F-3
922. H ₂ CO ⁺	• M		• H ₂ CO ⁺	• H ₂ O	• M	6.7E-05	-2.77 18115 PAR. 11-D, 11-F-3
948. O ⁺ CO ⁺	• M		• H ₂ CO ⁺	• O ₄	• M	6.5E-01	-1.00 13612 5, PAR. 11-F-1, 11-F-3
1214. H ₂ O ⁺	• M		• O ₂ ⁺	• H ₂ O	• M	3.3E-05	-1.50 10102 PAR. 11-D, 11-F-3
1278. H ₂ O ⁺	• M		• H ⁺	• H ₂ O	• M	7.8E-04	.89 83100 PAR. 11-D, 11-F-3
1540. H ₂ CO ⁺	• M		• H ₂ CO ⁺	• H ₂ O	• M	1.0E+00	.54 8755 PAR. 11-D, 11-F-3
CATEGORY 21. RADIATION-STABILIZED NEGATIVE-ION-NEUTRAL ASSOCIATION							
2533. O ⁻	• O ₂		• O ₃ ⁻			1.0E-17	0.00 0 5
CATEGORY 23. THREE-BODY NEGATIVE-ION-NEUTRAL ASSOCIATION							
139. O ₂ ⁻	• O ₂	• M	• O ₄ ⁻	• M		3.5E-31	-1.00 0 5
187. O ⁻	• O ₂	• M	• O ₃ ⁻	• M		1.1E-30	-1.00 0 5
495. O ⁻	• O ₂	• M	• NO ₂ ⁻	• M		1.0E-29	-1.00 0 5
741. O ₂ ⁻	• CO ₂	• M	• CO ₄ ⁻	• M		2.0E-29	-1.00 0 5
1229. O ₂ ⁻	• H ₂ O	• M	• H ₂ O ₂ ⁻	• M		3.0E-28	-1.00 0 5
1341. O ⁻	• H ₂ O	• M	• H ₂ O ⁻	• M		1.0E-28	-1.00 0 5
1343. O ₃ ⁻	• H ₂ O	• M	• H ₂ O ₃ ⁻	• M		2.1E-28	-1.00 0 5
1345. H ₂ O ₂ ⁻	• H ₂ O	• M	• H ₂ O ₂ ⁻	• M		4.0E-28	-1.00 0 5
1751. O ⁻	• CO ₂	• M	• CO ₃ ⁻	• M		8.0E-29	-1.00 0 5
1945. NO ₂ ⁻	• H ₂ O	• M	• H ₂ NO ₂ ⁻	• M		1.3E-28	-1.00 0 5
2051. O ₄ ⁻	• H ₂ O	• M	• H ₂ O ₄ ⁻	• M		1.0E-28	-1.00 0 PAR. 11-C-9
2053. NO ⁻	• H ₂ O	• M	• H ₂ NO ⁻	• M		1.0E-28	-1.00 0 PAR. 11-C-9
2055. NO ₃ ⁻	• H ₂ O	• M	• H ₂ NO ₃ ⁻	• M		1.0E-28	-1.00 0 PAR. 11-C-9
2057. O ₄ ⁻	• H ₂ O	• M	• H ₂ O ₄ ⁻	• M		1.0E-28	-1.00 0 PAR. 11-C-9
2059. CO ₃ ⁻	• H ₂ O	• M	• H ₂ CO ₃ ⁻	• M		1.0E-28	-1.00 0 PAR. 11-C-9
2061. CO ₄ ⁻	• H ₂ O	• M	• H ₂ CO ₄ ⁻	• M		1.0E-28	-1.00 0 PAR. 11-C-9
CATEGORY 24. NEGATIVE-ION COLLISIONAL DISSOCIATION							
140. O ₄ ⁻	• M		• O ₂ ⁻	• O ₂	• M	1.5E-05	.16 6834 PAR. 11-D

TABLE II (cont)

NO.				A	B	C	REFERENCE
CATEGORY 24. NEGATIVE-ION COLLISIONAL DISSOCIATION							
188. O ³⁻	+ M	= O ⁻	+ O ²⁻	+ M	8.2E-06	-1.00	19249 PAR. 11-D
496. NO ²⁻	+ M	= O ⁻	+ NO	+ M	3.1E-04	-.80	46805 PAR. 11-D
742. CO ⁴⁻	+ M	= O ²⁻	+ CO ²⁻	+ M	1.9E-05	.24	9857 PAR. 11-D
1230. NO ²⁻	+ M	= O ²⁻	+ H ² O	+ M	8.5E-05	-1.42	9248 PAR. 11-D
1942. NO ⁻	+ M	= O ⁻	+ H ² O	+ M	4.9E-06	-1.53	9334 PAR. 11-D
1944. NO ³⁻	+ M	= O ³⁻	+ H ² O	+ M	2.9E-04	-1.15	7497 PAR. 11-D
1946. H ² O ²⁻	+ M	= NO ²⁻	+ H ² O	+ M	1.3E-01	.54	8854 PAR. 11-D
1752. CO ³⁻	+ M	= O ⁻	+ CO ²⁻	+ M	4.2E-05	.13	23293 PAR. 11-D
1946. HNO ²⁻	+ M	= NO ²⁻	+ H ² O	+ M	1.7E-04	-1.34	7194 PAR. 11-D
2052. HO ⁴⁻	+ M	= O ⁴⁻	+ H ² O	+ M	8.6E-04	-2.19	9238 PAR. 11-D
2054. HNO ⁻	+ M	= NO ⁻	+ H ² O	+ M	8.2E-05	-1.98	9461 PAR. 11-D
2056. HNO ³⁻	+ M	= NO ³⁻	+ H ² O	+ M	3.8E-05	-.91	6280 PAR. 11-D
2058. HO ⁴⁺	+ M	= O ⁴⁺	+ H ² O	+ M	2.6E-06	-1.77	11238 PAR. 11-D
2060. HCO ³⁻	+ M	= CO ³⁻	+ H ² O	+ M	5.9E-04	-2.19	4779 PAR. 11-D
2062. HCO ⁴⁻	+ M	= CO ⁴⁻	+ H ² O	+ M	1.9E-02	-2.19	7195 PAR. 11-D
CATEGORY 25. RADIATION-STABILIZED NEUTRAL RECOMBINATION							
2535. O	+ NO	= NO ²			8.0E-17	-2.00	0 5
2537. N	+ N	= N ²			1.0E-17	-.90	0 5
CATEGORY 27. THREE-BODY NEUTRAL RECOMBINATION							
3. N	+ N	+ M	= N ²	+ M	4.6E-33	-1.70	0 5
101. O	+ O ²	+ M	= O ³	+ M	1.1E-34	0.00	-510 5
105. O	+ O	+ M	= O ²	+ M	3.0E-33	-2.90	0 5
209. O	+ N	+ M	= NO	+ M	1.1E-32	-.50	0 5
219. O	+ NO	+ M	= NO ²	+ M	1.0E-31	-2.50	0 5
497. O	+ N ²	+ M	= N ² O	+ M	1.0E-34	0.00	7500 5
805. H	+ O ²	+ M	= H ² O	+ M	2.1E-32	0.00	-300 5
817. NO	+ OH	+ M	= HNO ²	+ M	3.3E-32	0.00	-605 28
819. NO ²	+ OH	+ M	= HNO ³	+ M	1.1E-31	0.00	-906 28
983. H ² O	+ H ² O	+ M	= H ²	+ M	2.3E-35	.29	0 PAR. 11-D
1215. H	+ H	+ M	= H ²	+ M	8.3E-33	-.60	0 5
1217. H	+ OH	+ M	= H ² O	+ M	7.0E-32	0.00	0 5
1733. CO	+ O	+ M	= CO ²	+ M	1.4E-35	0.00	0 5
1949. H ² O	+ NO	+ M	= HNO ³	+ M	3.3E-33	0.00	0 34
2425. N ²	+ O(1D)	+ M	= N ² O	+ M	2.6E-36	0.00	0 16
2433. O	+ O	+ M	= O ² (SG)	+ M	1.7E-37	0.00	0 5
2436. O	+ O ²	+ O ²	= O ³	+ O ² (DL)	2.1E-36	-.03	2191 PAR. 11-D
2439. O	+ O ²	+ O ²	= O ³	+ O ² (SG)	6.9E-37	-.03	6346 PAR. 11-D
2503. NO ²	+ O	+ M	= NO ³	+ M	1.5E-31	0.00	0 PAR. 11-F-2
2506. NO	+ O ²	+ NO ²	= NO ³	+ NO ²	2.9E-40	.26	742 PAR. 11-D
2507. NO	+ O ²	+ NO	= NO ³	+ NO	6.6E-39	0.00	-526 PAR. 11-F-2
CATEGORY 28. NEUTRAL COLLISIONAL DISSOCIATION							
4. N ²	+ M	= N	+ N	+ M	2.5E-08	-1.29	113246 PAR. 11-D
102. O ³	+ M	= O	+ O ²	+ M	2.3E-09	.04	11873 PAR. 11-D
106. O ²	+ M	= O	+ O	+ M	1.6E-08	-2.43	59370 PAR. 11-D
210. NO	+ M	= O	+ N	+ M	1.5E-08	-.13	73511 PAR. 11-D
220. NO ²	+ M	= O	+ NO	+ M	2.6E-06	-2.14	35161 PAR. 11-D

TABLE II (cont)

NO.				A	B	C	REFERENCE
CATEGORY 28. NEUTRAL COLLISIONAL DISSOCIATION							
498. N2O	* H	* O	* N2	* H	3.1E-09	.09	38804 PAR. 11-D
806. NO2	* H	* H	* O2	* H	5.1E-09	.60	28815 PAR. 11-D
818. HNO2	* H	* NO	* OH	* H	2.9E-06	.17	23127 PAR. 11-D
820. HNO3	* H	* NO2	* OH	* H	4.1E-05	.03	23083 PAR. 11-D
984. H2	* H	* H2O	* H2O	* H	1.0E-10	0.00	2735 PAR. 11-D
1216. H2	* H	* H	* H	* H	6.0E-09	-.10	51884 PAR. 11-D
1218. H2O	* H	* H	* OH	* H	1.0E-07	.87	58423 PAR. 11-D
1794. CO2	* H	* CO	* O	* H	1.7E-08	.23	63283 PAR. 11-D
1950. HNO3	* H	* NO2	* NO	* H	9.4E-06	-.18	28838 PAR. 11-D
2426. N2O	* H	* N2	* O(1D)	* H	6.2E-11	-.02	42821 PAR. 11-D
2434. O2(1G)	* H	* O	* O	* H	1.9E-12	.47	40821 PAR. 11-D
2436. O3	* O2(1D)	* O	* O2	* O2	4.2E-11	0.00	2800 5
2437. O3	* O2(1G)	* O	* O2	* O2	2.2E-11	0.00	0 5
2504. NO3	* H	* NO2	* O	* H	3.4E-05	-.12	24881 PAR. 11-D
2505. NO3	* NO2	* NO	* O2	* NO2	3.8E-13	0.00	2215 30
2508. NO3	* NO	* NO	* O2	* NO	7.3E-12	-.23	947 PAR. 11-D
CATEGORY 29. NEUTRAL REARRANGEMENT							
103. O	* O3	* O2	* O2		1.5E-11	0.00	2240 5
104. O2	* O2	* O	* O3		3.8E-12	.44	48407 PAR. 11-D
201. N	* O2	* NO	* O		2.4E-11	0.00	4000 5
202. NO	* O	* N	* O2		6.3E-12	-.11	20141 PAR. 11-D
203. N	* NO	* O	* N2		5.1E-11	0.00	250 27
204. O	* N2	* N	* NO		2.0E-10	.02	37886 PAR. 11-D
207. O3	* N	* NO	* O2		3.1E-11	.50	1200 5
208. NO	* O2	* O3	* N		2.1E-12	.83	84508 PAR. 11-D
213. N	* NO2	* NO	* NO		6.0E-12	0.00	0 5
214. NO	* NO	* N	* NO2		3.1E-13	.01	38349 PAR. 11-D
215. N	* NO2	* O2	* N2		2.0E-12	0.00	0 5
216. O2	* N2	* N	* NO2		1.5E-12	-.16	80844 PAR. 11-D
217. N	* NO2	* O	* N2O		8.0E-12	0.00	0 5
218. O	* N2O	* N	* NO2		3.7E-11	-.23	20878 PAR. 11-D
221. O	* NO2	* NO	* O2		1.7E-11	0.00	300 15
222. NO	* O2	* O	* NO2		3.4E-12	.11	23508 PAR. 11-D
235. O3	* NO	* NO2	* O2		9.5E-13	0.00	1300 5
236. NO2	* O2	* O3	* NO		1.2E-12	.33	25298 PAR. 11-D
237. O3	* N2O	* O2	* O2	* N2	1.0E-20	0.00	0 33
238. O2	* O2	* O3	* N2O		7.2E-47	.37	27783 PAR. 11-D
239. O3	* NO2	* NO3	* O2		9.8E-12	0.00	3500 5
240. NO3	* O2	* O3	* NO2		1.1E-10	-.16	15878 PAR. 11-D
243. N	* N2O	* NO	* N2		1.0E-12	0.00	0 33
244. NO	* N2	* N	* N2O		4.3E-14	.28	56107 PAR. 11-D
499. O	* N2O	* O2	* N2		5.0E-11	0.00	14000 5
500. O2	* N2	* O	* N2O		8.2E-12	.39	53885 PAR. 11-D
501. O	* N2O	* NO	* NO		1.3E-10	0.00	14000 5
502. NO	* NO	* O	* N2O		1.7E-12	.23	32371 PAR. 11-D
505. N	* NO2	* O	* O	* N2	2.0E-12	0.00	0 5
506. O	* O	* N	* NO2		2.7E-37	-.30	1574 PAR. 11-D
801. O3	* H	* OH	* O2		2.0E-11	0.00	0 5
802. OH	* O2	* O3	* H		4.0E-13	.46	38759 PAR. 11-D
807. O	* OH	* H	* O2		5.0E-11	0.00	0 5
808. H	* O2	* O	* OH		8.1E-10	-.02	8407 PAR. 11-D
809. O	* NO2	* OH	* O2		2.0E-11	0.00	0 35

TABLE II (cont)

NO.	A	B	C	REFERENCE
CATEGORY 29. NEUTRAL REARRANGEMENT				
810. OH	• O	• H2O	2.7E-11	-10 27847 PAR. 11-D
811. OH	• O	• H2O	4.9E-11	0.00 400 5
812. O	• O	• OH	2.2E-10	.38 8880 PAR. 11-D
813. H2O	• O3	• O2	3.0E-15	0.03 0 20
814. OH	• O2	• H2O	1.0E-40	-.12 19944 PAR. 11-D
815. O3	• O4	• O2	1.3E-12	0.00 950 5
816. H2O	• O2	• O3	2.4E-13	.94 20389 PAR. 11-D
821. OH	• H2O2	• H2O	1.7E-11	0.03 910 5
822. H2O	• H2O	• OH	1.3E-11	.95 19871 PAR. 11-D
823. OH	• H2O2	• H2O	1.7E-11	0.00 1850 34
824. H2O	• H2O	• OH	2.2E-11	.57 28889 PAR. 11-D
825. OH	• H2O3	• H2O	1.7E-11	0.00 1850 22
826. H2O	• H2O3	• OH	4.9E-11	.23 10793 PAR. 11-D
827. OH	• H2O	• O2	2.0E-10	0.00 0 26
828. H2O	• O2	• OH	1.3E-09	.28 35307 PAR. 11-D
829. H2O	• H2O	• H2O2	9.4E-12	0.00 0 26
830. H2O2	• O2	• H2O2	7.9E-11	-.28 21346 PAR. 11-D
833. O	• H2O2	• OH	1.7E-11	0.00 0 34
834. H2O	• OH	• H2O2	4.6E-12	.20 12179 PAR. 11-D
835. O	• H2O3	• OH	1.7E-11	0.00 0 34
836. OH	• H2O3	• O	9.6E-12	-.15 882 PAR. 11-D
847. OH	• H2	• H	3.6E-11	0.00 2580 5
848. H	• H2O	• OH	7.9E-11	.37 10048 PAR. 11-D
849. H2O	• H	• OH	1.2E-09	0.00 971 29
850. NO	• OH	• H	1.2E-11	.14 15772 PAR. 11-D
1221. H	• OH	• H	1.2E-11	0.00 3880 5
1222. H2	• O	• OH	2.6E-11	.01 4652 PAR. 11-D
1223. H	• H2O2	• H2	2.6E-12	0.00 1900 5
1224. H2	• H2O2	• H	9.6E-13	.19 9403 PAR. 11-D
1225. O3	• OH	• CO2	9.3E-13	0.00 940 5
1226. CO2	• H	• CO	3.4E-10	-.27 12861 PAR. 11-D
1547. OH	• H2O	• OH	4.2E-10	0.00 950 5
1548. OH	• OH	• H2O	3.4E-11	-.07 20380 PAR. 11-D
1549. H	• H2O	• H2	4.2E-11	0.00 350 5
1550. H2	• O2	• H	1.2E-10	-.09 29199 PAR. 11-D
1761. N	• OH	• NO	5.3E-11	0.00 0 9
1762. NO	• H	• N	2.3E-10	-.13 24548 PAR. 11-D
1951. NO	• H2O3	• H2O2	1.9E-10	0.00 0 22
1952. H2O2	• H2O2	• NO	1.7E-11	.49 11480 PAR. 11-D
1953. NO	• H2O2	• H2O2	2.0E-37	0.00 0 16
1954. H2O2	• H2O2	• NO	1.4E-11	-.40 3343 PAR. 11-D
2401. O3	• O(1D)	• O2	2.9E-10	0.00 0 5
2402. O2	• O3	• O(1D)	4.9E-11	.33 66883 PAR. 11-D
2403. H2O	• O(1D)	• OH	2.0E-10	0.00 0 5
2404. OH	• OH	• H2O	3.1E-11	-.48 14357 PAR. 11-D
2411. O2	• N(2D)	• NO	7.0E-12	.50 0 5
2412. NO	• O	• N(2D)	4.6E-12	.40 44020 PAR. 11-D
2421. H2O	• O(1D)	• H2	6.6E-11	0.00 0 21
2422. H2	• O2	• NO	7.6E-12	.29 62783 PAR. 11-D
2423. H2O	• O(1D)	• NO	6.6E-11	0.00 0 21
2424. NO	• NO	• O(1D)	5.2E-13	.13 41188 PAR. 11-D
2439. N	• O2(DL)	• NO	2.0E-14	0.00 500 5
2440. N	• O	• N	5.2E-15	-.11 28335 PAR. 11-D
2541. NO3	• NO3	• NO2	5.0E-12	0.00 3000 9
2542. H2O2	• H2O2	• NO3	4.1E-40	.76 13007 PAR. 11-D

TABLE II (cont)

NO.				A	B	C	REFERENCE
CATEGORY 29. NEUTRAL REARRANGEMENT							
2343. N2O	• H	• OH	• N2	1.7E-10	0.00	7600	9
2344. OH	• N2	• N2O	• H	1.2E-12	.42	30150	PAR. 11-D
2351. N	• CO2	• NO	• CO	3.2E-13	0.00	1711	12
2352. NO	• CO	• N	• CO2	3.2E-15	.14	13030	PAR. 11-D
2355. H2O	• CO	• OH	• CO2	2.2E-12	.50	0	12
2356. OH	• CO2	• H2O	• CO	7.0E-11	.15	31760	PAR. 11-D
2357. H2O	• CO2	• NO	• CO2	2.2E-11	0.00	19000	12
2358. NO	• CO2	• H2O	• CO	1.0E-10	-.14	42721	PAR. 11-D
2359. NO3	• CO2	• NO2	• CO2	1.0E-11	0.00	3250	12
2360. H2O	• CO2	• NO3	• CO	8.4E-12	.35	41052	PAR. 11-D
2361. H2O	• NO	• NO2	• OH	8.0E-11	.50	900	12
2362. H2O	• OH	• H2O	• NO	5.9E-10	.29	9530	PAR. 11-D
2363. O3	• CO	• CO2	• O2	1.0E-25	0.00	0	11
2364. CO2	• O2	• O3	• CO	5.9E-25	.19	51080	PAR. 11-D
2365. H2O2	• NO	• OH	• H2O2	1.0E-18	0.00	1040	10, PAR. 11-F-1
2366. OH	• H2O2	• H2O2	• NO	6.3E-18	-.23	0	PAR. 11-D
CATEGORY 30. RADIATIVE ELECTRONIC-STATE DEEXCITATION							
2405. O(1D)		• O		6.0E-03	0.00	0	5
2413. N(2D)		• N		1.0E-05	0.00	0	5
2441. O2(1D)		• O2		2.0E-04	0.00	0	5
2443. O2(1G)		• O2		8.3E-02	0.00	0	5
CATEGORY 32. COLLISIONAL ELECTRONIC-STATE QUENCHING							
2407. E	• O(1D)	• E	• O	1.5E-09	0.00	0	5
2409. O(1D)	• H	• O	• H	9.0E-11	0.00	0	5
2415. E	• N(2D)	• E	• N	5.0E-10	0.00	0	5
2417. N(2D)	• H	• N	• H	5.0E-15	0.00	0	5
2445. O(1D)	• O2	• O	• O2(1G)	7.0E-11	0.00	0	5
2447. O2(1D)	• H	• O2	• H	6.0E-19	0.00	0	5
2449. O2(1G)	• H	• O2	• H	1.7E-15	0.00	0	5
CATEGORY 62. COLLISIONAL ELECTRONIC-STATE EXCITATION							
2408. E	• O	• E	• O(1D)	1.1E-09	-.10	22017	PAR. 11-D
2410. O	• H	• O(1D)	• H	5.7E-11	-.10	22017	PAR. 11-D
2416. E	• N	• E	• N(2D)	1.3E-09	.00	27070	PAR. 11-D
2418. N	• H	• N(2D)	• H	1.2E-14	.00	27070	PAR. 11-D
2446. O	• O2(1G)	• O(1D)	• O2	8.2E-11	-.10	4208	PAR. 11-D
2448. O2	• H	• O2(1D)	• H	6.0E-19	0.00	11504	PAR. 11-D
2450. O2	• H	• O2(1G)	• H	1.0E-15	-0.00	18949	PAR. 11-D

III. COMPUTER CODES

The systems of differential equations describing the chemical kinetics of a set of reacting species is numerically solved using the stiffly stable multistep methods developed by C. W. Gear.³⁶ Gear's methods permit the economical integration of "stiff" systems of ordinary differential equations, i.e., systems whose solution components contain both very rapidly changing terms and very slowly changing terms, all of a decaying nature.

The right-hand side of the system of differential equations

$$\frac{dy_i}{dt} = f_i(y_1(t), \dots, y_N(t), t), \quad i = 1, \dots, N,$$

involves sums of the product of a rate constant and concentrations of up to three chemical species. An equation-writer code is used to generate the FORTRAN code required to calculate the f_i for systems involving large numbers of reactions. In addition the equation-writer code produces code to calculate the Jacobian matrix

$$J = \left(\frac{\partial f_i}{\partial y_j} \right)_{i,j=1}^N.$$

This is required if the implicit equations of Gear's methods are solved by a Newton-Raphson iteration. The input to the equation-writer code is a set of cards listing the reactants and products, one card per reaction.

IV. COMPUTED RESULTS

A. Equilibria and Relaxation Times

Our own recent computations of chemical species concentrations in thermodynamic equilibrium have been described in Ref. 1. To demonstrate that the present chemical reaction kinetics set is consistent with thermodynamics, we present here a series of computations in which the equilibrium code

was used to provide initial conditions for the kinetics code. The computations are for moist air (1 mole % H_2O) at 1 atmosphere pressure at various temperatures. To add interest to the scenario we hold the temperature at the input level (the temperature for which the input equilibrium concentrations apply) for 1 s, satisfying ourselves that the concentrations remain essentially constant (the same as the equilibrium concentrations), and then drop the temperature abruptly by 500 K, with the density held constant. The response of the system after the temperature drop indicates the relaxation times for equilibration of chemical composition at the lower temperature. Computed results for four pairs of temperatures are plotted in Fig. 1. No radiation source is included in this set of computations (i.e., - no photochemical reactions).

One will note that some of the concentration vs time curves exhibit small inflections at $t = 0.1$ s when the chemical kinetics calculations are commenced, showing that the ratios of forward and reverse reaction rates are not quite the same as the thermodynamic equilibrium constants. This difficulty (which we do not regard as serious) comes from our procedure of force-fitting computed reverse rate constants to the standard functional form

$$k = A(T/300)^B e^{-C/T}. \quad (7)$$

The fits are made by least squares over the temperature range 300 - 2300 K, as described in Ref. 1.

One will also note that some of the curves are perfectly straight and horizontal. In some cases this shows that the species in question have the same equilibrium concentration at both temperatures, but in other cases it means simply that the reaction rates are too slow to permit a readjustment within the allowed 10^3 s. The latter interpretation applies to the NO concentrations in Fig. 1 (a and b).

Parenthetically, these results relate

Fig. 1(a) Equilibria and relaxation times for moist air (1 atom % hydrogen) at 1000 K (T_1) and 500 K (T_2): For $t < 0.1$ s the system is in thermodynamic equilibrium at 1000 K and 1 atmosphere pressure. Between 0.1 and 1 s chemical reactions are allowed to proceed at 1000 K. At 1 s the temperature is dropped to 500 K at constant density (3.7×10^{-4} g/cm³), and reactions proceed at the lower temperature. All species with concentrations between 10^{11} and 10^{17} cm⁻³ are plotted. (O₂ and N₂ are off scale.)

(b) Analogous results for temperatures $T_1 = 2000$ K and $T_2 = 1500$ K. $\rho = 1.8 \times 10^{-4}$ g/cm³.

(c) $T_1 = 2500$ K and $T_2 = 1000$ K. $\rho = 1.5 \times 10^{-4}$ g/cm³.

(d) $T_1 = 3000$ K and $T_2 = 2500$ K. $\rho = 1.2 \times 10^{-4}$ g/cm³.

to the matter of fixation of atmospheric nitrogen by lightning or nuclear explosions. One will note from Fig. 1 that the decay times for larger-than-equilibrium concentrations of NO_x ($\text{NO} + \text{NO}_2$) are about 0.1 s at 2500 K, 10 s at 2000 K, and greater than 1000 s at 1500 K. In situations where the air is heated above 2500 K and then cooled abruptly, the high-temperature NO_x fraction tends to become "frozen in." In lightning, where the cooling occurs in less than 0.01 s, the frozen-in NO_x mole fraction should be about 0.035, corresponding to a temperature between 2500 and 3000 K. For a nuclear fireball, where the cooling times are slightly longer, the frozen-in NO_x fraction would be slightly lower--probably between 0.01 and 0.02. Similar estimates have been made by H. S. Johnston,³⁷ F. R. Gilmore,³⁸ and others.

B. Concentrations vs Time in Impulsively Ionized Air

1. Without Photochemical Reactions:

In this series of computations we assume that the air before zero time is in its normal state at 300 K and 1 atmosphere, with 1 mole % H_2O . At zero time it is dosed instantaneously with ionizing radiation of an amount specified in terms of a number of ion pairs produced per cm^3 . The initial state therefore is one of intense ionization far out of equilibrium, and we compute the subsequent changes of composition. The temperature, which governs the reaction rates, is assumed to be that corresponding to the initial radiation dosage, assuming an energy requirement of 35 eV per ion-electron pair. The density is constant, the same as before the dosage. Results, corresponding to initial ionization levels of 10^{14} , 10^{15} , 10^{16} , and 10^{17} ion pairs per cm^3 (and corresponding kinetic temperatures of 300, 300, 350, and 810 K, respectively), are plotted in Figs. 2(a,b,c) through 5(a,b,c). No photochemical reactions are included.

The initial ionization step is assumed in each case to produce the following spe-

cies in the following proportions:³⁹

electrons	1.00
N_2^+	0.63
N^+	0.14
$\text{N}/\text{N}({}^2\text{D})$	0.50/0.51
O_2^+	0.16
O^+	0.07
$\text{O}/\text{O}({}^1\text{D})/\text{O}_2({}^1\Delta_g)/\text{O}_2({}^1\Sigma_g^+)$	0.21/0.12/0.78/0.12
H_2O^+	0.002
$\text{H}, \text{OH}, \text{H}^+, \text{OH}^+$	5×10^{-4}

It is assumed that for all $t > 0$ the temperature is that corresponding to complete equilibration of the ionization energy (35 eV/ion pair) over all chemical and quantum mechanical degrees of freedom, at constant density. This is an oversimplification of the physical situation that we intended to represent. For a fixed total energy input, the kinetic temperature would actually decrease with time as more and more degrees of freedom are populated.

2. With Photochemical Reactions: The above calculations could serve as a model for the chemical relaxation of air close to a nuclear explosion, after irradiation by prompt neutrons and gamma rays. However, they do not include the photochemical reactions that would be produced by the optical and uv radiations from the fireball. The influence of the fireball radiation is illustrated in the next figure [Fig. 6(a,b,c)] which is equivalent to Fig. 2(a,b,c) with an initial ionization level of 10^{14} ion-pairs/ cm^3 , except that in this case an intense optical-uv photon source is included. The source is represented by a temperature $T_s = 1$ eV, a flux scale factor $f = 0.5$ (infinite planar fireball on one side), and a high energy spectral cutoff $h\nu_m = 5$ eV ($\lambda_m = 2479 \text{ \AA}$).

The assumed spectral cutoff at $h\nu_m = 5$ eV is intended to mock up in a crude way the removal, by O_2 Schumann-Runge absorption, of all photons with energies above 5 eV. That absorption would lead, of course,

Fig. 2(a,b,c) Computed negative, positive, and neutral species concentrations vs time following an impulsive ionization event leading to 10^{14} ion-pairs per cm^3 . $T = 300 \text{ K}$ and $\rho = 0.00123 \text{ g/cm}^3$. For $t > 0$ the fluxes of ionizing radiation and optical-uv radiation are assumed to be zero.

Fig. 3(a,b,c) Analogous results for an initial ionization level of 10^{15} cm^{-3} . $T = 300 \text{ K}$.

Fig. 4(a,b,c) Computed negative, positive, and neutral species concentrations vs time following an impulsive ionization event leading to 10^{16} ion-pairs per cm^3 . The initial temperature and density are 300 K and 0.00123 g/cm^3 , respectively. For $t > 0$ the fluxes of ionizing radiation and optical-uv radiation are assumed to be zero, the temperature is 350 K, and the density is unchanged.

Fig. 5(a,b,c) Analogous results for an initial ionization level of 10^{17} cm^{-3} and $T = 810 \text{ K}$.

to dissociation of O_2 , with resultant heating and burnup of the absorbing layer. The problem is properly one of chemistry coupled with radiation transport, which we pursue no further in this report.

An important effect of the optical-uv flux is to detach electrons from negative ions. Comparing Figs. 2(a) and 6(a), it is evident that the photon flux produces a quasi equilibrium between electron and negative ion concentrations after 10^{-7} s, so that the electron concentration history from that time on is controlled by recombination instead of attachment. Other effects on the negative species populations are minor. No changes at all are noticeable in the positive ion populations [comparing Figs. 2(b) and 6(b)]. Comparing neutral species densities in Figs. 2(c) and 6(c), the optical-uv flux begins to make a difference after 10^{-6} s, tending to destroy O_3 , NO_2 , and N_2O and to increase concentrations of O , $O_2(^1\Delta_g)$, $O_2(^1\Sigma_g^+)$, H , and OH , HO_2 , HNO_2 , HNO_3 , and H_2O_2 .

Figure 7(a,b,c) shows results of a similar calculation, but with an initial ionization level of 10^{15} cm^{-3} . It is therefore the counterpart of Fig. 3(a,b,c) with the 1 eV optical-uv flux added.

3. At 1/100 of Normal Density, Without Photochemical Reactions: Figures 8(a,b,c) and 9(a,b,c) show results of two computations representing the relaxation of impulsively dosed air at 1/100 of normal density with no flux of optical-uv radiation. In Fig. 8(a,b,c) the initial electron density is 10^{12} cm^{-3} , and in Fig. 9(a,b,c) it is 10^{14} cm^{-3} . These two sets of figures are analogous to Figs. 2(a,b,c) and 4(a,b,c) in that a fluence of radiation that would produce 10^{14} electrons/ cm^3 at normal density would produce 10^{12} electrons/ cm^2 at 1/100 of normal density. While this fluence produces a lower electron concentration initially [Fig. 8(a) vs Fig. 2(a)], the ionization decays more slowly in the low density case, because of the smaller attachment rate. By 1 μs the electron density in

Fig. 8(a) exceeds the value in Fig. 2(a).

C. Effects of Duration and Rate of Delivery of the Ionization Pulse

In problems involving ionization sources (e.g. due to gamma rays), it would seem reasonable to expect that the concentrations of some chemical species would depend primarily on the *rate* of ionization, while others would depend mainly on the *integrated dose* and the time. Still others, presumably, would depend on the detailed dose-time history. To explore these possibilities we have run a series of computations where the time-integrated ionization dose is fixed while the dose rate and time duration are varied. Results for one pair of comparisons of this type are shown in Figs. 10(a,b,c) and 11(a,b,c). The time-integrated ion-pair production is 10^{14} cm^{-3} in both cases. However, in Fig. 10(a,b,c) the dose rate is $10^{22} \text{ cm}^{-3} \text{ s}^{-1}$, with duration 10^{-8} s, and in Fig. 11(a,b,c) the rate is $10^{20} \text{ cm}^{-3} \text{ s}^{-1}$ for 10^{-6} s. These two sets of computations can also be compared with Fig. 2(a,b,c) where the same time-integrated number of ion pairs is created, but impulsively as a δ -function in time.

It is impractical to discuss the time-dependent concentrations of each species individually, but certain simple features are evident.

1. Positive Ions: On a time scale of about 1 μs , $H_3O^+ \cdot (H_2O)_3$ tends to become the dominant positive ion (no higher hydrates are included in the computations). The positive ion concentration appears to follow a simple differential equation of the form

$$\frac{dn_+}{dt} = \dot{Q} - \alpha n_+^2 \quad (8)$$

with $\alpha = 8 \times 10^{-6} \text{ cm}^3 \text{ s}^{-1}$ (the complex ion-ion recombination rate coefficient), n_+ the positive concentration, and $\dot{Q}$ the given ion-pair production rate. At very early times $n_+ = \int \dot{Q} dt$; at intermediate times

$$n_+ = \text{Min} \left\{ (\dot{Q}/\alpha)^{1/2}, \int \dot{Q} dt \right\}$$

Fig. 6(a,b,c) Computed negative, positive, and neutral species concentrations vs time following an impulsive ionization event leading to 10^{14} ion-pairs per cm^3 . $T = 300 \text{ K}$ and $\rho = 0.00123 \text{ g/cm}^3$. For $t > 0$ the flux of ionizing radiation is assumed to be zero, while an optical-uv flux is applied, equal to that produced by an infinite surface radiation with a temperature of 1 eV , but with a cutoff for photons above 5 eV .

Fig. 7(a,b,c) Analogous results for an initial ionization level of 10^{15} cm^{-3} . $T = 300 \text{ K}$.

Fig. 8(a,b,c) Computed negative, positive, and neutral species concentrations vs time following an impulsive ionization event leading to 10^{12} ion pairs/cm³ in air at 300 K and $\rho = 1.23 \times 10^{-5}$ g/cm³ (1/100 of sea level density). No optical-uv flux included.

Fig. 9(a,b,c) Analogous results for an initial ionization level of 10^{14} cm⁻³ at the same temperature and density.

Fig. 10(a,b,c) Computed negative, positive, and neutral species concentrations vs time during and after an ionization pulse of strength 10^{22} ion pairs/cm³ s and duration 10^{-8} s. $T = 300$ K and $\rho = 0.00123$ g/cm³. No optical-uv radiation is included.

Fig. 11(a,b,c) Analogous results for an ionization source of 10^{20} ion pairs/cm³ s lasting for 10^{-6} s.

still later, after $\dot{Q}$ has dropped to zero,

$$n_+ \rightarrow 1/\alpha t \quad .$$

Before 1 μ s, ions other than $H_3O^+ \cdot (H_2O)_3$ are dominant, such as O_2^+ , N_2^+ , and NO^+ .

2. Electrons and Negative Ions: Free electrons tend to predominate for about 2×10^{-8} s (the attachment time). They are subsequently replaced by $O_2^-(H_2O)_2$, which is in turn replaced (after 10^{-4} s) by $O_3 \cdot H_2O$ and $NO_3 \cdot H_2O$. The total electron and negative ion concentration follows the positive ion concentration, given by Eq. (8).

3. Neutral Species: The neutral species exhibit a more diverse variety of behavior. The most reactive species are $O(^1D)$ and $N(^2D)$, which decay or reach quasi-steady concentrations within 10^{-7} s, and H, which decays in about 10^{-6} s. The next most reactive are O, NO_3 , and $O_2(^1\Sigma_g^+)$, in order of increasing decay times. Species whose concentrations increase during the ionization pulse and remain level thereafter include NO, $O_2(^1\Delta_g)$, CO, and H_2 . O_3 concentration continues to increase rapidly after termination of the pulse. Some that increase more slowly, with induction times of 10^{-6} to 10^{-4} s, are NO_2 , N_2O , H_2O_2 , HNO_2 , and HNO_3 .

Upon comparing Figs. 2(a,b,c), 10(a,b,c), and 11(a,b,c) at fixed times, it is evident that the concentrations of N and O and "odd-nitrogen" compounds ($N + NO + NO_2 + NO_3 + HNO_2$) are independent of the duration and rate of delivery of the ionization pulse, depending only on the time integral (ion-pairs/cm³). Other species concentrations do depend (rather weakly) on the pulse duration (τ). Concentrations of HO_2 , OH, and HNO_2 are increasing functions of τ , while NO is a decreasing function.

D. Systems with Steady Ionization Sources

The next series of figures [Figs. 12 (a,b,c) through 15(a,b,c)] show composition changes in systems whose temperatures are raised abruptly, simultaneously with application of a steady flux of ionizing radia-

tion. In each case the system (air with 1 mole % water) is started at 300 K. At $t = 0$ a steady ionization source of strength $\dot{Q}_Y = 10^{14}$ ion pairs/cm³ s is turned on and the temperature is simultaneously raised to T. (No optical-uv source is included.) The density is that corresponding to 1 atmosphere pressure at T. Figures 12(a,b,c) through 15(a,b,c) show changes in composition over the interval 10^{-4} to 1 s.

It will be noted that the concentrations of some species reach their steady state levels within 10^{-3} s. Others respond more slowly and do not level off in the first second. Electrons and ions tend to reach their quasi-steady concentrations in less than 10^{-4} s, although the individual ion populations sort out more gradually. The quasi-steady electron and total positive ion concentrations are influenced slightly by the slow reordering of ion populations, due to differences in individual recombination, attachment, and detachment rates. Most neutral species are formed relatively slowly, and their concentrations are still increasing at $t = 1$ s. Exceptions are O, N, H, NO, OH, HO_2 , $O_2(^1\Delta_g)$, and $O_2(^1\Sigma_g^+)$.

The relative values of the quasi-steady concentrations of electrons and the various ions depend on the temperature. At 300 K the complex hydrated ions predominate over electrons and simple ions. Above 1000 K, electrons and simple ions predominate. Moreover, the magnitude of the quasi-steady electron concentration is a strongly increasing function of temperature.

We have performed similar sets of computations with different ionization source strengths, and with the addition of various optical-uv photochemical source terms. Of particular interest are the quasi-steady electron concentrations, and their functional dependence on the temperature, optical-uv source strengths, ionization source strengths, and pressure. Because of the occasional slow readjustment of the electron density with changing ion populations (see, for example, Fig. 13a), it is necessary to

Fig. 12(a,b,c) Computed negative, positive, and neutral species concentrations vs time in 300 K air at atmospheric pressure in the presence of a steady ionization source producing 10^{14} ion pairs/ cm^3 s. The source is turned on at $t = 0$, and there is no optical-uv flux.

Fig. 13(a,b,c) Analogous results for a temperature of 1000 K. Same ionization source strength of $10^{14} \text{ cm}^{-3} \text{ s}^{-1}$.

Fig. 14(a,b,c) Computed negative, positive, and neutral species concentrations vs time in 1500 K air at atmospheric pressure in the presence of a steady ionization source producing 10^{14} ion pairs/cm³ s. The source is turned on at $t = 0$, and there is no optical-uv flux.

Fig. 15(a,b,c) Analogous results for $T = 2000$ K. Same ionization source strength of 10^{14} cm⁻³ s⁻¹.

Fig. 16. "Quasi-steady" (0.01 s) values of electron number density for $P = 1$ atmosphere and temperatures between 300 and 4000 K. The radiation-induced ionization rates are $\dot{Q}_Y = 0$ ("Equilibrium" curve) and $\dot{Q}_Y = 10^{14}$ ion pairs/cm³ s. Three blackbody optical-uv flux levels are assumed, corresponding to $T_s = 0$ (no flux), $T_s = 0.5$ eV, and $T_s = 1.0$ eV.

define what we mean by "quasi-steady" electron density. We shall define it to be the computed concentration at 10^{-2} s. Results of several computations are collected in Fig. 16, which shows quasi-steady (10^{-2} s) electron densities created by a 10^{14} ion pair per cm³ s source as a function of temperature and at 1 atmosphere pressure. The three curves that merge above 2000 K represent three different levels of optical-uv flux, specified by (1) $T_s = 0$ (no flux), (2) $T_s = 0.5$ eV with $f = 0.5$ and $h\nu_m = 5$ eV,

and (3) $T_s = 1.0$ eV, $f = 0.5$, $h\nu_m = 5$ eV. The lower curve, which merges with the other three above 3000 K, is a plot of computed *thermodynamic equilibrium* electron densities¹ at the same temperatures (with no applied ionization source or optical-uv flux). The merging of the three quasi-steady electron density curves above 2000 K demonstrates that collisional detachment of electrons from negative ions is more important, for $T > 2000$ K, than photodetachment by the 1.0 or 0.5 eV blackbody radiation fluxes. Similarly, the merging of the three upper curves with the thermodynamic equilibrium curve above 3000 K demonstrates that for $T > 3000$ K ordinary collisions produce ionizations at a rate greater than the applied source rate of 10^{14} cm⁻³ s⁻¹.

Results of four similar sets of computations are summarized in Figs. 17 through 20. Figures 17 and 18 give quasi-steady electron density vs temperature for source strengths ($\dot{Q}_Y$) of 10^{15} and 10^{16} ion pairs/cm³ s at $P = 1$ atm. Figures 19 and 20 are similar plots for $\dot{Q}_Y = 10^{12}$ and 10^{14} ion pairs/cm³ s at $P = 0.01$ atm.

The intent of these calculations is to develop simple semi-analytic relationships to describe electron and ion densities as functions of ionizing radiation flux density (ionization source strength), optical-uv flux density, temperature, and pressure (see Section V). In this connection it may be noted that, for a given gamma-ray, beta, or neutron flux density (erg/cm² s), the ionization source strength $\dot{Q}_Y$ (i.p./cm³ s) is proportional to the air density, or to P/T . Therefore Figs. 17 and 19 correspond to similar flux densities (which, however, in each figure, are proportional to T .) The same applies to Figs. 18 and 20.

Comparing Figs. 16, 17, and 18, one notes the obvious fact that the larger the value of $\dot{Q}_Y$ the larger the electron density, below the temperature where the equilibrium and nonequilibrium curves merge. Also, the larger the $\dot{Q}_Y$ the higher the temperature at which the merging occurs.

Fig. 17. "Quasi-steady" (0.01 s) values of electron number density for $P = 1$ atmosphere and temperatures between 300 and 4000 K. The radiation-induced ionization rates are $\dot{Q}_Y = 0$ ("Equilibrium" curve) and $\dot{Q}_Y = 10^{15}$ ion pairs/cm³ s. Three blackbody optical-uv flux levels are assumed, corresponding to $T_s = 0$ (no flux), $T_s = 0.5$ eV, and $T_s = 1.0$ eV.

Comparing Figs. 16 and 20, with the same values of $\dot{Q}_Y$ but different pressures, one notes that the n_e values are similar at 2500 K where they are determined by dissociative recombination in equilibrium with the applied ionization source $\dot{Q}_Y$. At 3000 K collisional ionizations begin to dominate in the 1 atmosphere case, where they are not yet important at the lower pressure. Below 2000 K negative ion formation leads to lower electron densities in the 1 atmosphere case. At 0.01 atmosphere negative ions are important only at temperatures below 1000 K.

Fig. 18. "Quasi-steady" (0.01 s) values of electron number density for $P = 1$ atmosphere and temperatures between 300 and 4000 K. The radiation-induced ionization rates are $\dot{Q}_Y = 0$ ("Equilibrium" curve) and $\dot{Q}_Y = 10^{16}$ ion pairs/cm³ s. Three blackbody optical-uv flux levels are assumed, corresponding to $T_s = 0$ (no flux), $T_s = 0.5$ eV, and $T_s = 1.0$ eV.

E. Other Quasi-Equilibria

It has been pointed out recently by F. R. Gilmore that at temperatures below 2000 K the presence of excess NO₂ can reduce quasi-equilibrium electron densities by shifting the attachment-detachment equilibrium, owing to the large attachment energies of NO₂⁻, WNO₂⁻, and NO₃⁻ relative to those of O₂⁻, WO₂⁻, etc. Abnormally high NO₂ concentrations tend to occur in situations where the air temperature is abruptly decreased from a high value to a lower one below about 2000 K [see Fig. 1(c)], a situation

Fig. 19. "Quasi-steady" (1 s) values of electron number density for $P = 0.01$ atmosphere and temperatures between 300 and 4000 K. The radiation-induced ionization rates are $\dot{Q}_Y = 0$ ("Equilibrium" curve) and $\dot{Q}_Y = 10^{12}$ ion pairs/cm³ s. Three blackbody optical-uv flux levels are assumed, corresponding to $T_s = 0$ (no flux), $T_s = 0.5$ eV, and $T_s = 1.0$ eV.

Fig. 20. "Quasi-steady" (0.01 s) values of electron number density for $P = 0.01$ atmosphere and temperatures between 300 and 4000 K. The radiation-induced ionization rates are $\dot{Q}_Y = 0$ ("Equilibrium" curve) and $\dot{Q}_Y = 10^{14}$ ion pairs/cm³ s. Three blackbody optical-uv flux levels are assumed, corresponding to $T_s = 0$ (no flux), $T_s = 0.5$ eV, and $T_s = 1.0$ eV.

that occurs, for example, behind an expanding shock wave, or in a rising fireball.

Now the quasi-steady n_e values in Figs. 16-20 are not really true steady-state values. Instead, we have defined them as the values existing 0.01 s after applying the source $\dot{Q}_Y$ and simultaneously raising the temperature to T . The composition is seldom constant at 0.01 s, but drifts gradually for tens of seconds.

The 0.01 s n_e values would be different if, for example, we started with some high-temperature equilibrium composition and then

suddenly lowered the temperature to T , with the simultaneous application of $\dot{Q}_Y$. Figure 21 shows results of a set of calculations of this sort, where the temperature before $t = 0$ was 2500 K and at $t = 0$ it was changed to T (at constant density). Because of the large equilibrium concentrations of NO and NO₂ at 2500 K, the system contains excess NO_x if the final temperature T is below 2500 K. As a result, electrons tend to become attached to NO₂ in preference to O₂ or other available molecules. Accordingly, for values of T below 2000 K, in the absence of

Fig. 21. Values of electron number density for $P = 1$ atmosphere, $\dot{Q}_Y = 10^{14}$ ion pairs/cm³ s, 0.01 s after changing the temperature discontinuously from 2500 K to T , $300 < T < 4000$ K. Three blackbody optical-uv flux levels are assumed, corresponding to $T_S = 0$ (no flux), $T_S = 0.5$ eV, and $T_S = 1.0$ eV. The thermodynamic equilibrium ($\dot{Q}_Y = 0$) curve is also shown.

an optical-uv source the n_e values in Fig. 21 are smaller than those in Fig. 16. Above 2500 K the n_e values in Figs. 16 and 21 are similar.

We have done a similar set of computations with the initial temperature ($t < 0$) equal to 3000 K. The computed 0.01 s n_e values are almost identical to those of Fig. 21, showing that the initial temperature does not matter greatly as long as it exceeds 2500 K.

F. Stratospheric Ozone Problems

We have adapted the computer code, with a subset of the reactions listed in Table II, as a subroutine for computing the distribution of stratospheric ozone. In this case it is necessary to (1) integrate the rate equations simultaneously in several individual atmospheric layers (presently 30, representing altitudes from 0 to 60 km); (2) compute the time-dependent spectrum of transmitted sunlight at each altitude, as conditioned by the computed distribution of O_2 and O_3 concentrations; (3) compute the resulting photodissociation rates for O_2 , O_3 , NO_2 , NO , H_2O , CO_2 , N_2O , NO_3 , HO_2 , H_2O_2 , HNO_2 , N_2O_5 , and HNO_3 ; (4) follow the continuous redistribution of species concentrations produced by eddy diffusion, with appropriate boundary conditions; and (5) include a model for the precipitation of water as it attempts to diffuse across the tropopause. Results of these computations, and comparisons with observational data, are described in a separate report, which is in preparation.⁴⁰

V. APPROXIMATIONS VIA LUMPED-PARAMETER MODELS

One of the main purposes of this work is to develop a simple air chemistry model for systems near atmospheric pressure, applicable over a wide range of temperatures, and of a size suitable for inclusion within a fluid dynamics code. We require the model to provide electron and ion concentrations in reasonable agreement with the full reaction set. Also of special interest are the species NO , NO_2 , O_3 , O , and N , and the interactions between NO_2 and the electron concentration.

We have constructed two models. The first considers only electrons and ions, and is based on the well-known DNA "WEPH" models.⁴¹ We have reevaluated the lumped-parameter rate coefficients to extend its temperature range, and have included the effects

of optical-uv sources. It gives good results *except* for situations involving rapid cooling or excess concentrations of NO_x .

The second model includes explicitly the species NO , NO_2 , O_3 , N , and O , as well as ions, electrons, and the special negative ion " NO_x^- ."

In the first model positive ions are treated collectively, as are negative ions, and the electron concentration is equal to the difference between the positive and negative ion concentrations, exactly as in Ref. 41. Five types of reaction processes are considered, namely ion-pair production (rate $\dot{Q} \text{ cm}^{-3} \text{ s}^{-1}$), ion-electron recombination (rate coefficient $\alpha_d \text{ cm}^3 \text{ s}^{-1}$), ion-ion recombination (rate coefficient $\alpha_i \text{ cm}^3 \text{ s}^{-1}$), attachment (rate coefficient $A \text{ s}^{-1}$), and detachment (rate coefficient $D \text{ s}^{-1}$). The rate equations governing the concentrations of electrons (n_e), positive ions (n_+), and negative ions (n_-) are

$$\frac{dn_e}{dt} = \dot{Q} - \alpha_d n_+ n_e + D n_- - A n_e \quad (9)$$

$$\frac{dn_+}{dt} = \dot{Q} - \alpha_d n_+ n_e - \alpha_i n_+ n_- \quad (10)$$

$$\frac{dn_-}{dt} = A n_e - D n_- - \alpha_i n_+ n_- \quad (11)$$

A set of recommended values of α_i , α_d , A , and D has been given in Ref. 41 for moderately disturbed environments under various conditions of ambient temperature, pressure, and atmospheric O and O_3 concentrations. Several recent refinements in the model have been added to extend its range of applicability, as described in classified literature. None, to our knowledge, have been

designed to pressures up to 1 atm or temperatures higher than about 500 K.

To extend the model to high temperatures, it is necessary to add collisional detachment and collisional ionization. These processes are, at least formally, the reverses of attachment and recombination, and when they are included the model can be made to give results consistent with thermodynamic equilibrium. The total detachment coefficient D is then the sum of the photo-detachment rate coefficient D_{hv} and the collisional detachment coefficient D_c . The ionization rate $\dot{Q}$ is the sum of an applied ionization rate $\dot{Q}_Y$ and a collisional rate $\dot{Q}_c$.

Steady-state solutions of Eqs. (9) to (11) are given by the algebraic equations:

$$\alpha n_+^2 + \frac{\dot{Q}(\alpha_d - \alpha_i)n_+}{A + D + (\alpha_d + D)n_+} - \dot{Q} = 0 \quad (12)$$

and

$$n_e = \dot{Q} / [A + D + (\alpha_d + D)n_+] \quad (13)$$

$$n_- = n_+ - n_e \quad (14)$$

(see also Ref. 41). Equation (12) has only one positive root.

We have derived a set of lumped-parameter rate coefficients α_d , α_i , A , D_c , D_{hv} , and $\dot{Q}_c$ with the property that when they are used in Eqs. (12) to (14) they produce a reasonable fit to the steady-state results of the full 1360-reaction code, examples of which are shown in Figs. 16 to 20. The fitted coefficients are:

$$\alpha_d = 1.7 T^{-2.2} + 2.3 \times 10^{-7} P^{0.5} \exp \left[-(T-1650)^2 / 9 \times 10^4 \right] (\text{cm}^3/\text{s}) \quad (15)$$

$$\alpha_i = 5.0 \times 10^{-7} + 3.97 P T^{-2.25} (\text{cm}^3/\text{s}) \quad (16)$$

$$A = 8.1 \times 10^{12} P^2 T^{-2} (\text{s}^{-1}) \quad (17)$$

$$D_c = \begin{cases} P \left[4. \times 10^6 T^{-1} + 7.57 \times 10^{24} T^{-4.7} \exp(-9880/T) \right] & \text{for } T \leq 2000 \text{ K} \\ P \times 8.1 \times 10^{12} T^{-2} \exp(+0.001 T) & \text{for } T > 2000 \text{ K} (\text{s}^{-1}) \end{cases} \quad (18)$$

Fig. 22. 0.01 s ("quasi-steady") values of electron and negative ion number densities for $P = 1$ atmosphere and $300 \leq T \leq 4000$ K, as computed with the lumped-parameter model. The radiation-induced ionization rates are $\dot{Q}_Y = 0$ and $\dot{Q}_Y = 10^{14}$ ion pairs/cm³ s. Three levels of optical-uv flux are represented by $T_S = 0$ (no flux), $T_S = 0.5$ eV, and $T_S = 1$ eV. The negative ion curve is for $T_S = 0$ only. These curves are intended to approximate the curves in Fig. 16.

Fig. 23. 0.01 s ("quasi-steady") values of electron and negative ion number densities for $P = 1$ atmosphere and $300 \leq T \leq 4000$ K, as computed with the lumped-parameter model. The radiation-induced ionization rates are $\dot{Q}_Y = 0$ and $\dot{Q}_Y = 10^{16}$ ion pairs/cm³ s. Three levels of optical-uv flux are represented by $T_S = 0$ (no flux), $T_S = 0.5$ eV, and $T_S = 1$ eV. The negative ion curve is for $T_S = 0$ only. These curves are intended to approximate the curves in Fig. 18.

$$D_{hv} = 3. \times 10^5 F T_S^{-1} \exp(-7000/T_S) \text{ (s}^{-1}\text{)} \quad (19)$$

$$\dot{Q}_c = 4.1 \times 10^{46} T^{-4.2} \left[\exp(-1.22 \times 10^5/T) \right] P (1 + 9.4 \times 10^{-12} T^3) \text{ (s}^{-1}\text{)} \quad (20)$$

Fig. 24. 1 s ("quasi-steady") values of electron and negative ion number densities for $P = 0.01$ atmosphere and $300 < T < 4000$ K, as computed with the lumped-parameter model. The radiation-induced ionization rates are $\dot{Q}_\gamma = 0$ and $\dot{Q}_\gamma = 10^{12}$ ion pairs/cm³ s. Three levels of optical-uv flux are represented by $T_s = 0$ (no flux), $T_s = 0.5$ eV, and $T_s = 1$ eV. The negative ion curve is for $T_s = 0$ only. These curves are intended to approximate the curves in Fig. 19.

$$D = D_c + D_{hv} \text{ (s}^{-1}\text{)} \quad (21)$$

$$\dot{Q} = \dot{Q}_c + \dot{Q}_\gamma \text{ (s}^{-1}\text{)} \quad (22)$$

F is the local optical-uv flux (W/cm^2) and T_s is its color temperature (kelvin). T is in kelvin and P is in atmospheres. In these calculations we assume the source is a perfect blackbody subtending 2π sr, so that $F = \sigma T_s^4$.

The results of combining Eqs. (12) through (22) with a few combinations of T , P , T_s , and $\dot{Q}_\gamma$ are plotted in Figs. 22, 23, and 24. These are equivalent to Figs. 16, 18, and 19. Figures 22 to 24 include plots of n_- as well as n_e , and our criteria for selection of parameters required that the n_- curves as well as the n_e curves should fit concentrations computed with the 1360-reaction code.

The fits provided by these lumped rate coefficients are within a factor of two in electron concentration in all the cases we have checked, which include pressures from 10^{-3} to 10 atm and temperatures from 300 to 4000 K. They are also usable for time-dependent computations.

For situations involving the formation and freezing-in of NO_x , as in cases where the air is rapidly cooled from temperatures above 2500 K (see Section IV-E and Fig. 21), additional species and reactions must be included. A minimum set to describe the NO and NO_2 formation seems to be:

$$\text{rate } \dot{Q} \text{ cm}^{-3} \text{ s}^{-1}$$

$$k_1 = 2.4 \times 10^{-11} \exp(-4000/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_2 = 6.3 \times 10^{-12} (T/300)^{-0.1} \exp(-20140/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_3 = 2.0 \times 10^{-10} \exp(-38000/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_4 = 5.1 \times 10^{-11} \exp(-250/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_5 = 3.8 \times 10^{-12} (T/300)^{0.4} \exp(-49410/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_6 = 1.5 \times 10^{-11} \exp(-2240/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_7 = 1.0 \times 10^{-31} (T/300)^{-1.5} \text{ cm}^6 \text{ s}^{-1}$$

$$k_8 = 2.6 \times 10^{-6} (T/300)^{-1.1} \exp(-36160/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_9 = 1.7 \times 10^{-11} \exp(-300/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_{10} = 3.4 \times 10^{-12} (T/300)^{0.1} \exp(-23510/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_{11} = 1.1 \times 10^{-34} \exp(+510/T) \text{ cm}^6 \text{ s}^{-1}$$

$$k_{12} = 2.26 \times 10^{-9} \exp(-11690/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_{13} = 9.5 \times 10^{-13} \exp(-1300/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_{14} = 1.2 \times 10^{-12} (T/300)^{0.3} \exp(-25260/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_{15} = 3.1 \times 10^{-11} (T/300)^{0.5} \exp(-1200/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_{16} = 2.07 \times 10^{-12} (T/300)^{0.8} \exp(-64510/T) \text{ cm}^3 \text{ s}^{-1}$$

$$k_{17} = 6.6 \times 10^{-39} \exp(+526/T)$$

$$k_{18} = 7.3 \times 10^{-12} (T/300)^{-0.23} \exp(-947/T)$$

$$k_{19} = 0.02 \alpha_i \text{ cm}^3 \text{ s}^{-1}$$

The first equation [Eq. (23)] represents the reaction sequence, $\text{N}_2 + \gamma \rightarrow \text{N} + \text{N}(^2\text{D})$ followed by $\text{N}(^2\text{D}) + \text{O}_2 \rightarrow \text{NO} + \text{O}$, where the first reaction is rate-controlling.

The last equation [Eq. (35)] is intended to represent reactions between hydrated NO^+ and hydrated O_2^- ions, products of which are assumed to be NO_3 and water. The NO_3 reacts rapidly with NO to make NO_2 .

Equations (23) to (35) are to be combined with the basic lumped-parameter ion-electron equations, which can be written in the form

The rate parameters $\dot{Q}$, α_d , α_i , A , D_{hv} , and D_c are given by Eqs. (15) through (22). To include the suppression of electron concentrations by attachment to NO_2 , three additional equations are needed, namely,

$$k_{20} = 3.0 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$$

$$k_{21} = 3. \times 10^{-10} \exp (-20000/T) \text{ cm}^3 \text{ s}^{-1}$$

This reaction set [Eqs. (23) - (43)] is intended to follow explicitly the concentrations of eight chemical species, namely N, O, NO, NO_2 , O_3 , electrons, NO_X^- , and other negative ions (i^-). O_2 and N_2 concentrations are assumed to remain constant, given by

$$[O_2] = 0.2[M] = 1.6 \times 10^{21} \text{ PT}^{-1}$$

$$[N_2] = 0.8[M] = 6.4 \times 10^{21} \text{ PT}^{-1}$$

$$[M] = 8.0 \times 10^{21} \text{ PT}^{-1}.$$

Also, the positive ion concentration [i^+] is equal to the sum of [e^-], [i^-], and [NO_X^-].

The reactions do not include H_2O or compounds derived from water, such as HNO_2 . Calculated NO_X concentrations should therefore be interpreted as $NO_X + HNO_X$. Likewise,

calculated concentrations of NO_X^- should be interpreted as $NO_2^- + WNO_2^- + W_2NO_2^- + NO_3^- + WNO_3^- + \dots$ etc.

With this abbreviated reaction set we have run the sets of computations described in Sections IV-B, D, and E above, and find that the results are in fairly good agreement with the full-scale computations. As in Section IV-E we find that large frozen-in concentrations of NO_2 can suppress the concentration of free electrons.

For the quasi-steady situations represented in Figs. 22 to 24, the 8-species model gives results identical to the simpler 2-species model. On the other hand, in situations involving rapid cooling (as in nuclear fireballs), the 8-species model gives results in good agreement with the 1360-reaction set, while the 2-species model fails badly. The 8-species model also generates NO and NO_2 concentrations in fair agreement with the 1360-reaction model.

Figure 25 contains a set of curves of electron and ion concentration vs temperature for systems starting at equilibrium at 2500 K and cooled abruptly to T, for various values of T. The pressure is 1 atmosphere, $\dot{Q}_Y = 10^{14}$ ion pairs/cm³ s, and the plotted n_e and n_i values are for 0.01 s after the cool-down. Figure 25 is therefore the counterpart of Fig. 21. The agreement between the $T_S = 0$ curves (zero uv flux) of Figs. 21 and 25 is almost perfect. For cases with nonzero uv flux, the agreement is less good.

VI. CONCLUSIONS

We have generated a forward-reverse-matched reaction set for air chemical kinetics computations over the temperature range 300 - 4000 K. Where appropriate, the system gives results consistent with thermodynamic equilibrium requirements. Photochemical reactions are included. Dead-end reaction paths have been systematically purged (though probably not eliminated). Where necessary, we have estimated reaction rate coefficients on the basis of analogies to similar reactions.

Fig. 25. Electron and negative ion number densities calculated with the 8-species lumped-parameter model, representing systems started at $T \geq 2500$ K, $P = 1$, $\dot{Q}_e = 0$, and 10^{12} ion pairs/cm³ s, $300 < T < 4000$ K, $T_e = 0, 0.5$ eV, 1 eV. These curves are intended to approximate the curves in Fig. 21.

Guided by the computed results, we have constructed a much simpler reaction set with 8 species and 31 chemical reactions, which can be used with reasonable confidence and reasonable computer storage within a hydrodynamics code.

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