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DNA 3880T

TN 248

AN EXAMINATION OF THE ADEQUACY OF THE THREE-SPECIES AIR CHEMISTRY TREATMENT FOR THE PREDICTION OF SURFACE-BURST EMP

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December 1975

Topical Report for Period April 1974—December 1975

CONTRACT No. DNA 001-75-C-0094

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Prepared for
Director
DEFENSE NUCLEAR AGENCY
Washington, D. C. 20305

PREFACE

The author expresses his thanks to Conrad Longmire for his help in establishing the basis for the reaction rate coefficients employed in previous EMP calculations. Also the efforts of Trella McCartor and Murray Scheibe in performing and providing an understanding of the DCHEM calculations are hereby acknowledged.

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SECTION 1

INTRODUCTION

During the past 10 years or so several computational models have been developed to calculate the electromagnetic pulse (EMP) produced by a nuclear surface burst detonation[1-5]. More recently similar numerical techniques have been employed to predict the internal electromagnetic pulse (IEMP) generated during flash X-ray experiments in the HIFX and Aurora facilities[6-9], and to predict the system-generated EMP (SGEMP) produced in the close-in coupling region of a surface or near-surface detonation[10-12].

In all of these numerical models the driving source for the electromagnetic fields are high-energy photons which have been produced directly in the device material or created by inelastic scattering or capture of high-energy neutrons in the surrounding air and ground material. These photons in turn will produce an electron current density in the air through Compton scattering, and the Compton electrons through collisions with air molecules will ionize the air forming a conducting plasma.

At sea level the electron-neutral and ion-neutral collision frequencies are approximately 1.7×10^{11} and 8.4×10^{9} sec^{-1}, respectively[13], and given that the maximum EMP frequencies of interest are of the order of a few hundred megahertz and below, it is reasonable to treat the air conductivity as Ohmic in nature. Therefore all of the computational models which predict the surface-burst EMP calculate the air conductivity with a form of the equation

$$\sigma = q(\mu_e n_e + \mu_- n_- + \mu_+ n_+) \ , \qquad (1)$$

where σ is the air conductivity in mhos/cm, μ_e, μ_-, and μ_+ are the electron and ion mobilities in [(cm/sec)/(v/cm)], n_e, n_-, and n_+ are the electron and ion densities in cm^{-3}, and q is the charge of an electron (1.6×10^{-19} coul). The functional dependences of these quantities will be discussed later in this report.

Of the quantities in Equation 1, only the electron mobility has been given a great deal of attention, and its precise variation for the range of air densities, water vapor fractions and electric fields of interest to the calculation of EMP has been the subject of continued discussion[14,15]. The other quantities, in particular the electron and ion densities, have been calculated in the past by assuming that the appropriate air chemistry reactions could be modeled satisfactorily with three species (electrons, positive ions and negative ions). The reaction rates assumed in each of the air chemistry equations were then chosen by each EMP calculator based upon what were thought to be the dominant reactions taking place. Because of apparent differences in the selection of these "lumped" coefficients, and due to the recent extension of EMP calculations to later times ($t > 10^{-4}$ sec), it is appropriate to investigate the accuracy of the three species air chemistry treatment for sea level air density conditions.

SECTION 2

DISCUSSION OF THE THREE SPECIES TREATMENT

The three-species air-chemistry treatment as employed in the solution of sea-level EMP takes the form of the following differential equations:

$$\frac{dn_e(t)}{dt} + [\beta n_+(t) + \alpha_e(|\vec{E}(t)|) - G(|\vec{E}(t)|)]n_e(t) = Q(t) \ , \qquad (2)$$

$$\frac{dn_-(t)}{dt} + [\gamma n_+(t)]n_-(t) = \alpha_e(|\vec{E}(t)|)n_e(t) \ , \qquad (3)$$

$$\frac{dn_+(t)}{dt} + [\beta n_e(t) + \gamma n_-(t)]n_+(t) = Q(t) + G(|\vec{E}(t)|)n_e(t) \ , \qquad (4)$$

$$n_+(t) = n_e(t) + n_-(t) \ , \qquad (5)$$

where β is the lumped electron-ion recombination coefficient [cm^3/sec], γ is the lumped ion-ion neutralization coefficient [cm^3/sec], α_e is the lumped electron attachment rate [sec^{-1}] as a function of electric field, G is the avalanche rate [sec^{-1}] (also a function of electric field), and Q is the ionization rate [ion pairs/$cm^3 \cdot$ sec].

Upon examination of Equations 2 through 5 it can be noted that only Equations 2, 3 and 5 are necessary to obtain a complete solution. It is also apparent why those in the EMP community have desired to simplify the solution of the air chemistry equations. The presence of the electric field dependence in the attachment and avalanche rates requires a simultaneous solution of these equations with the solution of Maxwell's field equations at every position where the ionization rate varies. Fortunately, the primary spatial variation in the ionization rate is related to the absorption mean free path of energetic photons (>1 MeV) in sea-level air which is several hundred meters, thereby allowing spatial charge transport terms in Equations 2 through 5 to be ignored.*

In order to solve for the electron and ion densities, it is necessary to specify the lumped parameter coefficients and rates. As many organizations performing EMP calculations employ slightly different rates, the remaining discussion will apply to those values used in the EMP computer codes at Mission Research Corporation; the conclusions obtained from this analysis, however, should be applicable to all EMP environment codes.

The attachment rate α_e and the avalanche rate G as functions of the electric field were curve fit by Longmire[16], and for sea-level conditions are stated as follows:

$$\alpha_e[\mathrm{sec}^{-1}] = \frac{1.09 \times 10^{10}}{\sqrt{|E| + 3000}} + 1.3 \times 10^{8} \exp\left(- \frac{7.5 \times 10^{5}}{|E| + 3}\right) \quad (6)$$

$$G[\mathrm{sec}^{-1}] = \frac{5.7 \times 10^{8} y^{5}}{1 + 0.3 y^{2.5}} \;, \quad y = \frac{|E|}{3 \times 10^{6}} \;, \qquad (7)$$

where E is the electric field in volts/meter. Longmire employed the two- and three-body electron attachment data of Chanin, Phelps, and Biondi[17] for dry air and the drift velocity data of Phelps[18] to obtain Equation 6. Equation 7 was also derived by folding the first ionization coefficients in various gases[19,20] with the dependence of the electron drift velocity versus electric field.

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* Even in the case of photon simulators where the ionizing flux may vary significantly over 1 meter, the path length of a conduction electron under pulsed electric field conditions is of the order of centimeters at sea level air density.

The electron-ion recombination and the ion-ion recombination coefficients were specified as $\beta = 2.5 \times 10^{-7}$ cm^3/sec and $\gamma = 2.3 \times 10^{-6}$ cm^3/sec (Reference 4). The former coefficient is representative of the primary dissociative recombination reaction

$$O_2^+ + e \rightarrow O + O \; , \tag{8}$$

as the positive-ion charge transfer reaction

$$N_2^+ + O_2 \rightarrow N_2 + O_2^+ \; , \tag{9}$$

occurs at a rate of approximately 7×10^9 sec^{-1}[21] at sea-level air density, thereby quickly depleting the N_2^+ which was formed during the ionization process. The ion-ion recombination coefficient was chosen to represent the sum of the two- and three-body neutralization rates involving the O_2^- ion at sea level.

Given these air chemistry coefficients and reaction rates and an ionization rate Q as a function of time, Equations 2, 3 and 5 may be solved using finite difference techniques; this is accomplished by iterating between the calculation of the electron and ion densities (which yields an air conductivity through Equation 1) and the solution of Maxwell's field equations (which determines the electric field). It is now possible to examine the accuracy of this treatment by performing a comparative study between the given three species air chemistry model and calculations performed by a more complete reaction rate computer code.

SECTION 3

THE DCHEM REACTION RATE CODE

The DCHEM computer code was developed primarily to aid in the determination of the chemical response of the atmosphere to nuclear detonations within and above the atmosphere[22]. For a specified set of atmospheric constituents and conditions (pressure, temperature, density, and ionization rates), the DCHEM code solves a predetermined number of reaction rate equations as a function of time. The rate coefficients for each reaction are specified in the code and are updated continually based upon state-of-the-art improvements in reaction rate research.

In order to perform a comparison with the DCHEM code, the author felt it was necessary to eliminate the EMP electric field as a parameter in the study. This would hopefully minimize the complexity of the analysis but would still test the accuracy of the three species treatment under low electric field conditions. This assumption reduces the attachment rate in Equation 6 to a constant and the avalanche rate in Equation 7 to an insignificant value. The ionization rate for this study was specified as

$$Q\left[\frac{\text{ion pairs}}{\text{cm}^3 \cdot \text{sec}}\right] = \frac{2Q_{pk}t_0t}{t_0^2 + t^2}, \qquad (10)$$

with $t_0 = 10^{-8}$ seconds and Q_{pk} the input maximum ionization rate (at $t = t_0$). At times $t \ll t_0$, Q is proportional to t, while for $t \gg t_0$, Q decays as t^{-1}. Although this precise time dependence is not necessarily characteristic of any specific ionization rate, it will adequately serve the purposes of this study.

The input parameters for the DCHEM calculations are listed in Table 1. At the time of this effort* DCHEM modeled 53 species (1 electron, 24 molecular species, 19 positive ions and 9 negative ions) and solved 371 reaction rate equations. The details of these reactions are contained in the appendix for the reader's interest.

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* The DCHEM calculations to be shown in this report were performed in May 1974. Additional calculations were run in May 1975 with a completely updated set of species and reaction rates, however, no changes in the electron and total positive and negative ion densities were observed.

Table 1. Input parameters for the DCHEM code.

Atmospheric density (excluding water vapor), ρ		2.5×10^{19} molecules/cm^3
Atmospheric temperature, T		293°K
Atmospheric pressure, P		759 mm Hg
Constituent densities:	N_2	1.97×10^{19} molecules/cm^3
	O_2	5.25×10^{18}
	CO_2	7.5×10^{15}
	N_2O	1.25×10^{13}
	O_3	1.5×10^{11}
	NO_2	5.0×10^{10}
	H_2O	$f_{H_2O}\rho$*

* The water vapor fraction (f_{H_2O}) was initially set as a constant, however , results of this study indicated that in fact it was an important parameter (see the following section).

SECTION 4

RESULTS

In order to perform a consistent comparison between the three species and multi-species solutions of air chemistry, it was necessary (as mentioned in the previous section) to eliminate the known electric field dependence in the electron attachment rate and the possible dependence in other reaction rates. This assumption (E = 0) reduces the value of α_e in Equation 6 to 1.99×10^8 sec^{-1}. However, because Equation 6 was fit on the basis of data[18] for electric fields greater than 3000 v/m, the author has chosen instead a value of 1.0×10^8 sec^{-1} for the zero field attachment rate based upon the work of Vittitoe[23]. The three species equations to be solved here become:

$$\frac{dn_e(t)}{dt} + [\beta n_+(t) + \alpha_e]n_e(t) = Q(t) \ , \tag{11}$$

$$\frac{dn_-(t)}{dt} + [\gamma n_+(t)]n_-(t) = \alpha_e n_e(t) \ , \tag{12}$$

$$n_+ = n_e + n_- \ , \tag{13}$$

with $\alpha_e = 10^8$ sec^{-1}, $\beta = 2.5 \times 10^{-7}$ cm^3/sec, $\gamma = 2.3 \times 10^{-6}$ cm^3/sec and Q(t) defined in Equation 10.

Figure 1 illustrates the time variation of each of the three species for peak ionization rates between 10^{19} and 10^{22} ion pairs/cm^3 · sec as calculated numerically with finite difference techniques. As expected from Equation 11, the electron density rises proportionally to t^2, decays as t^{-1}, and scales directly with the peak ionization rate. The negative ion

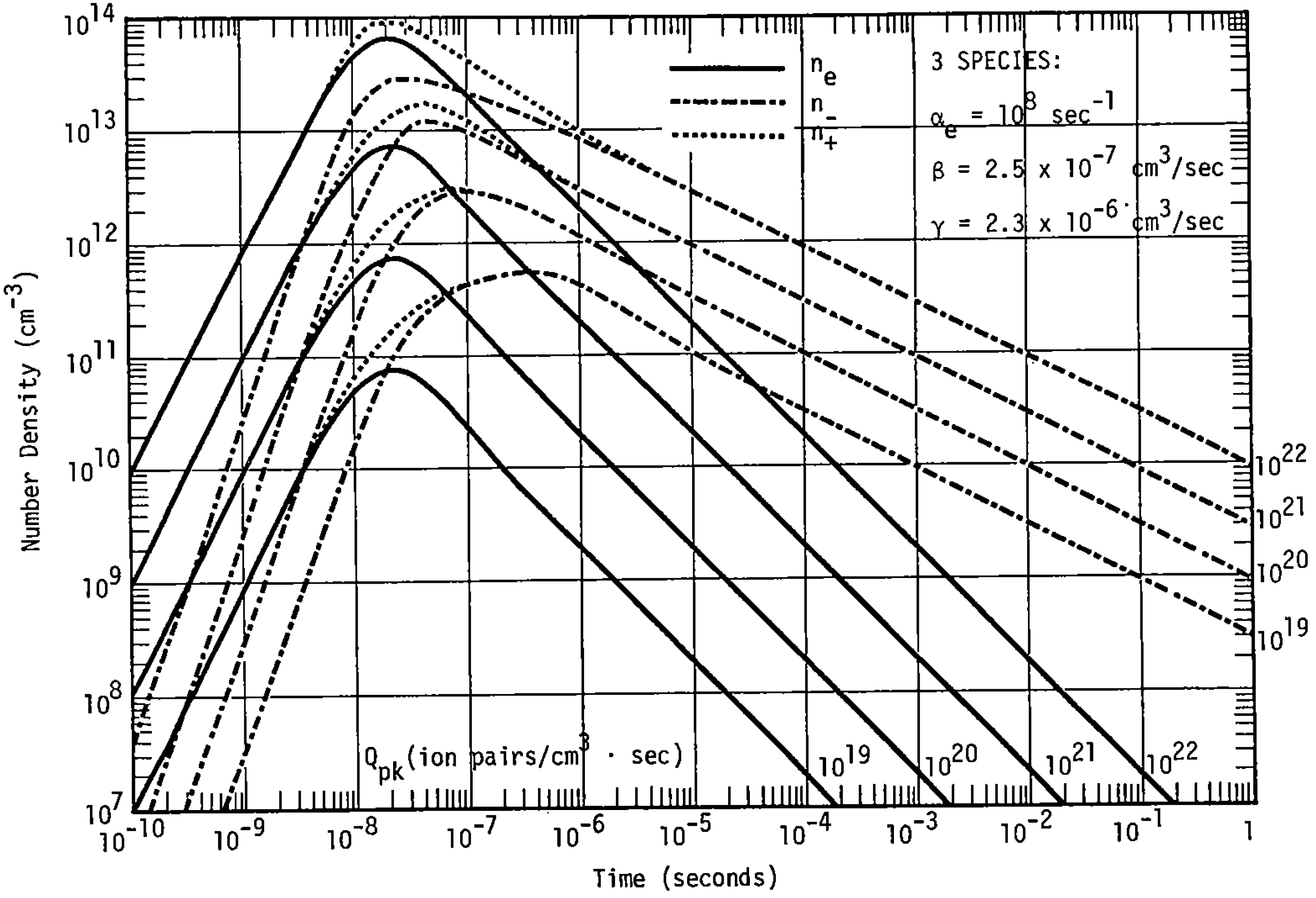

Figure 1. The time dependence of the electron, positive ion and negative ion densities as provided by the solution of the three species air chemistry equations for variations in the peak ionization rate.

density rises as t^3 and decays as $t^{-1/2}$ at later times. At early times the magnitude of n_- varies proportionally to the peak ionization rate and at late times to the square root of the ionization rate. The positive ion density is the sum of the electron and negative ion densities and therefore follows the predominating time dependence at early and late times.

Of special interest in Figure 1 is the relationship between the ion densities and the electron densities at late times. As shown in Equation 1 each of the three species contributes to the air conductivity; because the zero electric field, dry air electron mobility is roughly 10^4 times larger than each of the appropriate ion mobilities, ions do not contribute significantly until the time when the sum of their densities is approximately 10^4 times larger than the electron density. Upon examination of Figure 1 it is noted that this time occurs earliest for the smallest peak air ionization rate and latest for the largest ionization rate. The exact times that the ion conductivity becomes dominant is, however, a function of the specific time behavior of the ionization rate employed, in addition to the peak value of that rate.

A similar set of calulations was performed with the DCHEM code as described in the last section. In addition to the parameters specified in Table 1, the water vapor fraction was set at 0.01. The results of these calculations were summed to the form n_+, n_-, and n_e and are presented in Figure 2; the curves are remarkably similar to those in Figure 1. Upon close examination, however, the peak values of the electron densities are no longer directly proportional to the peak ionization rate.

In order to compare these curves more easily, Figure 3 presents the results of the highest ionization rate case. At times later than 10^{-4} seconds, the reaction rate code illustrates slightly higher densities for both electrons and ions indicating that the effective attachment rate and ion neutralization coefficient must be slightly smaller than those assumed

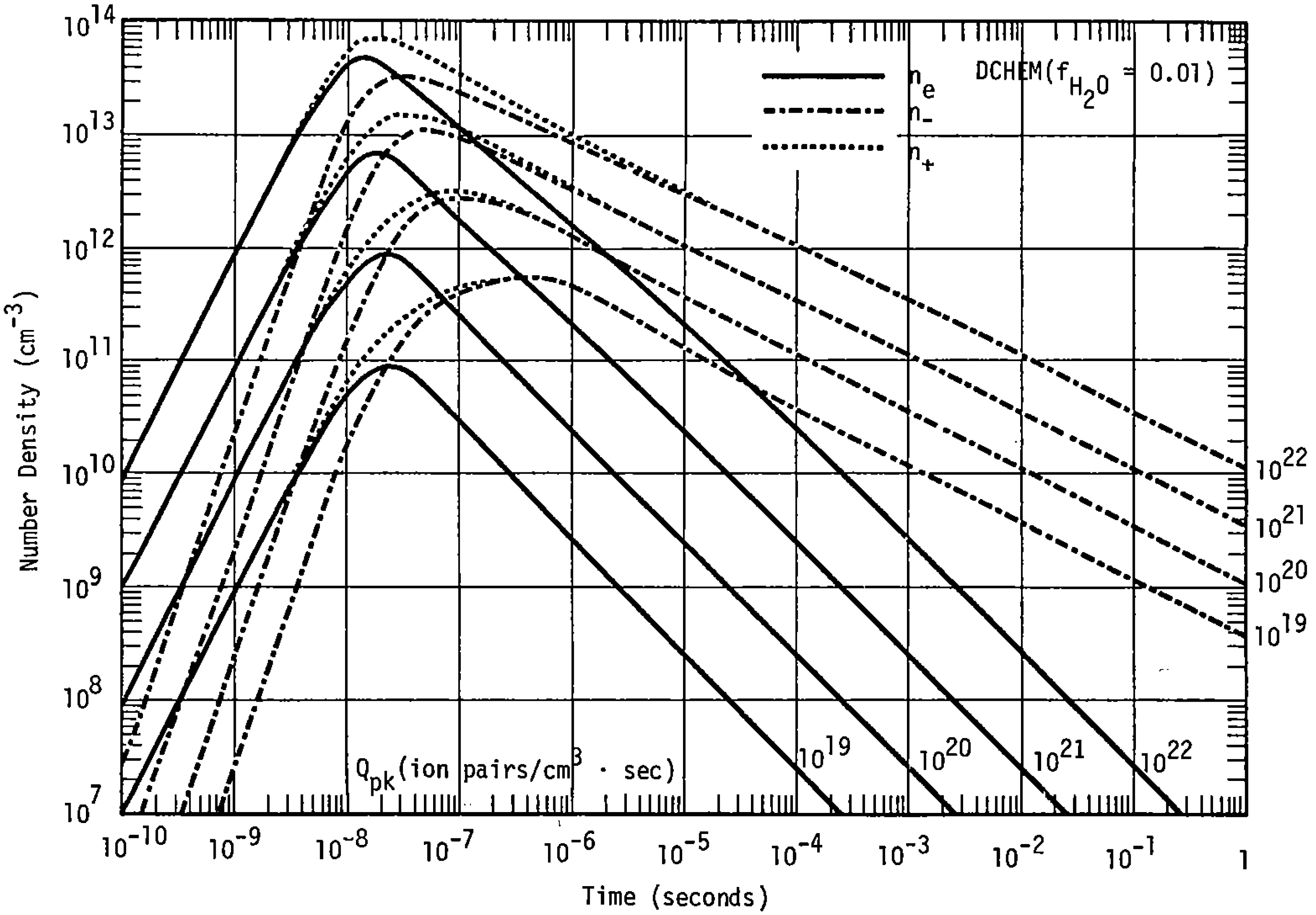

Figure 2. The time dependence of the electron densities and the sum of all positive and negative ion densities as calculated with the DCHEM code for variations in the peak ionization rate.

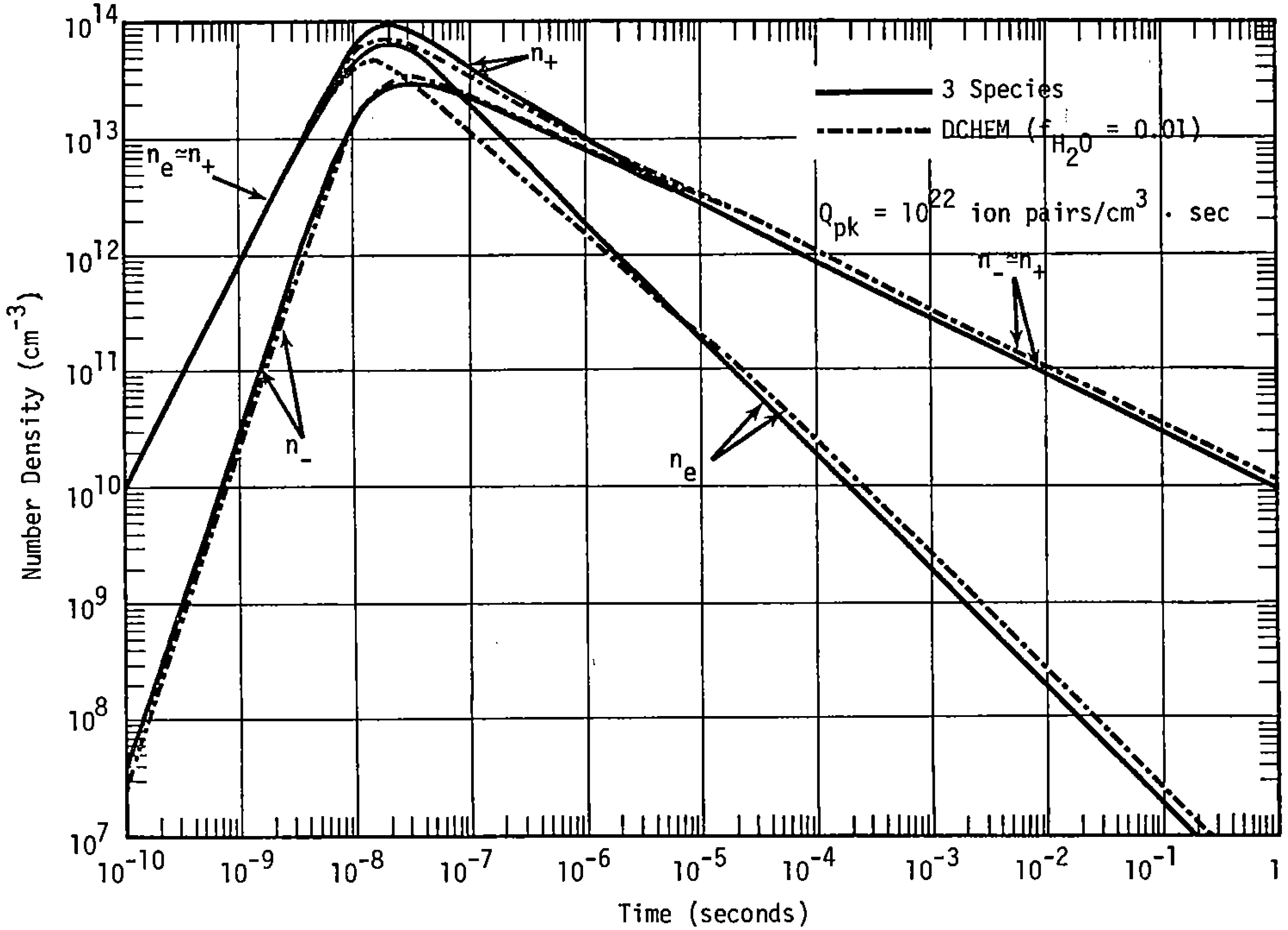

Figure 3. A comparison of the electron and ion densities as calculated from a three species and a multi-species treatment of the air chemistry.

in the three species code. The lower attachment rate is also exhibited through a smaller negative ion density at early times. Unfortunately the electron density predicted by the DCHEM code near the peak disagrees by roughly a factor of two.

After an examination of the dominate reaction rates in DCHEM, it was noted that the presence of water vapor was the likely contributor to the difference observed. Therefore two additional DCHEM calculations were made for water vapor fractions of 0.001 and 0.06 (equivalent to 100 percent relative humidity at approximately -20 and 36°C, respectively[24]). Although it is possible to achieve a smaller water vapor fraction through a decrease in the relative humidity, these values along with the 0.01 already specified should provide a reasonable range of values.

Figure 4 illustrates a comparison of the predicted electron densities from the water vapor dependent DCHEM results and the appropriate three species calculations for peak ionization rates of 10^{19} and 10^{22} ion pairs/cm^3 sec. At the lower ionization rate all of the results appear to be related by a constant factor after the peak, and the three species calculation is straddled by the other predictions. However, in the high flux case this linearity appears to hold only at later times. Near the peak the three species treatment is as much as 3.5 times larger than the 0.06 water vapor fraction case. It is apparent that the effective electron attachment rate (α_e) and electron-ion recombination coefficient (β) as employed in the three species equations (11-13) are both functions of the water vapor fraction.

To determine the attachment rate variation, the relevant DCHEM reactions were examined and are listed in Table 2 with their appropriate rate coefficients. All of the rates shown are in agreement with those in the DNA reaction rate handbook[21].

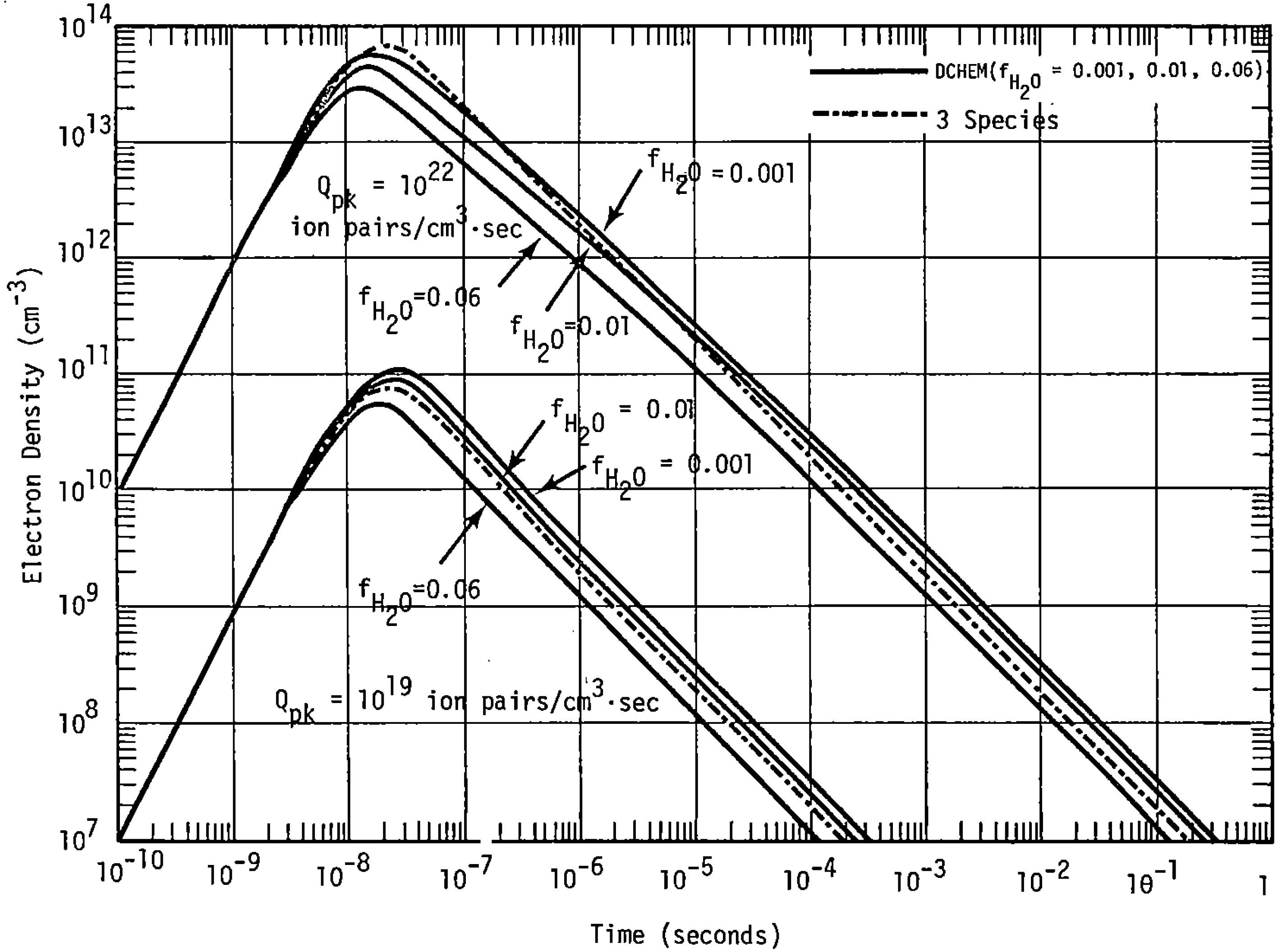

Figure 4. A comparison of the three species and the multi-species solution of the electron density for variations in water vapor fraction and peak ionization rate.

Table 2. Three-body attachment reactions and rate coefficients.

Reaction	Rate Coefficient $\left(\frac{cm^6}{sec}\right)$
$O_2 + e + O_2 \rightarrow O_2^- + O_2$	1.4×10^{-29} (T/300) exp(-600/T) $= 1.85 \times 10^{-30}$ for T = 293°K
$O_2 + e + N_2 \rightarrow O_2^- + N_2$	1.0×10^{-31}
$O_2 + e + H_2O \rightarrow O_2^- + H_2O$	1.4×10^{-29}

In order to calculate a sea-level reaction rate, the input parameters from Table 1 are substituted into the following equation

$$\alpha_e(\sec^{-1}) = 1.85 \times 10^{-30}(N_{O_2})^2 + 1.0 \times 10^{-31} N_{O_2} N_{N_2} + 1.4 \times 10^{-29} N_{O_2} N_{H_2O} , \quad (14)$$

where N_{O_2}, N_{N_2}, and N_{H_2O} are the molecular densities in cm^{-3} of O_2, N_2 and H_2O; this results in

$$\alpha_e(\sec^{-1}) = 6.133 \times 10^7 + 1.838 \times 10^9 f_{H_2O} . \quad (15)$$

Table 3 lists the effective attachment rates for the three selected water vapor fractions as determined by Equation 15. Upon reexamination of Figure 4 at times after the peak in the low flux case and for $t > 10^{-4}$ seconds in the high flux case, the magnitude of the electron density is inversely proportional to the attachment rate. This indicates that the attachment reaction alone adequately describes the late-time (and low flux) behavior of the electron density. The behavior of the peak electron density in the high flux case is clearly not uniquely described, however, by the attachment rate.

Table 3. Effective sea-level attachment rates as a function of water vapor content.

f_{H_2O}	$\alpha_e(\text{sec}^{-1})$
0.001	6.317×10^7
0.01	7.971×10^7
0.06	1.716×10^8

In the three species treatment, Equation 11 contains an additional non-linear term which may reduce the electron density in high flux cases. The reaction is loosely termed an electron-ion recombination reaction with an assumed rate coefficient of $\beta = 2.5 \times 10^{-7}$ cm^3/sec which is indicative of the dissociative recombination rate coefficient of O_2^+ with an electron. A survey of the important recombination coefficients in the DCHEM calculations performed here are listed in Table 4.

As the actual decay rate of electrons is determined by the product of these coefficients and the positive ion density of interest, Table 4 alone is not sufficient to allow the selection of a more accurate value for a lumped recombination rate coefficient. An examination of the individual positive ion densities in DCHEM at early times, however, clearly indicates that the O_4^+ reaction dominates the O_2^+ and N_2^+ reactions in the low water vapor content case; in the higher water vapor calculations the $(H_2O)_n \cdot H_3O^+$ species (hydrated ions) dominate the recombination reaction. Since the rate coefficients for these respective reactions are roughly a factor of 10 greater than the O_2^+ reaction, it is clear that our selection of β is not satisfactory. Also since the production rate of hydrated ions is a function of water vapor content and ionization rate, the selection of a constant value for β in Equation 11 does not appear appropriate.

Table 4. Dissociative recombination reactions and rate coefficients.

Reaction	Rate Coefficient (cm^3/sec)	Rate Coefficient at T = 293°K (cm^3/sec)
$O_4^+ + e \rightarrow O_2 + O_2$	$2.00 \times 10^{-6}\ (T/300)^{-1}$	2.05×10^{-6}
$H_2O_3^+ + e \rightarrow H_2O + O_2$	$1.50 \times 10^{-6}\ (T/300)^{-1}$	1.54×10^{-6}
$H_4O_2^+ + e \rightarrow H_2O + H_2O$	3.00×10^{-6}	3.00×10^{-6}
$N_2^+ + e \rightarrow N(2D) + N$	$2.70 \times 10^{-7}\ (T/300)^{-.2}$	2.71×10^{-7}
$O_2^+ + e \rightarrow O + O$	$2.10 \times 10^{-7}\ (T/300)^{-.7}$	2.13×10^{-7}
$H_3O^+ + e \rightarrow H_2O + H$	1.00×10^{-6}	1.00×10^{-6}
$H_5O_2^+ + e \rightarrow H_2O + H_2O + H$	2.20×10^{-6}	2.20×10^{-6}
$H_7O_3^+ + e \rightarrow (H_2O)_2 + H_2O + H$	4.60×10^{-6}	4.60×10^{-6}
$H_9O_4^+ + e \rightarrow (H_2O)_2 + (H_2O)_2 + H$	6.00×10^{-6}	6.00×10^{-6}
$H_{11}O_5^+ + e \rightarrow (H_2O)_2 + (H_2O)_3 + H$	6.00×10^{-6}	6.00×10^{-6}

In order to estimate a lumped recombination coefficient β, an empirical approach was chosen. Upon examination of specific DCHEM calculations, it was possible to compute an effective electron-ion recombination rate at each time of interest from

$$\overline{\beta n_+} = \sum \beta_i n_i^+ \ . \qquad (16)$$

Figure 5 illustrates the ratio of this quantity to the electron attachment rate (as given in Equation 15) as a function of time for the two largest ionization rates and the three water vapor fractions. It is apparent that the recombination rate is a function of peak ionization rate, water vapor fraction and time. It is also true that higher ionization rates might create a larger impact although increased ionization is usually accompanied by higher electric EMP fields which can directly remove energy from the high energy Compton electrons that produce the air ionization (a self-consistent effect). Lower ionization rates ($<10^{21}$ ion pairs/$\text{cm}^3 \cdot$ sec) will result in the reduction of the impact of electron-ion recombination for the assumptions made in this study.

Figure 6 describes the variation of the lumped parameter β from Figure 5 as a function of the same variables. From this figure the dependence on peak ionization rate is less than the corresponding time and water vapor variations. It was possible, therefore, to roughly fit this coefficient so that the resultant electron density calculated from a lumped parameter set of three species equations (Equations 11-13) would closely reproduce the solution from the multi-species code DCHEM over times of interest. This fit is given as

$$\beta(\text{cm}^3/\text{sec}) = 2.0 \times 10^{-7} + 1.30 \times 10^{-5} \, (f_{H_2O})^{1/3} \ , \qquad (17)$$

for $0.001 \le f_{H_2O} \le 0.06$.

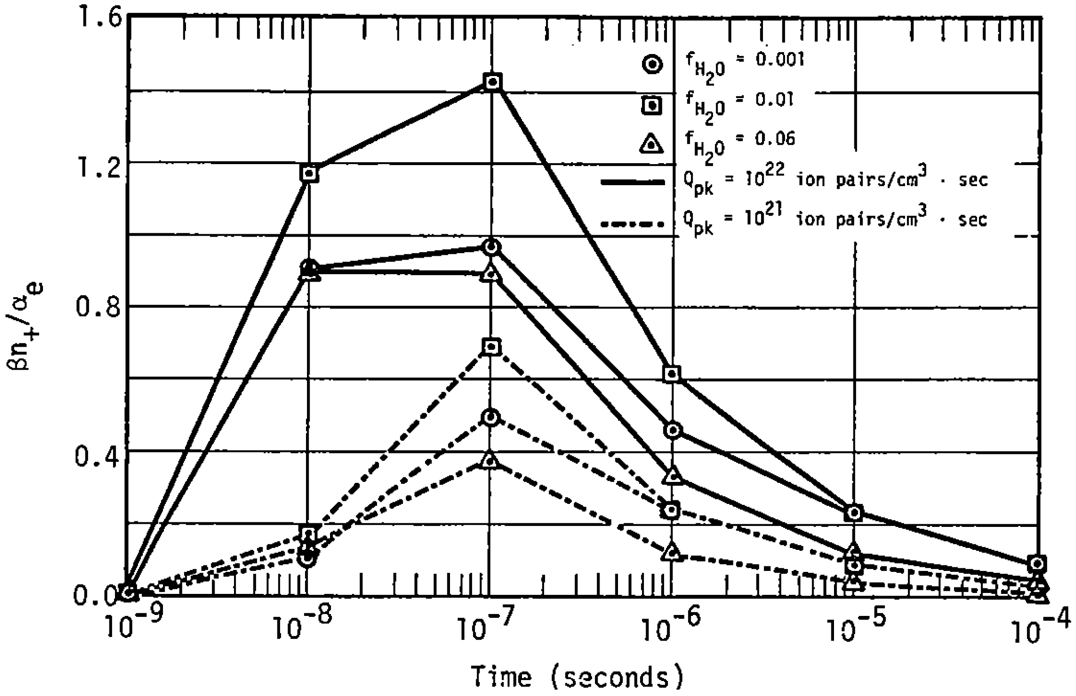

Figure 5. The variation of the ratio of the "average" recombination and attachment rates in the DCHEM code as functions of water vapor fraction, peak ionization rate and time.

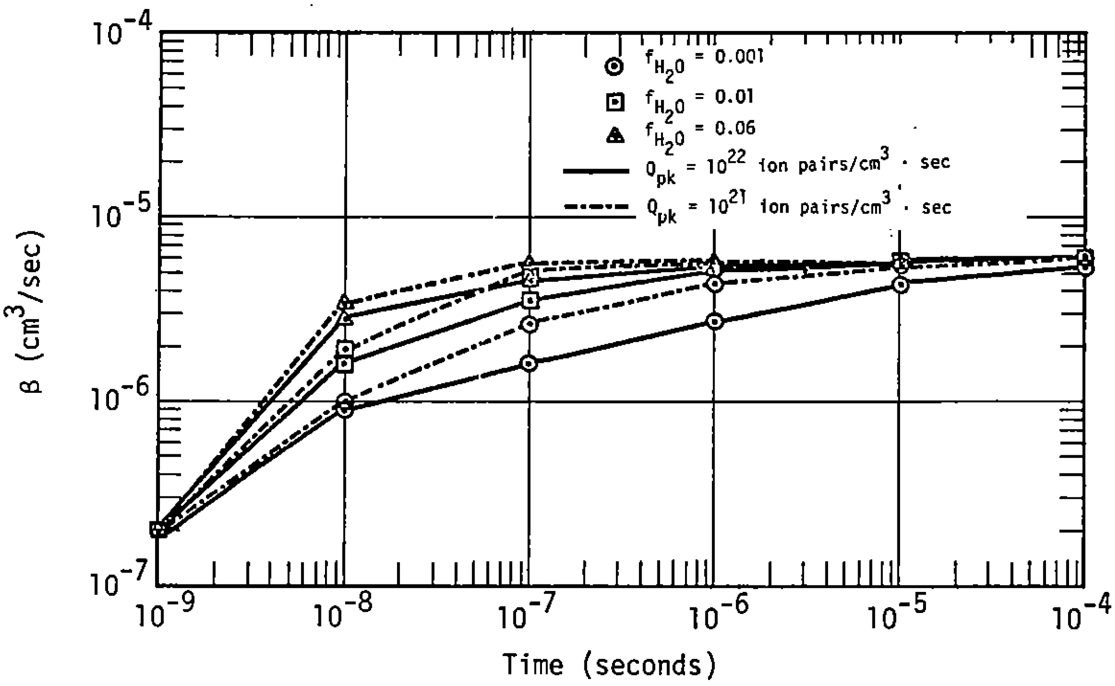

Figure 6. The variation of the "average"recombination rate coefficient in the DCHEM code as functions of water vapor fraction, peak ionization rate and time.

Using Equations 15 and 17 and further specifying $\gamma = 1.69 \times 10^{-6}$ cm^3/sec based upon the dominant two- and three-body mutual neutralization and recombination rate coefficients as employed in DCHEM, Equations 11-13 may be solved again. Figure 7 illustrates a comparison of these calculations with the DCHEM results and the previous three species treatment. The positive and negative ion species also agree quite well and are not shown here. The main disagreement in the ion species previously occurred (Figure 3) due to the differences in the values of α_e and γ which have now been established for the assumptions in this study.

A final piece of information which may be extracted from the DCHEM multi-species calculations is the specification of "lumped-parameter" values for the positive and negative ion mobilities. After surveying the ion constituents at times later than 10^{-4} seconds, the major negative ion species appeared to be NO_3^-, CO_3^-, CO_4^-, and O_4^-. The positive ion density was found in all cases to be composed nearly completely by hydrated ions $(H_2O)_n \cdot H_3O^+$, even in the 0.001 water vapor fraction case.

Table 5 lists the mobilities of these ions in air for T ≈ 300°K and $\rho = 2.5 \times 10^{19}$ molecules/cm^3 (scaled from Reference 21)*. Mobilities for the larger hydrated ions are not available in Reference 21 and may be somewhat lower than those shown in Table 5. Also the presence of hydrated negative ions at sea level is likely, and this study did not include those species[25]. In addition the mobilities of negative hydrated ions have not been accurately established. In spite of these difficulties, however, the author suggests the continued use of $\mu_+ = \mu_- = 2.5$ (cm/sec)/(v/cm) as in the past[4]. Developments in the reaction rate community may indicate a better value at some future date.

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* The data in Reference 21 were collected for radio-frequency transmission purposes (and altitudes above 60 km) and may not be entirely accurate for our purposes here.

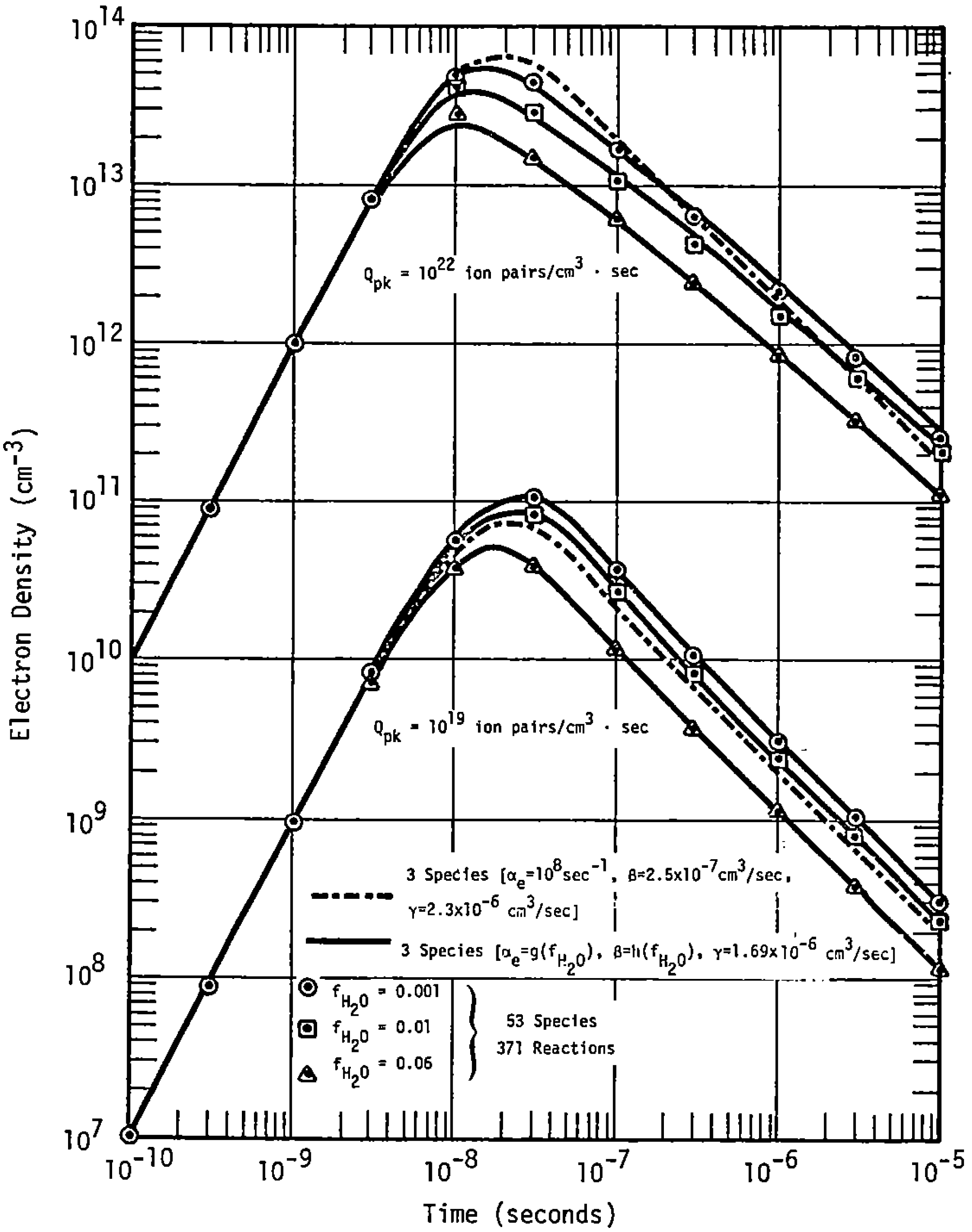

Figure 7. Comparison of the old and new three species treatment with the DCHEM code for variations in water vapor fraction and peak ionization rate.

Table 5. Ion mobilities in air for T = 300°K and $\rho = 2.5 \times 10^{19}$ molecules/cm^3.

Ion	Mobility [cm/sec)/(v/cm)]
NO_3^-	2.48
CO_3^-	2.52
CO_4^-	2.40
O_4^-	2.40
H_3O^+	3.24
$H_3O^+ \cdot H_2O$	2.72

SECTION 5

CONCLUSIONS

The purpose of this study was to determine whether or not the three species air chemistry treatment as employed in EMP ground-burst codes was adequate with respect to state-of-the-art multi-species air chemistry solutions. Within the constraints assumed (mainly no electric field dependence), it appears that a three species solution is possible given that the proper coefficients are employed. The coefficients as assumed by MRC in the past had the potential of overpredicting the electron density by as much as a factor of 3.5. However, the possibility of a strong electric field dependence may increase or decrease this potential error.

It is important, however, to understand that the coefficients employed in the DCHEM code are based upon reaction rate research which results in the continual updating of the coefficients and their respective uncertainties. For example the excellent late-time ion agreement between the three species and multi-species treatments was afforded primarily because DCHEM assumed the same two- and three-body neutralization rate coefficients for 138 of the 144 ion-ion reactions. It is likely that any improvements in these reaction rates will change the lumped parameter chosen for the three species treatment. Also the number of species and reactions carried in the reaction rate codes increases with time in an attempt to provide more accurate solutions.

Based upon this effort the author recommends the following lumped parameter coefficients as more suitable than those employed in the past for use in the solution of ground-burst EMP:

$$\alpha_e(\mathrm{sec}^{-1}) = 6.133 \times 10^7 + 1.838 \times 10^9 f_{H_2O} , \quad (18)$$

$$\beta(\mathrm{cm}^3/\mathrm{sec}) = 2.00 \times 10^{-7} + 1.30 \times 10^{-5}(f_{H_2O})^{1/3} , \quad (19)$$

and

$$\gamma(\mathrm{cm}^3/\mathrm{sec}) = 1.69 \times 10^{-6} , \quad (20)$$

for fractions of water vapor content, $0.001 \leq f_{H_2O} \leq 0.06$.

The author further recommends that additional study be directed toward the impact of electron temperature variations on the relevant reaction rates. This could be done through the use of typical electric EMP field time histories in the reaction rate codes or through a thorough review of the temperature dependence of the electron attachment and dissociative recombination coefficients.* Based upon the significant error arising in what was thought to be a well calculated quantity (the electron density) under constrained conditions (no electric field dependence), further study seems prudent. Also recent disagreements between predicted and measured EMP waveforms under well controlled conditions may be explained through a more complete understanding of the EMP-related air chemistry.

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* The electron attachment field dependence including the effect of water vapor as a third body has recently been specified by Longley and Longmire[26].

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APPENDIX

The following species and reactions were used in the DCHEM solution of the air chemistry for this report. The column labeled "rates" refers to the sea level rate coefficient actually employed in the code solution. The coefficients A, B, and C are to be used in Equation A-1.

$$k = A(T/300)^{-B} \exp(-1000\, c/T) \quad , \qquad \text{(A-1)}$$

for T in °K and k in the same units as A (for two-body reactions the units are cm^3/sec; for three-body reactions, cm^6/sec).

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***NUMBER OF REACTIONS FOR EACH SPECIES

E        IS INVOLVED IN  48 REACTIONS
N2       IS INVOLVED IN  34 REACTIONS
O2       IS INVOLVED IN 137 REACTIONS
CO2      IS INVOLVED IN  63 REACTIONS
N        IS INVOLVED IN  27 REACTIONS
N(2D)    IS INVOLVED IN   7 REACTIONS
O        IS INVOLVED IN  79 REACTIONS
NO       IS INVOLVED IN 111 REACTIONS
O3       IS INVOLVED IN  42 REACTIONS
NO2      IS INVOLVED IN  50 REACTIONS
N2O      IS INVOLVED IN   4 REACTIONS
H2O      IS INVOLVED IN  81 REACTIONS
O2(1D)   IS INVOLVED IN  15 REACTIONS
H        IS INVOLVED IN  48 REACTIONS
H2       IS INVOLVED IN   3 REACTIONS
OH       IS INVOLVED IN  28 REACTIONS
HO2      IS INVOLVED IN  24 REACTIONS
H2O2     IS INVOLVED IN   6 REACTIONS
NO3      IS INVOLVED IN  33 REACTIONS
O4       IS INVOLVED IN  20 REACTIONS
N2O2     IS INVOLVED IN   9 REACTIONS
(H2O)2   IS INVOLVED IN  27 REACTIONS
(H2O)3   IS INVOLVED IN  21 REACTIONS
(H2O)4   IS INVOLVED IN  11 REACTIONS
(H2O)5   IS INVOLVED IN  10 REACTIONS
NO+      IS INVOLVED IN  35 REACTIONS
N2+      IS INVOLVED IN   3 REACTIONS
O2+      IS INVOLVED IN  23 REACTIONS
N+       IS INVOLVED IN   7 REACTIONS
O+       IS INVOLVED IN   9 REACTIONS
O4+      IS INVOLVED IN  16 REACTIONS
N2O2+    IS INVOLVED IN  19 REACTIONS
H3O+     IS INVOLVED IN  14 REACTIONS
H2O3+    IS INVOLVED IN  17 REACTIONS
H4O2+    IS INVOLVED IN  13 REACTIONS
H5O2+    IS INVOLVED IN  15 REACTIONS
H7O3+    IS INVOLVED IN  15 REACTIONS
H9O4+    IS INVOLVED IN  14 REACTIONS
H11O5+   IS INVOLVED IN  12 REACTIONS
H2NO2+   IS INVOLVED IN  20 REACTIONS
H4NO3+   IS INVOLVED IN  14 REACTIONS
H6NO4+   IS INVOLVED IN  13 REACTIONS
NON2+    IS INVOLVED IN  15 REACTIONS
NOCO2+   IS INVOLVED IN  18 REACTIONS
O-       IS INVOLVED IN  30 REACTIONS
O2-      IS INVOLVED IN  36 REACTIONS
O3-      IS INVOLVED IN  29 REACTIONS
O4-      IS INVOLVED IN  27 REACTIONS
NO2-     IS INVOLVED IN  28 REACTIONS
NO3-     IS INVOLVED IN  29 REACTIONS
NR3-     IS INVOLVED IN  22 REACTIONS
CO3-     IS INVOLVED IN  24 REACTIONS
CO4-     IS INVOLVED IN  25 REACTIONS
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                         REACTIONS                                            RATES       COEFFICIENTS
                                                                                          A             B           C
 1   N2      +                 = N2+    + E                                  IIII     7.50E-01      0.00        0.00
 2   N2      +                 = N+     + E       + N                        IIII     4.00E-02      0.00        0.00
 3   O2      +                 = O2+    + E                                  IIII     1.90E-01      0.00        0.00
 4   O2      +                 = O+     + E       + O                        IIII     2.00E-02      0.00        0.00
 5   O2      +                 = O      + O                                  IIII     7.40E-01      0.00        0.00
 6   O2      +                 = O2(1D)+                                     IIII     2.00E+00      0.00        0.00
 7   N2      +                 = N(2D)  + N                                  IIII     1.60E-01      0.00        0.00
 8   N2      +                 = N(2D)  + N(2D)                              IIII     7.00E-02      0.00        0.00
 9   O2      +                 = O      + O                             0.            2.50E-07      0.00        0.00
10   O3      +                 = O2     + O                             0.            1.00E-02      0.00        0.00
11   O3      +                 = O2(1D)+ O                              0.            1.00E-02      0.00        0.00
12   NO2     +                 = NO     + O                             0.            1.00E-02      0.00        0.00
13   N2O     +                 = N2     + O                             0.            4.00E-07      0.00        0.00
14   N2O     +                 = N      + NO                            0.            6.00E-08      0.00        0.00
15   O2-     +                 = O2     + E                             0.            3.30E-01      0.00        0.00
16   O-      +                 = O      + E                             0.            1.40E+00      0.00        0.00
17   O3-     +                 = O3     + E                             0.            2.00E-01      0.00        0.00
18   NO2-    +                 = NO2    + E                             0.            4.00E-02      0.00        0.00
19   NO3-    +                 = NO     + O2      + E                   0.            1.00E-02      0.00        0.00
20   NO3-    +                 = NO     + O2      + E                   0.            1.00E-01      0.00        0.00
21   NO3-    +                 = NO     + O2-                           0.            1.00E-01      0.00        0.00
22   CO3-    +                 = CO2    + O       + E                   0.            1.00E-01      0.00        0.00
23   O4-     +                 = O2     + O2-                           0.            1.00E-01      0.00        0.00
24   O4-     +                 = O2     + O2      + E                   0.            1.00E-01      0.00        0.00
25   CO4-    +                 = CO2    + O2-                           0.            1.00E-01      0.00        0.00
26   CO4-    +                 = CO2    + O2      + E                   0.            1.00E-01      0.00        0.00
27   O       + O2      + M     = O3     +         + M                   6.27E-34      1.10E-34      0.00        -.51
28   O       + NO      + M     = NO2    +         + M                   1.01E-31      4.10E-33      0.00        -.94
29   N       + O2              = NO     + O                             6.91E-17      3.30E-12     -1.00        3.15
30   N(2D)   + O2              = NO     + O                             7.08E-12      7.00E-12       .50        0.00
31   N       + NO              = N2     + O                             2.80E-11      2.80E-11      0.00        0.00
32   N(2D)   + NO              = N2     + O                             6.00E-11      6.00E-11      0.00        0.00
33   N       + NO2             = NO     + NO                            9.00E-12      9.00E-12      0.00        0.00
34   N       + NO2             = N2O    + O                             9.00E-12      9.00E-12      0.00        0.00
35   O       + NO2             = NO     + O2                            9.10E-12      9.10E-12      0.00        0.00
36   NO      + O3              = NO2    + O2                            1.60E-14      1.50E-12      0.00        1.33
37   NO      + NO      + O2    = NO2    + NO2                           2.01E-38      3.30E-39      0.00        -.53
38   N       + O3              = NO     + O2                            5.59E-13      3.40E-11      -.50        1.20
39   O       + O       + M     = O2     +         + M                   7.45E-33      1.30E-32      1.00         .17
40   N       + N       + M     = N2     +         + M                   4.57E-33      8.30E-34      0.00        -.50
41   N       + O       + M     = NO     +         + M                   1.11E-32      1.10E-32       .50        0.00
42   N       + N               = N2     +                               1.02E-17      1.00E-17       .90        0.00
43   O       + NO              = NO2    +                               6.90E-17      6.60E-17      1.90        0.00
44   N       + O               = NO     +                               1.50E-17      1.50E-17      0.00        0.00
45   NO3     + NO              = NO2    + NO2                           5.33E-12      5.70E-11      0.00         .70
46   NO2     + O3              = NO3    + O2                            4.09E-17      6.20E-12      0.00        3.50
47   NO3     + O               = NO2    + O2                            5.98E-15      1.00E-12      0.00        1.50
48   NO3     + NO3             = NO2    + NO2     + O2                  1.79E-16      5.00E-12      0.00        3.00
49   N2+     + E               = N(2D)  + N                             2.71E-07      2.70E-07       .20        0.00
50   O2+     + E               = O      + O                             2.13E-07      2.10E-07       .70        0.00
51   NO+     + E               = N      + O                             1.02E-07      1.00E-07      1.00        0.00
52   NO+     + E               = N(2D)  + O                             3.07E-07      3.00E-07      1.00        0.00
53   O+      + E       + E     = O      + E                             1.11E-19      1.00E-19      4.50        0.00
54   N+      + E       + E     = N      + E                             1.11E-19      1.00E-19      4.50        0.00
55   O2(1D)+ O3                = O2     + O2      + O                   3.18E-15      4.50E-11      0.00        2.80
56   O2(1D)+ N                 = O2     + N                             1.55E-13      2.00E-14      0.00        -.60
57   O2(1D)+ O                 = O2     + O                             1.00E-16      1.00E-16      0.00        0.00
58   O2(1D)+ E                 = O2     + E                             1.00E-11      1.00E-11      0.00        0.00
59   O2(1D)+ N2                = O2     + N2                            1.00E-20      1.00E-20      0.00        0.00
60   O2(1D)+ O2                = O2     + O2                            2.16E-18      2.20E-18      -.80        0.00
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                                                                   A           B          C
 61   O2(1D)+                    = O2     +                 2.60E-04   2.60E-04     0.00       0.00
 62   O      + O3                = O2(1D)+ O2               3.90E-15   1.00E-11     0.00       2.50
 63   O      + O3                = O2     + O2              3.90E-15   1.00E-11     0.00       2.30
 64   H      + HO2               = OH     + OH              1.64E-11   4.20E-10     0.00        .95
 65   H      + HO2               = H2     + O2              1.27E-11   4.20E-11     0.00        .35
 66   H      + HO2               = H2O    + O               2.90E-12   1.60E-11     0.00        .50
 67   H      + NO2               = OH     + NO              4.64E-11   5.80E-10     0.00        .74
 68   O      + HO2               = OH     + O2              1.43E-11   7.90E-11     0.00        .50
 69   OH     + HO2               = H2O    + O2              2.90E-12   1.60E-11     0.00        .50
 70   OH     + O3                = HO2    + O2              5.27E-14   1.60E-12     0.00       1.00
 71   OH     + OH                = H2O    + O               1.82E-12   1.00E-11     0.00        .50
 72   H      + H2O2              = HO2    + H2              4.27E-15   2.80E-12     0.00       1.90
 73   H      + H2O2              = OH     + H2O             1.13E-16   5.30E-10     0.00       4.50
 74   OH     + OH      + M       = H2O2   +        + M      4.40E-30   4.00E-30     4.00       0.00
 75   OH     + H2O2              = HO2    + H2O             7.61E-13   1.70E-11     0.00        .91
 76   HO2    + HO2               = H2O2   + O2              5.45E-12   3.00E-11     0.00        .50
 77   H2O2   + O                 = OH     + HO2             1.53E-15   3.60E-11     0.00       2.95
 78   HO2    + NO                = OH     + NO2             2.00E-13   2.00E-13     0.00       0.00
 79   H      + O2      + M       = HO2    +        + M      5.65E-32   2.10E-32     0.00       -.29
 80   H      + O3                = OH     + O2              2.60E-11   2.60E-11     0.00       0.00
 81   OH     + H2                = H      + H2O             5.22E-15   3.60E-11     0.00       2.59
 82   OH     + N                 = H      + NO              5.30E-11   5.30E-11     0.00       0.00
 83   OH     + O       + M       = HO2    +        + M      1.00E-31   1.00E-31     0.00       0.00
 84   H      + OH      + M       = H2O    +        + M      4.51E-30   4.30E-30     2.00       0.00
 85   HO2    + O3                = OH     + O2     + O2     1.40E-13   1.00E-13     0.00       1.25
 86   O      + OH                = H      + O2              4.20E-11   4.20E-11     0.00       0.00
 87   O      + H       + M       = OH     +        + M      2.00E-32   2.00E-32     0.00       0.00
 88   (H2O)2+          + M       = H2O    + H2O    + M      1.00E-10   1.00E-10     0.00       0.00
 89   (H2O)3+          + M       = (H2O)2+ H2O     + M      1.00E-10   1.00E-10     0.00       0.00
 90   (H2O)4+          + M       = (H2O)3+ H2O     + M      1.00E-10   1.00E-10     0.00       0.00
 91   (H2O)5+          + M       = (H2O)4+ H2O     + M      1.00E-10   1.00E-10     0.00       0.00
 92   O4     +         + M       = O2     + O2     + M      1.00E-10   1.00E-10     0.00       0.00
 93   N2O2   +         + M       = NO     + NO     + M      1.00E-10   1.00E-10     0.00       0.00
 94   N2+    + NO                = NO+    + N2              3.30E-10   3.30E-10     0.00       0.00
 95   N2+    + O2                = O2+    + N2              5.06E-11   5.00E-11      .50       0.00
 96   N2+    + O                 = O+     + N2              6.00E-12   6.00E-12     0.00       0.00
 97   N2+    + N                 = N+     + N2              1.00E-11   1.00E-11     0.00       0.00
 98   N+     + NO                = N      + NO+             8.00E-10   8.00E-10     0.00       0.00
 99   N+     + O2                = N      + O2+             3.00E-10   3.00E-10     0.00       0.00
100   N+     + O                 = N      + O+              1.00E-12   1.00E-12     0.00       0.00
101   O+     + NO                = NO+    + O               1.30E-12   1.30E-12     0.00       0.00
102   O+     + O2                = O2+    + O               2.02E-11   2.00E-11      .50       0.00
103   O+     + N2      + M       = NO+    + N      + M      1.68E-29   1.60E-29     2.00       0.00
104   O2+    + NO                = NO+    + O2              6.30E-10   6.30E-10     0.00       0.00
105   O2+    + N2                = NO+    + NO              1.00E-16   1.00E-16     0.00       0.00
106   N+     + O2                = O      + NO+             3.00E-10   3.00E-10     0.00       0.00
107   O+     + N2                = NO+    + N               1.21E-12   1.20E-12      .50       0.00
108   O+     + N2O               = NO+    + NO              8.90E-10   6.90E-10     0.00       0.00
109   N2+    + O                 = NO+    + N(2D)           7.00E-11   7.00E-11     0.00       0.00
110   N2+    + O                 = NO+    + N               7.00E-11   7.00E-11     0.00       0.00
111   O2+    + NO2               = NO+    + O3              1.00E-11   1.00E-11     0.00       0.00
112   O2+    + N                 = NO+    + O               1.80E-10   1.80E-10     0.00       0.00
113   NO+    + NO      + M       = N2O2+  +        + M      5.12E-30   5.00E-30     1.00       0.00
114   N2O2+  +         + M       = NO+    + NO     + M      4.31E-16   1.00E-05     1.00       7.00
115   N2O2+  + O                 = NO+    + NO2             3.00E-10   3.00E-10     0.00       0.00
116   N2O2+  + CO2               = NOCO2++ NO               2.71E-16   2.50E-13     0.00       2.00
117   N2O2+  + H2O               = H2NO2++ NO               1.40E-09   1.40E-09     0.00       0.00
118   H2NO2++ NO                 = N2O2+  + H2O             7.80E-14   2.00E-10     0.00       2.30
119   H2NO2++ N2                 = NON2+  + H2O             5.10E-19   2.20E-09     0.00       6.50
120   H2NO2++ CO2                = NOCO2++ H2O              1.13E-13   2.67E-07     0.00       4.30
121   H2NO2++          + M       = NO+    + H2O    + M      3.36E-19   2.00E-05     1.00       9.30
122   NO+    + H2O     + M       = H2NO2++         + M      1.57E-28   1.50E-28     2.00       0.00
```

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                                                                              A            B          C
123   H2NO2++ H2O    + M    = H4NO3++         + M        1.15E-27     1.10E-27     2.00       0.00
124   H4NO3++        + M    = H2NO2++ H2O     + M        4.41E-15     1.00E-04     2.00       7.00
125   H4NO3++ H2O    + M    = H6NO4++         + M        1.68E-27     1.60E-27     2.00       0.00
126   H6NO4++        + M    = H4NO3++ H2O     + M        8.63E-13     2.00E-02     2.00       7.00
127   H6NO4++ H2O           = H7O3+ + OH      + NO       7.00E-11     7.00E-11     0.00       0.00
128   NO+    + N2    + M    = NON2+ +         + M        2.10E-31     2.00E-31     2.00       0.00
129   NON2+  +       + M    = NO+   + N2      + M        9.53E-13     1.20E-08     2.00       2.78
130   NON2+  + H2O          = H2NO2++ N2                 1.00E-09     1.00E-09     0.00       0.00
131   NON2+  + CO2          = NOCO2++ N2                 1.00E-09     1.00E-09     0.00       0.00
132   NON2+  + NO           = N2O2+ + N2                 1.50E-09     1.50E-09     0.00       0.00
133   N2O2+  + N2           = NON2+ + NO                 1.79E-17     3.00E-11     0.00       4.20
134   NOCO2++ N2            = NON2+ + CO2                4.57E-15     8.33E-12     0.00       2.20
135   NOCO2++ NO            = N2O2+ + CO2                1.00E-09     1.00E-09     0.00       0.00
136   NOCO2++ H2O           = H2NO2++ CO2                1.00E-09     1.00E-09     0.00       0.00
137   NO+    + CO2   + M    = NOCO2++         + M        2.10E-29     2.00E-29     2.00       0.00
138   NOCO2++        + M    = NO+   + CO2     + M        4.07E-16     1.00E-08     2.00       5.00
139   O2+    + O2    + M    = O4+   +         + M        2.94E-30     2.80E-30     2.00       0.00
140   O4+    +       + M    = O2+   + O2      + M        2.03E-14     5.00E-07     2.00       5.00
141   O4+    + O            = O2+   + O3                 3.00E-10     3.00E-10     0.00       0.00
142   O4+    + NO           = NO+   + O2      + O2       5.00E-10     5.00E-10     0.00       0.00
143   O2+    + H2O   + M    = H2O3+ +         + M        2.94E-28     2.80E-28     2.00       0.00
144   O4+    + H2O          = H2O3+ + O2                 1.50E-09     1.50E-09     0.00       0.00
145   H2O3+  + O2           = O4+   + H2O                7.80E-14     2.00E-10     0.00       2.30
146   H2O3+  + O2(1D)       = O2+   + H2O     + O2       1.00E-10     1.00E-10     0.00       0.00
147   H2O3+  + NO           = NO+   + O2      + H2O      1.00E-10     1.00E-10     0.00       0.00
148   H2O3+  + H2O          = H3O+  + O2      + OH       2.00E-10     2.00E-10     0.00       0.00
149   H2O3+  + H2O          = H4O2+ + O2                 1.00E-09     1.00E-09     0.00       0.00
150   H3O+   + H2O   + M    = H5O2+ +         + M        3.56E-27     3.40E-27     2.00       0.00
151   H5O2+  +       + M    = H3O+  + H2O     + M        1.75E-26     9.00E+00     2.00      18.00
152   H4O2+  + H2O          = H5O2+ + OH                 1.40E-09     1.40E-09     0.00       0.00
153   H4O2+  +       + M    = H3O+  + OH      + M        3.39E-19     1.00E-01     2.00      11.80
154   H5O2+  + H2O   + M    = H7O3+ +         + M        2.41E-27     2.30E-27     2.00       0.00
155   H7O3+  +       + M    = H5O2+ + H2O     + M        2.63E-18     1.00E-01     2.00      11.20
156   H7O3+  + H2O   + M    = H9O4+ +         + M        2.52E-27     2.40E-27     2.00       0.00
157   H9O4+  +       + M    = H7O3+ + H2O     + M        1.89E-14     1.00E-01     2.00       8.60
158   H9O4+  + H2O   + M    = H11O5++         + M        9.23E-28     8.60E-28     2.00       0.00
159   H11O5++        + M    = H9O4+ + H2O     + M        4.02E-12     3.00E-03     2.00       6.00
160   O4+    + E            = O2    + O2                 2.05E-06     2.00E-06     1.00       0.00
161   N2O2+  + E            = NO    + NO                 1.74E-06     1.70E-06     1.00       0.00
162   H3O+   + E            = H2O   + H                  1.00E-06     1.00E-06     0.00       0.00
163   H5O2+  + E            = H2O   + H2O     + H        2.20E-06     2.20E-06     0.00       0.00
164   H7O3+  + E            = (H2O)2+ H2O     + H        4.60E-06     4.60E-06     0.00       0.00
165   H9O4+  + E            = (H2O)2+ (H2O)2+ H          6.00E-06     6.00E-06     0.00       0.00
166   H11O5++ E             = (H2O)2+ (H2O)3+ H          6.00E-06     6.00E-06     0.00       0.00
167   H2O3+  + E            = H2O   + O2                 1.54E-06     1.50E-06     1.00       0.00
168   H4O2+  + E            = H2O   + H2O                3.00E-06     3.00E-06     0.00       0.00
169   H2NO2++ E             = H2O   + NO                 1.02E-06     1.00E-06     1.00       0.00
170   H4NO3++ E             = H2O   + NO      + H2O      2.05E-06     2.00E-06     1.00       0.00
171   H6NO4++ E             = (H2O)2+ NO      + H2O      3.07E-06     3.00E-06     1.00       0.00
172   NON2+  + E            = NO    + N2                 1.02E-06     1.00E-06     1.00       0.00
173   NOCO2++ E             = NO    + CO2                1.02E-06     1.00E-06     1.00       0.00
174   O2     + E     + O2   = O2-   +         + O2       1.35E-30     1.40E-29     1.00        .50
175   O2-    +       + O2   = O2    + E       + O2       1.36E-18     2.70E-10     -.50       5.59
176   O2     + E     + N2   = O2-   +         + N2       1.00E-31     1.00E-31     0.00       0.00
177   O2-    +       + N2   = O2    + E       + N2       7.36E-20     1.90E-12    -1.50       4.99
178   O2     + E     + H2O  = O2-   +         + H2O      1.40E-29     1.40E-29     0.00       0.00
179   NO2    + E            = NO2-  +                    4.00E-11     4.00E-11     0.00       0.00
180   O3     + E            = O-    + O2                 8.69E-12     9.00E-12    -1.50       0.00
181   O      + E            = O-    +                    1.30E-15     1.30E-15     0.00       0.00
182   O2-    + O            = O3    + E                  3.00E-10     3.00E-10     0.00       0.00
183   O2-    + N            = NO2   + E                  3.00E-10     3.00E-10     0.00       0.00
184   O-     + NO           = NO2   + E                  2.00E-10     2.00E-10     0.00       0.00
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                                                                                A            B          C
185  O-      + N               = NO     + E                2.20E-10    2.20E-10      0.00       0.00
186  O-      + O               = O2     + E                2.00E-10    2.00E-10      0.00       0.00
187  O2(1D)+ O2-               = O2     + O2     + E       2.00E-10    2.00E-10      0.00       0.00
188  O2(1D)+ O-                = O3     + E                3.00E-10    3.00E-10      0.00       0.00
189  O2-     + O               = O-     + O2               3.30E-10    3.30E-10      0.00       0.00
190  O2-     + N               = O-     + NO               1.00E-10    1.00E-10      0.00       0.00
191  O2-     + O3              = O3-    + O2               4.00E-10    4.00E-10      0.00       0.00
192  O2-     + NO2             = NO2-   + O2               8.00E-10    8.00E-10      0.00       0.00
193  O-      + O3              = O3-    + O                5.30E-10    5.50E-10      0.00       0.00
194  O-      + NO2             = NO2-   + O                1.20E-09    1.20E-09      0.00       0.00
195  O-      + CO2    + M      = CO3-   +        + M       3.17E-28    3.10E-28      1.00       0.00
196  O3-     + NO2             = NO2-   + O3               1.40E-10    1.40E-10      0.00       0.00
197  O3-     + NO2             = NO3-   + O2               1.40E-10    1.40E-10      0.00       0.00
198  O3-     + NO              = NO2-   + O2               1.00E-11    1.00E-11      0.00       0.00
199  NO2-    + O3              = NO3-   + O2               1.80E-11    1.80E-11      0.00       0.00
200  NO2-    + NO2             = NO3-   + NO               4.00E-12    4.00E-12      0.00       0.00
201  NO3-    + NO              = NO2-   + NO2              1.50E-11    1.50E-11      0.00       0.00
202  CO3-    + NO2             = NO3-   + CO2              8.00E-11    8.00E-11      0.00       0.00
203  CO3-    + NO              = NO2-   + CO2              1.80E-11    1.80E-11      0.00       0.00
204  CO3-    + O               = O2-    + CO2              8.00E-11    8.00E-11      0.00       0.00
205  CO4-    + NO3             = NO3-   + CO2    + O2      5.00E-10    5.00E-10      0.00       0.00
206  NO3-    + NO3             = NO3-   + NO     + O2      5.00E-10    5.00E-10      0.00       0.00
207  O3-     + CO2             = CO3-   + O2               5.50E-10    5.50E-10      0.00       0.00
208  O3-     + O               = O2-    + O2               1.00E-11    1.00E-11      0.00       0.00
209  O-      + O2     + M      = O3-    +        + M       1.13E-30    1.10E-30      1.00       0.00
210  O2-     + O2     + M      = O4-    +        + M       3.58E-31    3.50E-31      1.00       0.00
211  O4-     +        + M      = O2-    + O2     + M       7.63E-15    1.00E-03      1.00       7.50
212  O4-     + O               = O3-    + O2               4.00E-10    4.00E-10      0.00       0.00
213  O4-     + NO              = NO3-   + O2               2.50E-10    2.50E-10      0.00       0.00
214  O4-     + CO2             = CO4-   + O2               4.30E-10    4.30E-10      0.00       0.00
215  O4-     + NO2             = NO2-   + O2     + O2      5.00E-10    5.00E-10      0.00       0.00
216  O4-     + NO3             = NO3-   + O2     + O2      5.00E-10    5.00E-10      0.00       0.00
217  O4-     + O3              = O3-    + O2     + O2      5.00E-10    5.00E-10      0.00       0.00
218  CO4-    + O2              = O4-    + CO2              1.54E-14    4.30E-10      0.00       3.00
219  O2-     + CO2    + M      = CO4-   +        + M       2.00E-29    2.00E-29      1.00       0.00
220  CO4-    + NO              = NO3-   + CO2              4.80E-11    4.80E-11      0.00       0.00
221  CO4-    + O               = CO3-   + O2               1.50E-10    1.50E-10      0.00       0.00
222  CO4-    + O3              = O3-    + CO2    + O2      1.30E-10    1.30E-10      0.00       0.00
223  CO3-    + NO3             = NO3-   + CO2    + O       5.00E-10    5.00E-10      0.00       0.00
224  O-      + NO3             = NO3-   + O                5.00E-10    5.00E-10      0.00       0.00
225  NO2-    + NO3             = NO3-   + NO2              5.00E-10    5.00E-10      0.00       0.00
226  O2-     + NO3             = NO3-   + O2               5.00E-10    5.00E-10      0.00       0.00
227  O3-     + NO3             = NO3-   + O3               5.00E-10    5.00E-10      0.00       0.00
228  NO+     + O-              = NO     + O                1.98E-06    4.90E-07       .50       0.00
229  NO+     + O2-             = NO     + O2               2.07E-06    5.80E-07       .50       0.00
230  NO+     + O3-             = NO     + O3               1.69E-06    2.00E-07       .50       0.00
231  NO+     + O4-             = NO     + O2     + O2      1.69E-06    2.00E-07       .50       0.00
232  NO+     + NO2-            = NO     + NO2              1.84E-06    3.50E-07       .50       0.00
233  NO+     + NO3-            = NO     + NO3              1.69E-06    2.00E-07       .50       0.00
234  NO+     + NO3-            = NO     + NO     + O2      1.69E-06    2.00E-07       .50       0.00
235  NO+     + CO3-            = NO     + CO2    + O       1.69E-06    2.00E-07       .50       0.00
236  NO+     + CO4-            = NO     + CO2    + O2      1.69E-06    2.00E-07       .50       0.00
237  O2+     + O-              = O2     + O                1.58E-06    9.60E-08       .50       0.00
238  O2+     + O2-             = O2     + O2               1.91E-06    4.20E-07       .50       0.00
239  O2+     + O3-             = O2     + O3               1.69E-06    2.00E-07       .50       0.00
240  O2+     + O4-             = O2     + O2     + O2      1.69E-06    2.00E-07       .50       0.00
241  O2+     + NO2-            = O2     + NO2              1.40E-06    4.10E-07       .50       0.00
242  O2+     + NO3-            = O2     + NO3              1.69E-06    2.00E-07       .50       0.00
243  O2+     + NO3-            = O2     + NO     + O2      1.69E-06    2.00E-07       .50       0.00
244  O2+     + CO3-            = O2     + CO2    + O       1.69E-06    2.00E-07       .50       0.00
245  O2+     + CO4-            = O2     + CO2    + O2      1.69E-06    2.00E-07       .50       0.00
246  O4+     + O-              = O2     + O      + O2      1.69E-06    2.00E-07       .50       0.00
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                                                                                    A            B         C
247  O4+     + O2-          = O2      + O2      + O2          1.69E-06    2.00E-07     .50      0.00
248  O4+     + O3-          = O2      + O3      + O2          1.69E-06    2.00E-07     .50      0.00
249  O4+     + O4-          = O4      + O2      + O2          1.69E-06    2.00E-07     .50      0.00
250  O4+     + NO2-         = O2      + NO2     + O2          1.69E-06    2.00E-07     .50      0.00
251  O4+     + NO3-         = O2      + NO3     + O2          1.69E-06    2.00E-07     .50      0.00
252  O4+     + NR3-         = O4      + NO      + O2          1.69E-06    2.00E-07     .50      0.00
253  O4+     + CO3-         = O4      + CO2     + O           1.69E-06    2.00E-07     .50      0.00
254  O4+     + CO4-         = O4      + CO2     + O2          1.69E-06    2.00E-07     .50      0.00
255  N2O2+   + O-           = NO      + O       + NO          1.69E-06    2.00E-07     .50      0.00
256  N2O2+   + O2-          = NO      + O2      + NO          1.69E-06    2.00E-07     .50      0.00
257  N2O2+   + O3-          = NO      + O3      + NO          1.69E-06    2.00E-07     .50      0.00
258  N2O2+   + O4-          = NO      + O4      + NO          1.69E-06    2.00E-07     .50      0.00
259  N2O2+   + NO2-         = NO      + NO2     + NO          1.69E-06    2.00E-07     .50      0.00
260  N2O2+   + NO3-         = NO      + NO3     + NO          1.69E-06    2.00E-07     .50      0.00
261  N2O2+   + NR3-         = N2O2    + O2      + NO          1.69E-06    2.00E-07     .50      0.00
262  N2O2+   + CO3-         = N2O2    + CO2     + O           1.69E-06    2.00E-07     .50      0.00
263  N2O2+   + CO4-         = N2O2    + CO2     + O2          1.69E-06    2.00E-07     .50      0.00
264  H2NO2++ O-             = H2O     + O       + NO          1.69E-06    2.00E-07     .50      0.00
265  H2NO2++ O2-            = H2O     + O2      + NO          1.69E-06    2.00E-07     .50      0.00
266  H2NO2++ O3-            = H2O     + O3      + NO          1.69E-06    2.00E-07     .50      0.00
267  H2NO2++ O4-            = H2O     + O4      + NO          1.69E-06    2.00E-07     .50      0.00
268  H2NO2++ NO2-           = H2O     + NO2     + NO          1.69E-06    2.00E-07     .50      0.00
269  H2NO2++ NO3-           = H2O     + NO3     + NO          1.69E-06    2.00E-07     .50      0.00
270  H2NO2++ NR3-           = H2O     + O2      + N2O2        1.69E-06    2.00E-07     .50      0.00
271  H2NO2++ CO3-           = H2O     + CO2     + NO2         1.69E-06    2.00E-07     .50      0.00
272  H2NO2++ CO4-           = H2O     + CO2     + NO3         1.69E-06    2.00E-07     .50      0.00
273  H4NO3++ O-             = (H2O)2+ O         + NO          1.69E-06    2.00E-07     .50      0.00
274  H4NO3++ O2-            = (H2O)2+ O2        + NO          1.69E-06    2.00E-07     .50      0.00
275  H4NO3++ O3-            = (H2O)2+ O3        + NO          1.69E-06    2.00E-07     .50      0.00
276  H4NO3++ O4-            = (H2O)2+ O4        + NO          1.69E-06    2.00E-07     .50      0.00
277  H4NO3++ NO2-           = (H2O)2+ NO2       + NO          1.69E-06    2.00E-07     .50      0.00
278  H4NO3++ NO3-           = (H2O)2+ NO        + NO3         1.69E-06    2.00E-07     .50      0.00
279  H4NO3++ NR3-           = (H2O)2+ N2O2      + O2          1.69E-06    2.00E-07     .50      0.00
280  H4NO3++ CO3-           = (H2O)2+ CO2       + NO2         1.69E-06    2.00E-07     .50      0.00
281  H4NO3++ CO4-           = (H2O)2+ CO2       + NO3         1.69E-06    2.00E-07     .50      0.00
282  H6NO4++ O-             = (H2O)3+ O         + NO          1.69E-06    2.00E-07     .50      0.00
283  H6NO4++ O2-            = (H2O)3+ O2        + NO          1.69E-06    2.00E-07     .50      0.00
284  H6NO4++ O3-            = (H2O)3+ O3        + NO          1.69E-06    2.00E-07     .50      0.00
285  H6NO4++ O4-            = (H2O)3+ O4        + NO          1.69E-06    2.00E-07     .50      0.00
286  H6NO4++ NO2-           = (H2O)3+ NO2       + NO          1.69E-06    2.00E-07     .50      0.00
287  H6NO4++ NO3-           = (H2O)3+ NO        + NO3         1.69E-06    2.00E-07     .50      0.00
288  H6NO4++ NR3-           = (H2O)3+ N2O2      + O2          1.69E-06    2.00E-07     .50      0.00
289  H6NO4++ CO3-           = (H2O)3+ CO2       + NO2         1.69E-06    2.00E-07     .50      0.00
290  H6NO4++ CO4-           = (H2O)3+ CO2       + NO3         1.69E-06    2.00E-07     .50      0.00
291  H2O3+   + O-           = H2O     + O2      + O           1.69E-06    2.00E-07     .50      0.00
292  H2O3+   + O2-          = H2O     + O2      + O2          1.69E-06    2.00E-07     .50      0.00
293  H2O3+   + O3-          = H2O     + O3      + O2          1.69E-06    2.00E-07     .50      0.00
294  H2O3+   + O4-          = H2O     + O2      + O4          1.69E-06    2.00E-07     .50      0.00
295  H2O3+   + NO2-         = H2O     + NO2     + O2          1.69E-06    2.00E-07     .50      0.00
296  H2O3+   + NO3-         = H2O     + NO3     + O2          1.69E-06    2.00E-07     .50      0.00
297  H2O3+   + NR3-         = H2O     + NO      + O4          1.69E-06    2.00E-07     .50      0.00
298  H2O3+   + CO3-         = H2O     + CO2     + O3          1.69E-06    2.00E-07     .50      0.00
299  H2O3+   + CO4-         = H2O     + CO2     + O4          1.69E-06    2.00E-07     .50      0.00
300  H3O+    + O-           = H2O     + O       + H           1.69E-06    2.00E-07     .50      0.00
301  H3O+    + O2-          = H2O     + O2      + H           1.69E-06    2.00E-07     .50      0.00
302  H3O+    + O3-          = H2O     + O3      + H           1.69E-06    2.00E-07     .50      0.00
303  H3O+    + O4-          = H2O     + O4      + H           1.69E-06    2.00E-07     .50      0.00
304  H3O+    + NO2-         = H2O     + NO2     + H           1.69E-06    2.00E-07     .50      0.00
305  H3O+    + NO3-         = H2O     + NO3     + H           1.69E-06    2.00E-07     .50      0.00
306  H3O+    + NR3-         = H2O     + NO      + HO2         1.69E-06    2.00E-07     .50      0.00
307  H3O+    + CO3-         = H2O     + CO2     + OH          1.69E-06    2.00E-07     .50      0.00
308  H3O+    + CO4-         = H2O     + CO2     + HO2         1.69E-06    2.00E-07     .50      0.00
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309	H5O2+	+ O-	= (H2O)2+	O	+ H	1.69E-06	2.00E-07	.50	0.00
310	H5O2+	+ O2-	= (H2O)2+	O2	+ H	1.69E-06	2.00E-07	.50	0.00
311	H5O2+	+ O3-	= (H2O)2+	O3	+ H	1.69E-06	2.00E-07	.50	0.00
312	H5O2+	+ O4-	= (H2O)2+	O4	+ H	1.69E-06	2.00E-07	.50	0.00
313	H5O2+	+ NO2-	= (H2O)2+	NO2	+ H	1.69E-06	2.00E-07	.50	0.00
314	H5O2+	+ NO3-	= (H2O)2+	NO3	+ H	1.69E-06	2.00E-07	.50	0.00
315	H5O2+	+ NO3-	= (H2O)2+	NO	+ HO2	1.69E-06	2.00E-07	.50	0.00
316	H5O2+	+ CO3-	= (H2O)2+	CO2	+ OH	1.69E-06	2.00E-07	.50	0.00
317	H5O2+	+ CO4-	= (H2O)2+	CO2	+ HO2	1.69E-06	2.00E-07	.50	0.00
318	H7O3+	+ O-	= (H2O)3+	O	+ H	1.69E-06	2.00E-07	.50	0.00
319	H7O3+	+ O2-	= (H2O)3+	O2	+ H	1.69E-06	2.00E-07	.50	0.00
320	H7O3+	+ O3-	= (H2O)3+	O3	+ H	1.69E-06	2.00E-07	.50	0.00
321	H7O3+	+ O4-	= (H2O)3+	O4	+ H	1.69E-06	2.00E-07	.50	0.00
322	H7O3+	+ NO2-	= (H2O)3+	NO2	+ H	1.69E-06	2.00E-07	.50	0.00
323	H7O3+	+ NO3-	= (H2O)3+	NO3	+ H	1.69E-06	2.00E-07	.50	0.00
324	H7O3+	+ NO3-	= (H2O)3+	NO	+ HO2	1.69E-06	2.00E-07	.50	0.00
325	H7O3+	+ CO3-	= (H2O)3+	CO2	+ OH	1.69E-06	2.00E-07	.50	0.00
326	H7O3+	+ CO4-	= (H2O)3+	CO2	+ HO2	1.69E-06	2.00E-07	.50	0.00
327	H9O4+	+ O-	= (H2O)4+	O	+ H	1.69E-06	2.00E-07	.50	0.00
328	H9O4+	+ O2-	= (H2O)4+	O2	+ H	1.69E-06	2.00E-07	.50	0.00
329	H9O4+	+ O3-	= (H2O)4+	O3	+ H	1.69E-06	2.00E-07	.50	0.00
330	H9O4+	+ O4-	= (H2O)4+	O4	+ H	1.69E-06	2.00E-07	.50	0.00
331	H9O4+	+ NO2-	= (H2O)4+	NO2	+ H	1.69E-06	2.00E-07	.50	0.00
332	H9O4+	+ NO3-	= (H2O)4+	NO3	+ H	1.69E-06	2.00E-07	.50	0.00
333	H9O4+	+ NO3-	= (H2O)4+	NO	+ HO2	1.69E-06	2.00E-07	.50	0.00
334	H9O4+	+ CO3-	= (H2O)4+	CO2	+ OH	1.69E-06	2.00E-07	.50	0.00
335	H9O4+	+ CO4-	= (H2O)4+	CO2	+ HO2	1.69E-06	2.00E-07	.50	0.00
336	H11O5++	O-	= (H2O)5+	O	+ H	1.69E-06	2.00E-07	.50	0.00
337	H11O5++	O2-	= (H2O)5+	O2	+ H	1.69E-06	2.00E-07	.50	0.00
338	H11O5++	O3-	= (H2O)5+	O3	+ H	1.69E-06	2.00E-07	.50	0.00
339	H11O5++	O4-	= (H2O)5+	O4	+ H	1.69E-06	2.00E-07	.50	0.00
340	H11O5++	NO2-	= (H2O)5+	NO2	+ H	1.69E-06	2.00E-07	.50	0.00
341	H11O5++	NO3-	= (H2O)5+	NO3	+ H	1.69E-06	2.00E-07	.50	0.00
342	H11O5++	NO3-	= (H2O)5+	NO	+ HO2	1.69E-06	2.00E-07	.50	0.00
343	H11O5++	CO3-	= (H2O)5+	CO2	+ OH	1.69E-06	2.00E-07	.50	0.00
344	H11O5++	CO4-	= (H2O)5+	CO2	+ HO2	1.69E-06	2.00E-07	.50	0.00
345	H4O2+	+ O-	= H2O	+ O	+ H2O	1.69E-06	2.00E-07	.50	0.00
346	H4O2+	+ O2-	= H2O	+ O2	+ H2O	1.69E-06	2.00E-07	.50	0.00
347	H4O2+	+ O3-	= H2O	+ O3	+ H2O	1.69E-06	2.00E-07	.50	0.00
348	H4O2+	+ O4-	= H2O	+ O4	+ H2O	1.69E-06	2.00E-07	.50	0.00
349	H4O2+	+ NO2-	= H2O	+ NO2	+ H2O	1.69E-06	2.00E-07	.50	0.00
350	H4O2+	+ NO3-	= H2O	+ NO3	+ H2O	1.69E-06	2.00E-07	.50	0.00
351	H4O2+	+ NO3-	= (H2O)2+	NO	+ O2	1.69E-06	2.00E-07	.50	0.00
352	H4O2+	+ CO3-	= (H2O)2+	CO2	+ O	1.69E-06	2.00E-07	.50	0.00
353	H4O2+	+ CO4-	= (H2O)2+	CO2	+ O2	1.69E-06	2.00E-07	.50	0.00
354	NON2+	+ O-	= N2	+ NO	+ O	1.69E-06	2.00E-07	.50	0.00
355	NON2+	+ O2-	= N2	+ NO	+ O2	1.69E-06	2.00E-07	.50	0.00
356	NON2+	+ O3-	= N2	+ NO	+ O3	1.69E-06	2.00E-07	.50	0.00
357	NON2+	+ O4-	= N2	+ NO	+ O4	1.69E-06	2.00E-07	.50	0.00
358	NON2+	+ NO2-	= N2	+ NO	+ NO2	1.69E-06	2.00E-07	0.00	0.00
359	NON2+	+ NO3-	= N2	+ NO	+ NO3	1.69E-06	2.00E-07	.50	0.00
360	NON2+	+ NO3-	= N2	+ N2O2	+ O2	1.69E-06	2.00E-07	.50	0.00
361	NON2+	+ CO3-	= N2	+ NO2	+ CO2	1.69E-06	2.00E-07	.50	0.00
362	NON2+	+ CO4-	= N2	+ NO3	+ CO2	1.69E-06	2.00E-07	.50	0.00
363	NOCO2++	O-	= CO2	+ NO	+ O	1.69E-06	2.00E-07	0.00	0.00
364	NOCO2++	O2-	= CO2	+ NO	+ O2	1.69E-06	2.00E-07	.50	0.00
365	NOCO2++	O3-	= CO2	+ NO	+ O3	1.69E-06	2.00E-07	.50	0.00
366	NOCO2++	O4-	= CO2	+ NO	+ O4	1.69E-06	2.00E-07	.50	0.00
367	NOCO2++	NO2-	= CO2	+ NO	+ NO2	1.69E-06	2.00E-07	.50	0.00
368	NOCO2++	NO3-	= CO2	+ NO	+ NO3	1.69E-06	2.00E-07	.50	0.00
369	NOCO2++	NO3-	= CO2	+ N2O2	+ O2	1.69E-06	2.00E-07	.50	0.00
370	NOCO2++	CO3-	= CO2	+ CO2	+ NO2	1.69E-06	2.00E-07	.50	0.00
371	NOCO2++	CO4-	= CO2	+ CO2	+ NO3	1.69E-06	2.00E-07	.50	0.00