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

**Mission Research Corporation
735 State Street
Santa Barbara, California 93101**

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20. ABSTRACT (Continued)

electric EMP fields were, however, neglected in order to narrow the scope of the effort. The conclusions of this study indicate that the lumped parameter approach may be usable, but the coefficients employed in the past were in error.

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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.

TABLE OF CONTENTS

	<u>Page</u>
PREFACE	1
LIST OF ILLUSTRATIONS	3
LIST OF TABLES	4
SECTION 1—INTRODUCTION	5
SECTION 2—DISCUSSION OF THE THREE SPECIES TREATMENT	7
SECTION 3—THE DCHEM REACTION RATE CODE	10
SECTION 4—RESULTS	13
SECTION 5—CONCLUSIONS	28
REFERENCES	30
APPENDIX	33

LIST OF ILLUSTRATIONS

<u>Figure</u>		<u>Page</u>
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.	14
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.	16
3	A comparison of the electron and ion densities as calculated from a three species and a multi-species treatment of the air chemistry.	17
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.	19
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.	24
6	The variation of the "average" recombination rate coefficient in the DCHEM code as functions of water vapor fraction, peak ionization rate and time.	24
7	Comparison of the old and new three species treatment with the DCHEM code variations in water vapor fraction and peak ionization rate.	26

LIST OF TABLES

<u>Table</u>		<u>Page</u>
1	Input parameters for the DCHEM code.	12
2	Three-body attachment reactions and rate coefficients.	20
3	Effective sea-level attachment rates as a function of water vapor content.	21
4	Dissociative recombination reactions and rate coefficients.	22
5	Ion mobilities in air for $T = 300^{\circ}\text{K}$ and $\rho = 2.5 \times 10^{19}$ molecules/cm ³ .	27

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 detonation¹⁻⁵. 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 facilities⁶⁻⁹, and to predict the system-generated EMP (SGEMP) produced in the close-in coupling region of a surface or near-surface detonation¹⁰⁻¹².

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 $8.4 \times 10^9 \text{ sec}^{-1}$, respectively¹³, 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

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

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:

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

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

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

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

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/ $\text{cm}^3 \cdot \text{sec}$].

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 Longmire¹⁶, and for sea-level conditions are stated as follows:

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

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

where E is the electric field in volts/meter. Longmire employed the two- and three-body electron attachment data of Chanin, Phelps, and Biondi¹⁷ for dry air and the drift velocity data of Phelps¹⁸ 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.

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



as the positive-ion charge transfer reaction



occurs at a rate of approximately $7 \times 10^9 \text{ sec}^{-1}$ 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 atmosphere²². 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

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

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.

* 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 ₂ O	1.25×10^{13}
O ₃	1.5×10^{11}
NO ₂	5.0×10^{10}
H ₂ O	$f_{H_2O} \rho^*$

* 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 $1.99 \times 10^8 \text{ sec}^{-1}$. However, because Equation 6 was fit on the basis of data¹⁸ for electric fields greater than 3000 v/m, the author has chosen instead a value of $1.0 \times 10^8 \text{ sec}^{-1}$ for the zero field attachment rate based upon the work of Vittitoe²³. The three species equations to be solved here become:

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

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

$$n_+ = n_e + n_- , \quad (13)$$

with $\alpha_e = 10^8 \text{ sec}^{-1}$, $\beta = 2.5 \times 10^{-7} \text{ cm}^3/\text{sec}$, $\gamma = 2.3 \times 10^{-6} \text{ cm}^3/\text{sec}$ 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/cm³ · 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

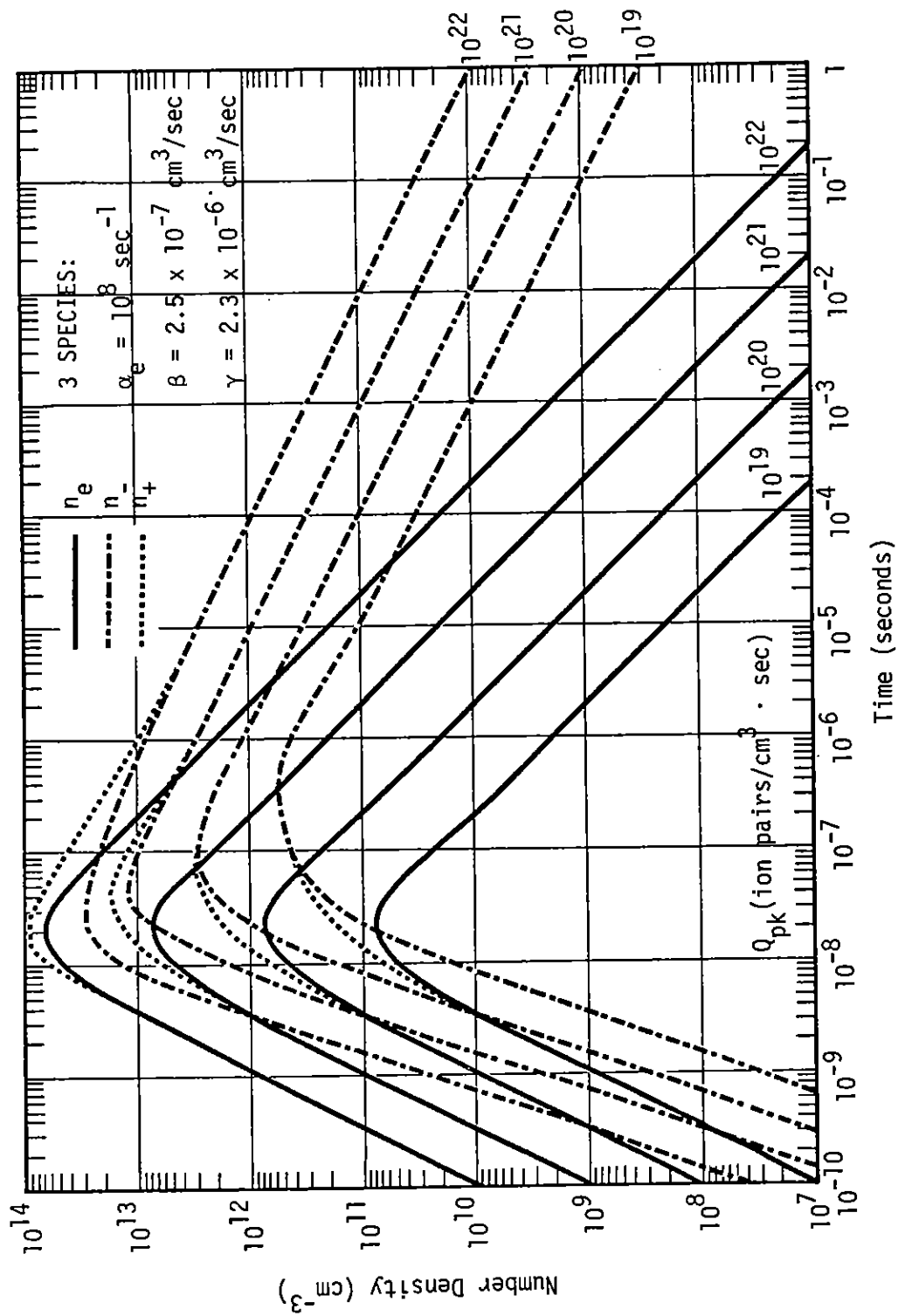


Figure 1. The time dependence of the electron, positive ion and negative ion densities as provided by the solution of the three species air chemistry equations for variations in the peak ionization rate.

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 calculations 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

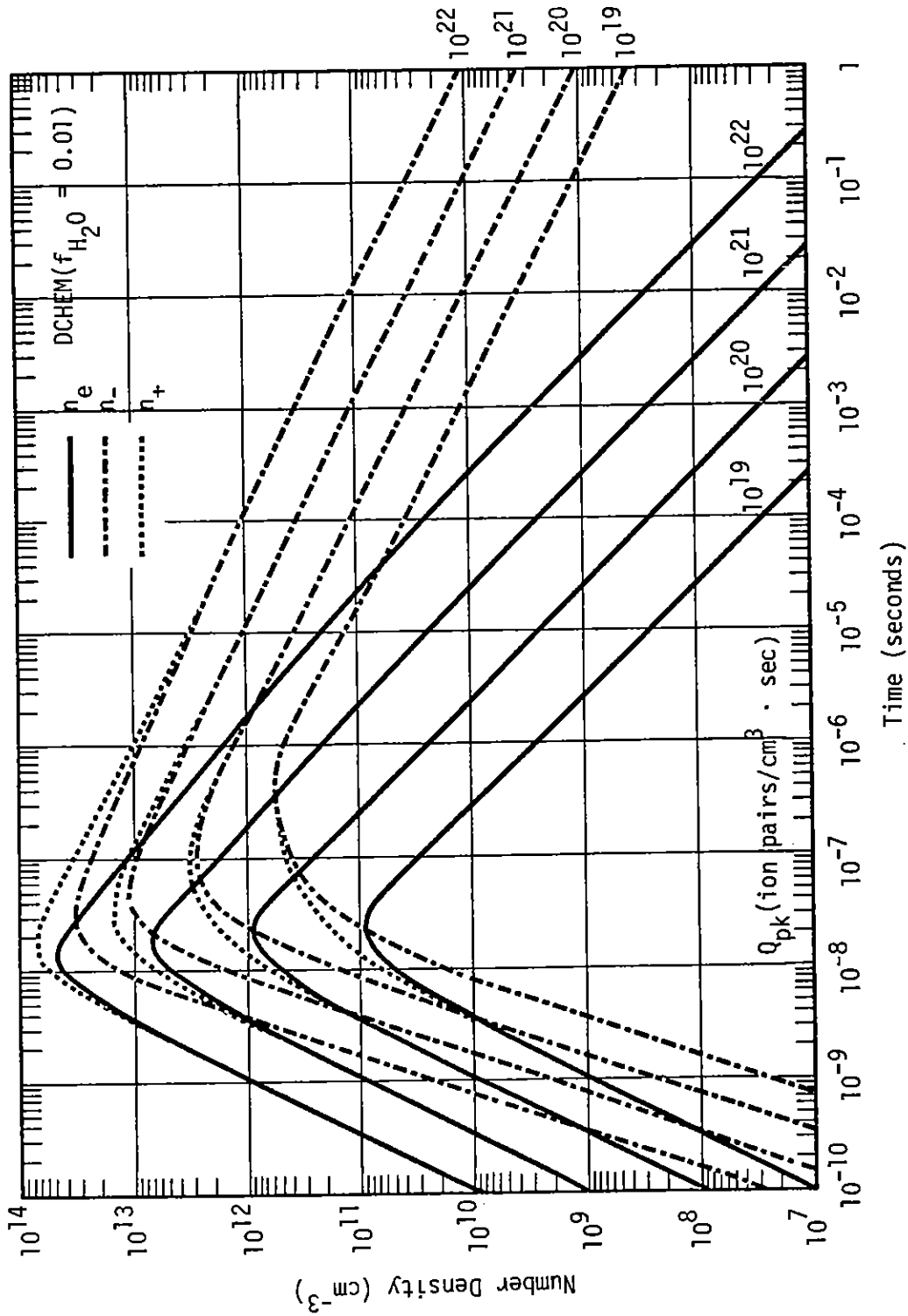


Figure 2. The time dependence of the electron densities and the sum of all positive and negative ion densities as calculated with the DCHEM code for variations in the peak ionization rate.

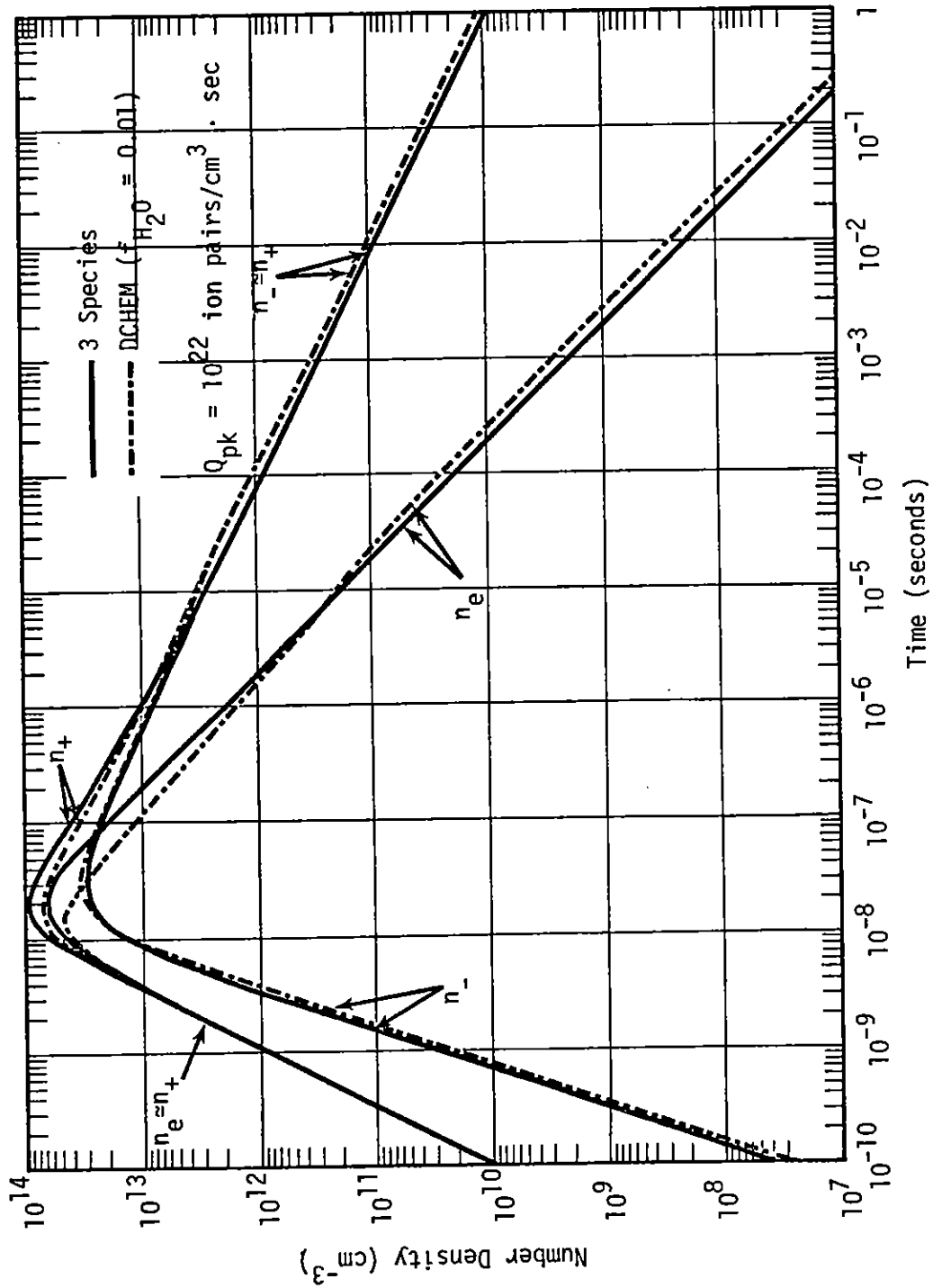


Figure 3. A comparison of the electron and ion densities as calculated from a three species and a multi-species treatment of the air chemistry.

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, respectively²⁴). 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/cm³ 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 handbook²¹.

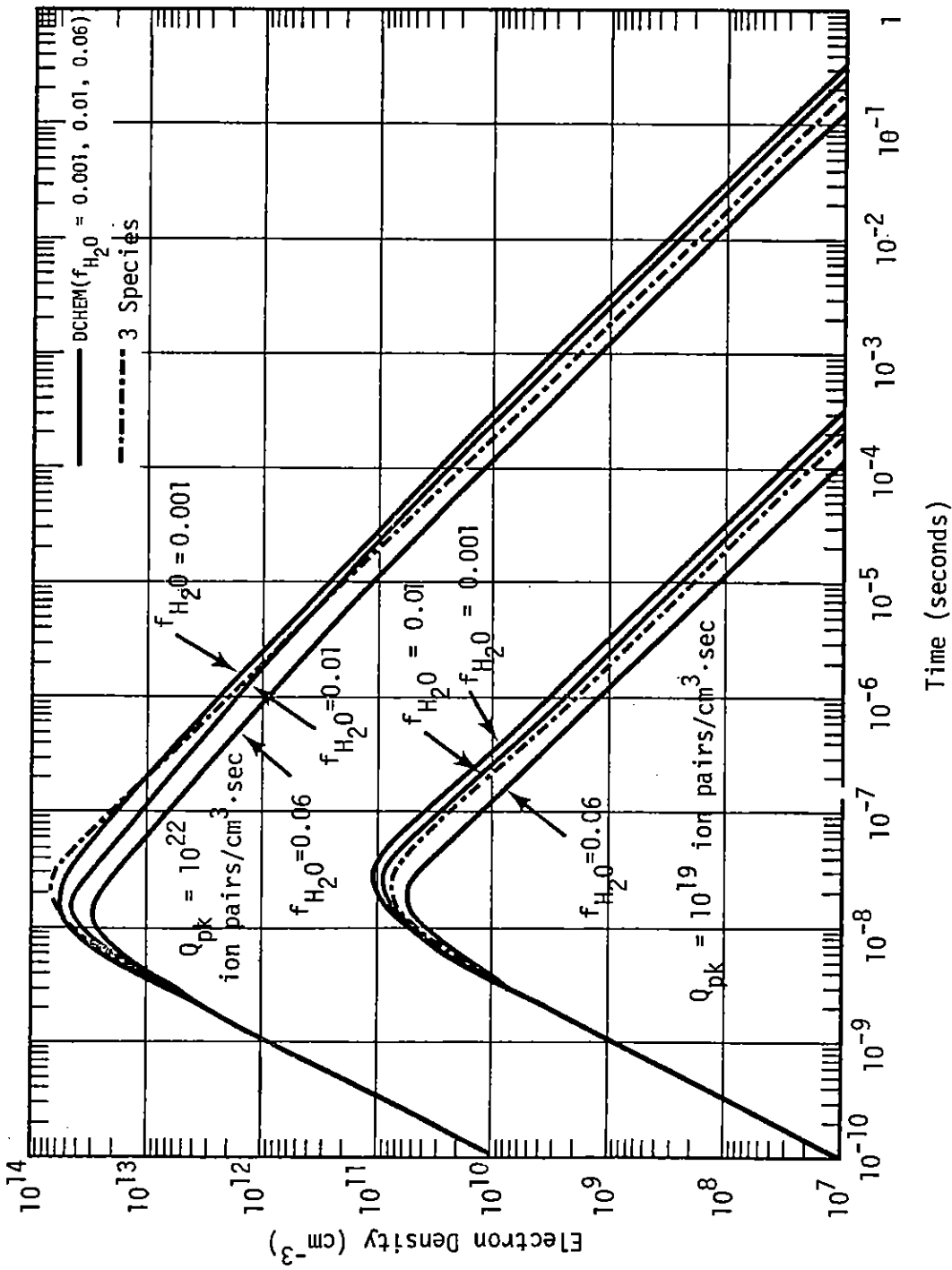


Figure 4. A comparison of the three species and the multi-species solution of the electron density for variations in water vapor fraction and peak ionization rate.

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

Reaction	Rate Coefficient $\left(\frac{\text{cm}^6}{\text{sec}}\right)$
$\text{O}_2 + e + \text{O}_2 \rightarrow \text{O}_2^- + \text{O}_2$	$1.4 \times 10^{-29} (T/300) \exp(-600/T)$ $= 1.85 \times 10^{-30}$ for $T = 293^\circ\text{K}$
$\text{O}_2 + e + \text{N}_2 \rightarrow \text{O}_2^- + \text{N}_2$	1.0×10^{-31}
$\text{O}_2 + e + \text{H}_2\text{O} \rightarrow \text{O}_2^- + \text{H}_2\text{O}$	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

$$\alpha_e (\text{sec}^{-1}) = 1.85 \times 10^{-30} (N_{\text{O}_2})^2 + 1.0 \times 10^{-31} N_{\text{O}_2} N_{\text{N}_2} + 1.4 \times 10^{-29} N_{\text{O}_2} N_{\text{H}_2\text{O}}, \quad (14)$$

where N_{O_2} , N_{N_2} , and $N_{\text{H}_2\text{O}}$ are the molecular densities in cm^{-3} of O_2 , N_2 and H_2O ; this results in

$$\alpha_e (\text{sec}^{-1}) = 6.133 \times 10^7 + 1.838 \times 10^9 f_{\text{H}_2\text{O}}. \quad (15)$$

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 $\beta = 2.5 \times 10^{-7} \text{ cm}^3/\text{sec}$ 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}
$N_2^+ + e \rightarrow N(2D) + N$	$2.70 \times 10^{-7} (T/300)^{-0.2}$	2.71×10^{-7}
$O_2^+ + e \rightarrow O + O$	$2.10 \times 10^{-7} (T/300)^{-0.7}$	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

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

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/cm³ · 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

$$\beta(\text{cm}^3/\text{sec}) = 2.0 \times 10^{-7} + 1.30 \times 10^{-5} (f_{\text{H}_2\text{O}})^{1/3} , \quad (17)$$

for $0.001 \leq f_{\text{H}_2\text{O}} \leq 0.06$.

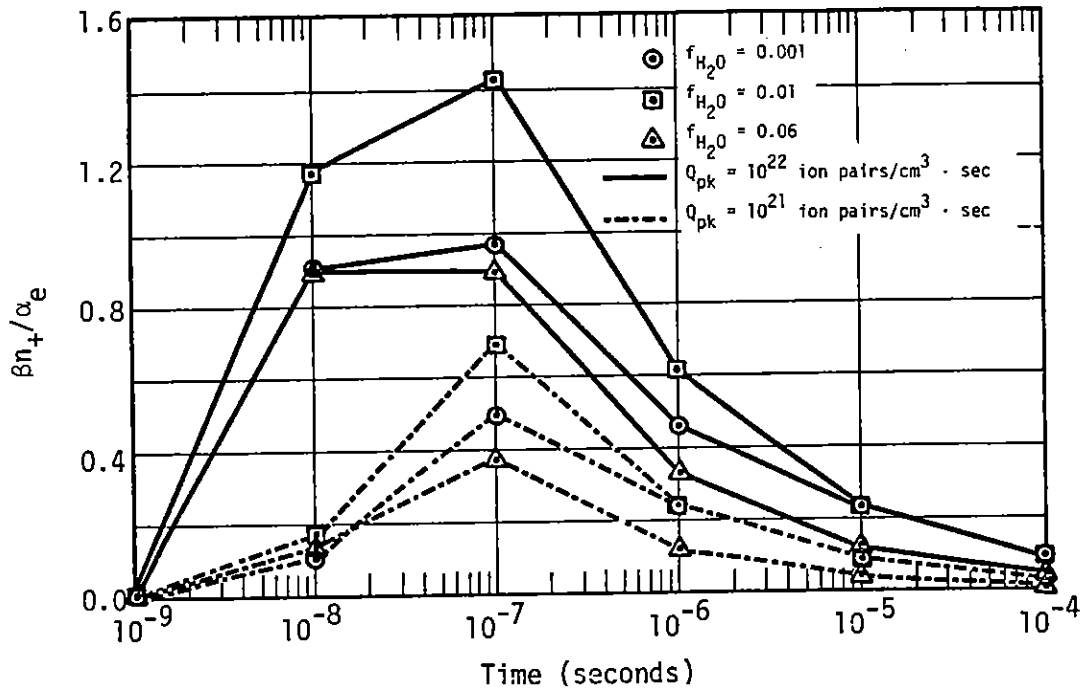


Figure 5. The variation of the ratio of the "average" recombination and attachment rates in the DCHEM code as functions of water vapor fraction, peak ionization rate and time.

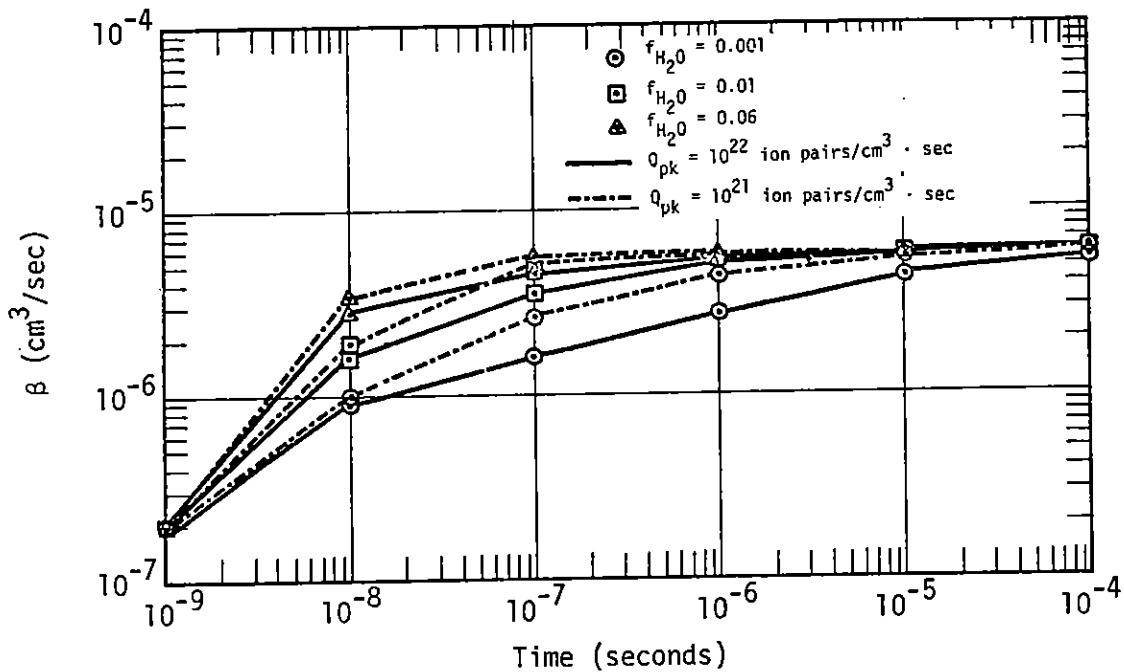


Figure 6. The variation of the "average" recombination rate coefficient in the DCHEM code as functions of water vapor fraction, peak ionization rate and time.

Using Equations 15 and 17 and further specifying $\gamma = 1.69 \times 10^{-6}$ cm³/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 $(\text{H}_2\text{O})_n \cdot \text{H}_3\text{O}^+$, even in the 0.001 water vapor fraction case.

Table 5 lists the mobilities of these ions in air for $T \approx 300^\circ\text{K}$ and $\rho = 2.5 \times 10^{19}$ molecules/cm³ (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 species²⁵. 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 past⁴. Developments in the reaction rate community may indicate a better value at some future date.

* 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.

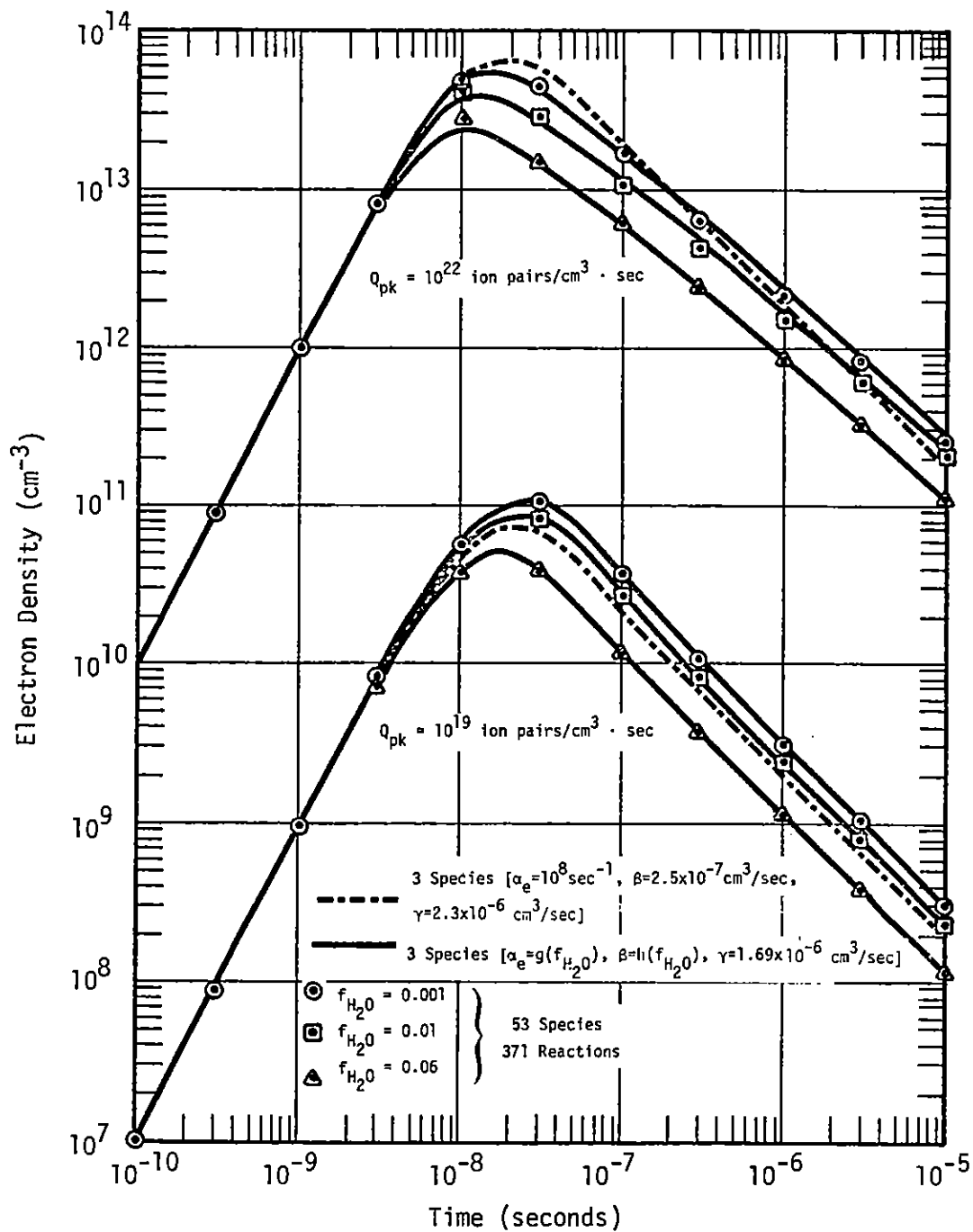


Figure 7. Comparison of the old and new three species treatment with the DCHEM code for variations in water vapor fraction and peak ionization rate.

Table 5. Ion mobilities in air for $T = 300^\circ\text{K}$ and $\rho = 2.5 \times 10^{19}$ molecules/cm³.

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
$\text{H}_3\text{O}^+ \cdot \text{H}_2\text{O}$	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:

$$\alpha_e(\text{sec}^{-1}) = 6.133 \times 10^7 + 1.838 \times 10^9 f_{\text{H}_2\text{O}}, \quad (18)$$

$$\beta(\text{cm}^3/\text{sec}) = 2.00 \times 10^{-7} + 1.30 \times 10^{-5} (f_{\text{H}_2\text{O}})^{1/3}, \quad (19)$$

and

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

for fractions of water vapor content, $0.001 \leq f_{\text{H}_2\text{O}} \leq 0.06$.

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.

* The electron attachment field dependence including the effect of water vapor as a third body has recently been specified by Longley and Longmire²⁶.

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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.

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

for T in °K and k in the same units as A (for two-body reactions the units are cm³/sec; for three-body reactions, cm⁶/sec).

***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	62 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	90 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	13 REACTIONS	
(H2O)5	IS INVOLVED IN	10 REACTIONS	
NO+	IS INVOLVED IN	35 REACTIONS	
N2+	IS INVOLVED IN	8 REACTIONS	
O2+	IS INVOLVED IN	23 REACTIONS	
A+	IS INVOLVED IN	7 REACTIONS	
C+	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	12 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	
NO3+	IS INVOLVED IN	18 REACTIONS	
NOO2+	IS INVOLVED IN	18 REACTIONS	
O-	IS INVOLVED IN	20 REACTIONS	
O2-	IS INVOLVED IN	36 REACTIONS	
O3-	IS INVOLVED IN	29 REACTIONS	
O4-	IS INVOLVED IN	27 REACTIONS	
NO2-	IS INVOLVED IN	26 REACTIONS	
NO3-	IS INVOLVED IN	29 REACTIONS	
NO3-	IS INVOLVED IN	22 REACTIONS	
CO3-	IS INVOLVED IN	24 REACTIONS	
CO4-	IS INVOLVED IN	25 REACTIONS	

REACTIONS				RATES	COEFFICIENTS		
					A	B	C
1	O2	+	= N2+ + O	IIII	7.50E-01	0.00	0.00
2	N2	+	= N+ + E	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-07	0.00	0.00
5	O2	+	= O + O	IIII	7.40E-01	0.00	0.00
6	O2	+	= O2(1D)+ + E	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	N2+	+	= N + N+	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 + L	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	= O3 + M	6.27E-34	1.10E-34	0.00	-0.51
28	O	+ NO	= NO2 + M	1.01E-31	4.10E-33	0.00	-0.94
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	2.00E-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	1.55
37	NO	+ NO	= NO2 + NO2	2.01E-39	3.30E-39	0.00	-0.53
38	N	+ O3	= NO + O2	5.59E-13	3.40E-11	-0.50	1.20
39	O	+ O	= O2 + M	7.45E-33	1.30E-32	1.00	.17
40	N	+ N	= N2 + M	4.57E-33	8.20E-34	0.00	-0.50
41	N	+ O	= NO + M	1.11E-32	1.10E-32	.50	0.00
42	N	+ N	= N2 + M	1.02E-17	1.00E-17	.70	0.00
43	O	+ NO	= NO2 +	6.90E-17	6.60E-17	1.90	0.00
44	O	+ O	= O2 +	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	4.07E-17	6.00E-12	0.00	3.50
47	NO3	+ O	= NO2 + O2	5.98E-15	1.00E-12	0.00	1.50
48	NO3	+ NO3	= N2 + 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	= O + E	1.11E-19	1.00E-19	4.50	0.00
54	N+	+ 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	-0.60
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	2.15E-18	2.20E-18	-0.80	0.00

					A	B	C
61	F2(10)+	= O2 +			2.60E-04	2.60E-04	0.00
62	O + O3	= O2(10)+ C2			3.90E-15	1.00E-11	0.00
63	O + O5	= O2 + C2			3.90E-15	1.00E-11	0.00
64	H + H2	= OH + CH			1.64E-11	4.20E-10	0.00
65	H + H22	= H2 + O2			1.27E-11	4.20E-11	0.00
66	H + H22	= H2O + O			2.90E-12	1.20E-11	0.00
67	H + H22	= OH + NO			4.64E-11	5.80E-10	0.00
68	O + H2	= OH + O2			1.43E-11	7.90E-11	0.00
69	OH + H2	= H2O + O2			2.90E-12	1.60E-11	0.00
70	OH + O5	= H2 + O2			5.27E-14	1.60E-12	0.00
71	OH + OH	= H2O + O			1.82E-12	1.00E-11	0.00
72	H + H2O2	= H2O + H2			4.27E-15	2.80E-12	0.00
73	H + H2O2	= OH + H2O			1.13E-16	5.30E-10	0.00
74	CH + OH + M	= H2O2 + + M			4.40E-30	4.00E-30	4.00
75	CH + H2O2	= H2 + H2O			7.61E-13	1.70E-11	0.00
76	H2O2 + H2O2	= H2O2 + C2			5.45E-12	3.00E-11	0.00
77	H2O2 + O	= OH + H2			1.53E-15	3.50E-11	0.00
78	H2O2 + NO	= OH + NO2			2.00E-13	2.00E-13	0.00
79	H + O2 + M	= H2 + + M			5.65E-32	2.10E-32	0.00
80	H + O2	= OH + C2			2.60E-11	2.60E-11	0.00
81	CH + H2	= H + H2O			5.22E-15	3.60E-11	0.00
82	CH + N	= H + NO			5.20E-11	5.30E-11	0.00
83	CH + O + M	= H2 + + M			1.00E-31	1.00E-31	0.00
84	H + OH + M	= H2O + + M			4.51E-30	4.30E-30	2.00
85	H2O2 + O3	= OH + C2			1.40E-13	1.00E-13	0.00
86	C + OH	= H + C2			4.70E-11	4.20E-11	0.00
87	C + H	= OH + + M			2.00E-32	2.00E-32	0.00
88	(H2O)2 +	= H2O + H2O + M			1.00E-10	1.00E-10	0.00
89	(H2O)3 +	= (H2O)2 + H2O + M			1.00E-10	1.00E-10	0.00
90	(H2O)4 +	= (H2O)3 + H2O + M			1.00E-10	1.00E-10	0.00
91	(H2O)5 +	= (H2O)4 + H2O + M			1.00E-10	1.00E-10	0.00
92	O4 +	= O2 + O2 + M			1.00E-10	1.00E-10	0.00
93	H2O2 +	= HO + NO + M			1.00E-10	1.00E-10	0.00
94	N2+ + N2	= NO+ + N2			3.30E-10	3.30E-10	0.00
95	N2+ + O2	= O2+ + N2			5.00E-11	5.00E-11	0.50
96	N2+ + O	= O+ + N2			6.00E-12	6.00E-12	0.00
97	N2+ + N	= N+ + N2			1.00E-11	1.00E-11	0.00
98	N+ + NO	= N + NO+			8.00E-10	8.00E-10	0.00
99	N+ + O2	= N + O2+			3.00E-10	3.00E-10	0.00
100	N+ + O	= N + O+			1.00E-12	1.00E-12	0.00
101	O+ + O3	= O3+ + O			1.30E-12	1.30E-12	0.00
102	O+ + O2	= O2+ + O			2.02E-11	2.00E-11	0.50
103	O+ + N2 + M	= NO+ + N + + M			1.68E-29	1.60E-29	2.00
104	O2+ + NO	= NO+ + O2			6.30E-10	6.20E-10	0.00
105	O2+ + N2	= N3+ + NO			1.00E-16	1.00E-16	0.00
106	H+ + O2	= O + HO+			3.00E-10	3.00E-10	0.00
107	O+ + N2	= NO+ + N			1.21E-12	1.20E-12	0.50
108	O+ + N2O	= NO+ + NO			8.90E-10	8.90E-10	0.00
109	N2+ + O	= NO+ + N(2D)			7.90E-11	7.00E-11	0.00
110	N2+ + O	= NO+ + N			7.00E-11	7.00E-11	0.00
111	O2+ + N(2D)	= NO+ + O3			1.30E-11	1.00E-11	0.00
112	O2+ + N	= NO+ + O			1.80E-10	1.80E-10	0.00
113	NO+ + N3	= N2O2+ + + M			5.12E-70	5.00E-30	1.00
114	N2O2+ + + M	= NO+ + NO + + M			4.31E-16	1.00E-05	7.00
115	N2O2+ + O	= NO+ + N(2D)			3.00E-10	3.00E-10	0.00
116	N2O2+ + O2	= NO2O2+ + NO			2.71E-16	2.50E-13	0.00
117	N2O2+ + H2O	= H2NO2+ + NO			1.40E-09	1.40E-09	0.00
118	H2NO2+ + NO	= N2O2+ + H2O			7.80E-14	2.00E-10	0.00
119	H2NO2+ + N2	= N2NO2+ + H2O			5.10E-19	2.20E-09	0.00
120	H2NO2+ + O(2D)	= NO2O2+ + H2O			1.13E-13	2.67E-07	0.00
121	H2NO2+ +	= NO+ + H2O + M			3.36E-19	2.00E-05	1.00
122	O5+ + H2O + K	= H2NO2+ + + K			1.57E-28	1.50E-28	2.00

							A	B	C	
123	H2N02++	H20	+ M	= H2N03++	+ M		1.156-27	1.10E-27	2.00	0.00
124	H2N03++		+ M	= H2N02++	H20	+ M	4.41E-15	1.00E-04	2.00	7.00
125	H2N03++	H20	+ M	= H2N04++		+ M	1.66E-27	1.60E-27	2.00	0.00
126	H2N04++		+ M	= H2N03++	H20	+ M	8.63E-13	2.00E-02	2.00	7.00
127	H2N04++	H20	+ M	= H203+	GH	+ M	7.00E-11	7.00E-11	0.00	0.00
128	H2+	+ H2	+ M	= H2+	+ H2	+ M	2.10E-31	2.00E-31	2.00	0.00
129	H2+	+ H2	+ M	= H2+	+ H2	+ M	9.53E-13	1.20E-08	2.00	2.78
130	H2N2+	+ H20		= H2N02++	N2		1.00E-09	1.00E-09	0.00	0.00
131	H2N2+	+ C02		= H2N02++	N2		1.00E-09	1.00E-09	0.00	0.00
132	H2N2+	+ N0		= H2N02+ + N2			1.50E-09	1.50E-09	0.00	0.00
133	H2N2+	+ H2		= H2N2+ + N0			1.79E-17	3.00E-11	0.00	4.20
134	H2N02++	N2		= H2N2+ + C02			4.57E-15	8.33E-12	0.00	2.20
135	H2N02++	N0		= H2N2+ + C02			1.00E-09	1.00E-09	0.00	0.00
136	H2N02++	H20		= H2N02++	C02		1.00E-09	1.00E-09	0.00	0.00
137	H2+	+ C02	+ M	= H2N02++		+ M	2.10E-29	2.00E-29	2.00	0.00
138	H2N02++		+ M	= H2+ + C02		+ M	4.07E-15	1.00E-08	2.00	5.00
139	C2+	+ H2	+ M	= C2+ + H2		+ M	2.94E-30	2.80E-30	2.00	0.00
140	C2+	+ H2	+ M	= C2+ + H2		+ M	2.03E-14	5.00E-07	2.00	5.00
141	C2+	+ H2		= C2+ + H2			3.00E-10	3.00E-10	0.00	0.00
142	C2+	+ H2		= C2+ + H2		+ H2	3.00E-10	5.00E-10	0.00	0.00
143	C2+	+ H20	+ M	= H203+ +		+ M	2.94E-28	2.80E-28	2.00	0.00
144	C2+	+ H20		= H203+ +			1.50E-09	1.50E-09	0.00	0.00
145	H23+ + H2			= H2+ + H20			7.80E-14	2.00E-10	0.00	2.30
146	H23+ + C2(10)			= H2+ + H20	+ H2		1.00E-10	1.00E-10	0.00	0.00
147	H203+ + H2			= H2+ + H20	+ H20		1.00E-10	1.00E-10	0.00	0.00
148	H203+ + H20			= H20+ + H2	+ H2		2.00E-10	2.00E-10	0.00	0.00
149	H203+ + H20			= H20+ + H2	+ H20		1.00E-09	1.00E-09	0.00	0.00
150	H203+ + H20			= H20+ + H2	+ H20		3.56E-27	3.40E-27	2.00	0.00
151	H202+ + H20	+ M		= H20+ + H20	+ M		1.75E-26	3.00E+00	2.00	16.00
152	H202+ + H20	+ M		= H20+ + H20	+ M		1.40E-09	1.40E-09	0.00	0.00
153	H2+ + H2	+ M		= H20+ + GH	+ M		3.09E-19	1.00E-01	2.00	11.80
154	H203+ + H20	+ M		= H203+ +			2.41E-27	2.50E-27	2.00	0.00
155	H203+ + H20	+ M		= H203+ +			2.41E-27	2.50E-27	2.00	11.20
156	H203+ + H20	+ M		= H203+ +			2.41E-27	2.50E-27	2.00	0.00
157	H203+ + H20	+ M		= H203+ +			2.41E-27	2.50E-27	2.00	8.60
158	H204+ + H20	+ M		= H203+ + H20	+ M		9.25E-23	8.80E-28	2.00	0.00
159	H204+ + H20	+ M		= H204+ + H20	+ M		4.02E-12	3.00E-03	2.00	6.30
160	C2+ + E			= C2+ + C2			2.05E-06	2.00E-06	1.00	0.00
161	H2N2+ + E			= H2+ + N0			1.74E-06	1.70E-06	1.00	0.00
162	H20+ + E			= H20+ + H			1.00E-06	1.00E-06	0.00	0.00
163	H202+ + E			= H20+ + H20	+ H		2.30E-06	2.20E-06	0.00	0.00
164	H203+ + E			= (H20)2+ + H20	+ H		4.60E-06	4.60E-06	0.00	0.00
165	H204+ + E			= (H20)2+ + (H20)2+ + H			6.50E-06	6.00E-06	0.00	0.00
166	H205+ + E			= (H20)2+ + (H20)3+ + H			6.00E-06	6.00E-06	0.00	0.00
167	H206+ + E			= H20+ + C2			1.54E-06	1.50E-06	1.00	0.00
168	H207+ + E			= H20+ + H20			3.00E-06	3.00E-06	0.00	0.00
169	H208+ + E			= H20+ + H20			1.02E-06	1.00E-06	1.00	0.00
170	H209+ + E			= H20+ + H20	+ H20		2.05E-06	2.00E-06	1.00	0.00
171	H210+ + E			= (H20)2+ + H20	+ H20		3.07E-06	3.00E-06	1.00	0.00
172	H211+ + E			= H20+ + H20			1.02E-06	1.00E-06	1.00	0.00
173	H212+ + E			= H20+ + C02			1.02E-06	1.00E-06	1.00	0.00
174	C2- + H	+ H2		= C2- +	+ H2		1.35E-30	1.40E-29	1.00	.50
175	C2- + H	+ H2		= C2- + E	+ H2		1.38E-13	2.70E-10	-1.50	5.50
176	C2- + H	+ H2		= C2- +	+ H2		1.00E-31	1.00E-31	0.00	0.00
177	C2- + H	+ H2		= C2- + F	+ H2		7.06E-20	1.90E-12	-1.50	4.00
178	C2- + H	+ H2		= C2- +	+ H20		1.40E-29	1.40E-29	0.00	0.00
179	C2- + H	+ H2		= C2- +			4.00E-11	4.00E-11	0.00	0.00
180	C2- + H	+ H2		= C2- +	+ H2		8.89E-12	9.00E-12	-1.50	0.00
181	C2- + H	+ H2		= C2- +			1.30E-15	1.30E-15	0.00	0.00
182	C2- + H	+ H2		= C2- +			3.00E-10	3.00E-10	0.00	0.00
183	C2- + H	+ H2		= C2- +			3.00E-10	3.00E-10	0.00	0.00
184	C2- + H	+ H2		= C2- +			2.00E-10	2.00E-10	0.00	0.00

						A	B	C
185	C-	+ N	= NG	+ E		2.20E-10	2.20E-10	0.00
186	C-	+ O	= C2	+ E		2.30E-10	2.30E-10	0.00
187	C2(10)+	O2-	= O2	+ O2	+ L	2.00E-10	2.00E-10	0.00
188	C2(10)+	O-	= O3	+ F		3.00E-10	3.00E-10	0.00
189	O2-	+ O	= O-	+ O2		3.30E-10	3.30E-10	0.00
190	O2-	+ N	= O-	+ NG		1.00E-10	1.00E-10	0.00
191	O2-	+ O3	= O3-	+ O2		4.00E-10	4.00E-10	0.00
192	O2-	+ NO2	= NO2-	+ O2		8.00E-10	8.00E-10	0.00
193	O-	+ O5	= O5-	+ O		5.30E-10	5.30E-10	0.00
194	O-	+ NO2	= NO2-	+ O		1.20E-09	1.20E-09	0.00
195	C-	+ CO2	+ M	= CO3-	+ M	3.17E-28	3.10E-28	1.00
196	O2-	+ NO2	= NO2-	+ O3		1.40E-10	1.40E-10	0.00
197	O3-	+ NO2	= NO3-	+ O2		1.40E-10	1.40E-10	0.00
198	O3-	+ NO	= NO2-	+ O2		1.00E-11	1.00E-11	0.00
199	NO2-	+ O3	= NO3-	+ O2		1.80E-11	1.80E-11	0.00
200	NO2-	+ NO2	= NO3-	+ NO		4.00E-12	4.00E-12	0.00
201	NO3-	+ NO	= NO2-	+ NO2		1.50E-11	1.50E-11	0.00
202	CO3-	+ NO2	= NO3-	+ CO2		8.00E-11	8.00E-11	0.00
203	CO3-	+ NO	= NO2-	+ CO2		1.80E-11	1.80E-11	0.00
204	CO3-	+ O	= O2-	+ CO2		8.00E-11	8.00E-11	0.00
205	CO4-	+ NO3	= NO3-	+ CO2	+ O2	5.00E-10	5.00E-10	0.00
206	NO3-	+ NO3	= NO3-	+ NO	+ O2	5.00E-10	5.00E-10	0.00
207	O3-	+ CO2	= CO3-	+ O2		5.50E-10	5.50E-10	0.00
208	O3-	+ O	= O2-	+ O2		1.00E-11	1.00E-11	0.00
209	O-	+ O2	+ M	= O3-	+ M	1.13E-30	1.10E-30	1.00
210	O2-	+ O2	+ M	= O4-	+ M	3.58E-51	3.50E-51	1.00
211	O4-	+ O	+ M	= O2-	+ O2	7.63E-15	1.00E-03	1.00
212	O4-	+ O		= O5-	+ O2	4.00E-10	4.00E-10	0.00
213	O4-	+ NO		= NO3-	+ O2	2.50E-10	2.50E-10	0.00
214	O4-	+ NO2		= NO4-	+ O2	4.30E-10	4.30E-10	0.00
215	O4-	+ NO2		= NO2-	+ O2	5.00E-10	5.00E-10	0.00
216	O4-	+ NO3		= NO3-	+ O2	5.00E-10	5.00E-10	0.00
217	O4-	+ O3		= O3-	+ O2	5.00E-10	5.00E-10	0.00
218	O4-	+ O2		= O4-	+ CO2	1.54E-14	4.50E-10	0.00
219	O2-	+ NO2	+ M	= CO4-	+ M	2.00E-29	2.00E-29	1.00
220	CO4-	+ NO		= NO3-	+ CO2	4.80E-11	4.80E-11	0.00
221	CO4-	+ O		= CO3-	+ O2	1.50E-10	1.50E-10	0.00
222	CO4-	+ O3		= O3-	+ CO2	1.30E-10	1.30E-10	0.00
223	CO3-	+ NO3		= NO3-	+ CO2	5.00E-10	5.00E-10	0.00
224	O-	+ NO3		= NO3-	+ O	5.00E-10	5.00E-10	0.00
225	NO2-	+ NO3		= NO3-	+ NO2	5.00E-10	5.00E-10	0.00
226	O2-	+ NO3		= NO3-	+ O2	5.00E-10	5.00E-10	0.00
227	O3-	+ NO3		= NO3-	+ O3	5.00E-10	5.00E-10	0.00
228	NO+	+ O-		= NO	+ O	1.98E-06	4.90E-07	.50
229	NO+	+ O2-		= NO	+ O2	2.07E-06	5.30E-07	.50
230	NO+	+ O3-		= NO	+ O3	1.69E-06	2.00E-07	.50
231	NO+	+ O4-		= NO	+ O2	1.69E-06	2.00E-07	.50
232	NO+	+ NO2-		= NO	+ NO2	1.84E-06	3.50E-07	.50
233	NO+	+ NO3-		= NO	+ NO3	1.89E-06	2.80E-07	.50
234	NO+	+ O2-		= NO	+ NO	1.89E-06	2.00E-07	.50
235	NO+	+ CO3-		= NO	+ CO2	1.69E-06	2.60E-07	.50
236	NO+	+ O4-		= NO	+ CO2	1.69E-06	2.00E-07	.50
237	O2+	+ O-		= O2	+ O	1.58E-06	9.60E-08	.50
238	O2+	+ O2-		= O2	+ O2	1.91E-06	4.20E-07	.50
239	O2+	+ O3-		= O2	+ O3	1.69E-06	2.30E-07	.50
240	O2+	+ O4-		= O2	+ O2	1.69E-06	2.00E-07	.50
241	O2+	+ NO2-		= O2	+ NO2	1.40E-06	4.10E-07	.50
242	O2+	+ NO3-		= O2	+ NO3	1.69E-06	2.00E-07	.50
243	O2+	+ NO3-		= O2	+ NO	1.69E-06	2.00E-07	.50
244	O2+	+ CO3-		= O2	+ CO2	1.69E-06	2.00E-07	.50
245	O2+	+ CO4-		= O2	+ CO2	1.69E-06	2.00E-07	.50
246	O4+	+ O-		= O2	+ O	1.59E-06	2.00E-07	.50

							A	B	C
247	H4+	+ H2-	= H2	+ H2	+ H2	1.69E-06	2.00E-07	.50	0.00
248	H4+	+ H3-	= H2	+ H3	+ H2	1.69E-06	2.00E-07	.50	0.00
249	H4+	+ H4-	= H4	+ H2	+ H2	1.69E-06	2.00E-07	.50	0.00
250	H4+	+ H22-	= H2	+ H22	+ H2	1.69E-06	2.00E-07	.50	0.00
251	H4+	+ H33-	= H2	+ H33	+ H2	1.69E-06	2.00E-07	.50	0.00
252	H4+	+ H43-	= H4	+ H4	+ H2	1.69E-06	2.00E-07	.50	0.00
253	H4+	+ H33-	= H4	+ H33	+ H2	1.69E-06	2.00E-07	.50	0.00
254	H4+	+ H44-	= H4	+ H22	+ H2	1.69E-06	2.00E-07	.50	0.00
255	H22+	+ H-	= H2	+ H-	+ H2	1.69E-06	2.00E-07	.50	0.00
256	H22+	+ H2-	= H2	+ H2	+ H2	1.69E-06	2.00E-07	.50	0.00
257	H22+	+ H3-	= H2	+ H3	+ H2	1.69E-06	2.00E-07	.50	0.00
258	H22+	+ H4-	= H2	+ H4	+ H2	1.69E-06	2.00E-07	.50	0.00
259	H22+	+ H22-	= H2	+ H22	+ H2	1.69E-06	2.00E-07	.50	0.00
260	H22+	+ H33-	= H2	+ H33	+ H2	1.69E-06	2.00E-07	.50	0.00
261	H22+	+ H43-	= H2	+ H43	+ H2	1.69E-06	2.00E-07	.50	0.00
262	H22+	+ H33-	= H22	+ H22	+ H2	1.69E-06	2.00E-07	.50	0.00
263	H22+	+ H44-	= H22	+ H44	+ H2	1.69E-06	2.00E-07	.50	0.00
264	H222+	+ H-	= H22	+ H-	+ H2	1.69E-06	2.00E-07	.50	0.00
265	H222+	+ H2-	= H22	+ H2	+ H2	1.69E-06	2.00E-07	.50	0.00
266	H222+	+ H3-	= H22	+ H3	+ H2	1.69E-06	2.00E-07	.50	0.00
267	H222+	+ H4-	= H22	+ H4	+ H2	1.69E-06	2.00E-07	.50	0.00
268	H222+	+ H22-	= H22	+ H22	+ H2	1.69E-06	2.00E-07	.50	0.00
269	H222+	+ H33-	= H22	+ H33	+ H2	1.69E-06	2.00E-07	.50	0.00
270	H222+	+ H43-	= H22	+ H43	+ H2	1.69E-06	2.00E-07	.50	0.00
271	H222+	+ H33-	= H22	+ H33	+ H2	1.69E-06	2.00E-07	.50	0.00
272	H222+	+ H44-	= H22	+ H44	+ H2	1.69E-06	2.00E-07	.50	0.00
273	H422+	+ H-	= (H22)2	+ H-	+ H2	1.69E-06	2.00E-07	.50	0.00
274	H422+	+ H2-	= (H22)2	+ H2	+ H2	1.69E-06	2.00E-07	.50	0.00
275	H422+	+ H3-	= (H22)2	+ H3	+ H2	1.69E-06	2.00E-07	.50	0.00
276	H422+	+ H4-	= (H22)2	+ H4	+ H2	1.69E-06	2.00E-07	.50	0.00
277	H422+	+ H22-	= (H22)2	+ H22	+ H2	1.69E-06	2.00E-07	.50	0.00
278	H422+	+ H33-	= (H22)2	+ H33	+ H2	1.69E-06	2.00E-07	.50	0.00
279	H422+	+ H43-	= (H22)2	+ H43	+ H2	1.69E-06	2.00E-07	.50	0.00
280	H422+	+ H33-	= (H22)2	+ H33	+ H2	1.69E-06	2.00E-07	.50	0.00
281	H422+	+ H44-	= (H22)2	+ H44	+ H2	1.69E-06	2.00E-07	.50	0.00
282	H422+	+ H-	= (H22)2	+ H-	+ H2	1.69E-06	2.00E-07	.50	0.00
283	H422+	+ H2-	= (H22)2	+ H2	+ H2	1.69E-06	2.00E-07	.50	0.00
284	H422+	+ H3-	= (H22)2	+ H3	+ H2	1.69E-06	2.00E-07	.50	0.00
285	H422+	+ H4-	= (H22)2	+ H4	+ H2	1.69E-06	2.00E-07	.50	0.00
286	H422+	+ H22-	= (H22)2	+ H22	+ H2	1.69E-06	2.00E-07	.50	0.00
287	H422+	+ H33-	= (H22)2	+ H33	+ H2	1.69E-06	2.00E-07	.50	0.00
288	H422+	+ H43-	= (H22)2	+ H43	+ H2	1.69E-06	2.00E-07	.50	0.00
289	H422+	+ H33-	= (H22)2	+ H33	+ H2	1.69E-06	2.00E-07	.50	0.00
290	H422+	+ H44-	= (H22)2	+ H44	+ H2	1.69E-06	2.00E-07	.50	0.00
291	H223+	+ H-	= H22	+ H-	+ H2	1.69E-06	2.00E-07	.50	0.00
292	H223+	+ H2-	= H22	+ H2	+ H2	1.69E-06	2.00E-07	.50	0.00
293	H223+	+ H3-	= H22	+ H3	+ H2	1.69E-06	2.00E-07	.50	0.00
294	H223+	+ H4-	= H22	+ H4	+ H2	1.69E-06	2.00E-07	.50	0.00
295	H223+	+ H22-	= H22	+ H22	+ H2	1.69E-06	2.00E-07	.50	0.00
296	H223+	+ H33-	= H22	+ H33	+ H2	1.69E-06	2.00E-07	.50	0.00
297	H223+	+ H43-	= H22	+ H43	+ H2	1.69E-06	2.00E-07	.50	0.00
298	H223+	+ H33-	= H22	+ H33	+ H2	1.69E-06	2.00E-07	.50	0.00
299	H223+	+ H44-	= H22	+ H44	+ H2	1.69E-06	2.00E-07	.50	0.00
300	H32+	+ H-	= H22	+ H-	+ H	1.69E-06	2.00E-07	.50	0.00
301	H32+	+ H2-	= H22	+ H2	+ H	1.69E-06	2.00E-07	.50	0.00
302	H32+	+ H3-	= H22	+ H3	+ H	1.69E-06	2.00E-07	.50	0.00
303	H32+	+ H4-	= H22	+ H4	+ H	1.69E-06	2.00E-07	.50	0.00
304	H32+	+ H22-	= H22	+ H22	+ H	1.69E-06	2.00E-07	.50	0.00
305	H32+	+ H33-	= H22	+ H33	+ H	1.69E-06	2.00E-07	.50	0.00
306	H32+	+ H43-	= H22	+ H43	+ H	1.69E-06	2.00E-07	.50	0.00
307	H32+	+ H33-	= H22	+ H33	+ H	1.69E-06	2.00E-07	.50	0.00
308	H32+	+ H44-	= H22	+ H44	+ H	1.69E-06	2.00E-07	.50	0.00

					A	B	C
304	H502+ + 0-	= (H20)12+ G	+ H	1.69E-06	2.00E-07	.50	0.00
310	H502+ + 02-	= (H20)12+ G2	+ H	1.69E-06	2.00E-07	.50	0.00
311	H502+ + 03-	= (H20)12+ G3	+ H	1.69E-06	2.00E-07	.50	0.00
312	H502+ + 04-	= (H20)12+ G4	+ H	1.69E-06	2.00E-07	.50	0.00
313	H502+ + N02-	= (H20)12+ N02	+ H	1.69E-06	2.00E-07	.50	0.00
314	H502+ + N03-	= (H20)12+ N03	+ H	1.69E-06	2.00E-07	.50	0.00
315	H502+ + N02-	= (H20)12+ N02	+ H02	1.69E-06	2.00E-07	.50	0.00
316	H502+ + C02-	= (H20)12+ C02	+ OH	1.69E-06	2.00E-07	.50	0.00
317	H502+ + C04-	= (H20)12+ C02	+ H02	1.69E-06	2.00E-07	.50	0.00
318	H703+ + 0-	= (H20)13+ 0	+ H	1.69E-06	2.00E-07	.50	0.00
319	H703+ + 02-	= (H20)13+ C2	+ H	1.69E-06	2.00E-07	.50	0.00
320	H703+ + 03-	= (H20)13+ C3	+ H	1.69E-06	2.00E-07	.50	0.00
321	H703+ + 04-	= (H20)13+ C4	+ H	1.69E-06	2.00E-07	.50	0.00
322	H703+ + N02-	= (H20)13+ N02	+ H	1.69E-06	2.00E-07	.50	0.00
323	H703+ + N03-	= (H20)13+ N03	+ H	1.69E-06	2.00E-07	.50	0.00
324	H703+ + N03-	= (H20)13+ N0	+ H02	1.69E-06	2.00E-07	.50	0.00
325	H703+ + C03-	= (H20)13+ C02	+ OH	1.69E-06	2.00E-07	.50	0.00
326	H703+ + C04-	= (H20)13+ C02	+ H02	1.69E-06	2.00E-07	.50	0.00
327	H904+ + 0-	= (H20)14+ 0	+ H	1.69E-06	2.00E-07	.50	0.00
328	H904+ + 02-	= (H20)14+ C2	+ H	1.69E-06	2.00E-07	.50	0.00
329	H904+ + 03-	= (H20)14+ C3	+ H	1.69E-06	2.00E-07	.50	0.00
330	H904+ + 04-	= (H20)14+ C4	+ H	1.69E-06	2.00E-07	.50	0.00
331	H904+ + N02-	= (H20)14+ N02	+ H	1.69E-06	2.00E-07	.50	0.00
332	H904+ + N03-	= (H20)14+ N03	+ H	1.69E-06	2.00E-07	.50	0.00
333	H904+ + N03-	= (H20)14+ N0	+ H02	1.69E-06	2.00E-07	.50	0.00
334	H904+ + C03-	= (H20)14+ C02	+ OH	1.69E-06	2.00E-07	.50	0.00
335	H904+ + C04-	= (H20)14+ C02	+ H02	1.69E-06	2.00E-07	.50	0.00
336	H1105+ + 0-	= (H20)15+ 0	+ H	1.69E-06	2.00E-07	.50	0.00
337	H1105+ + 02-	= (H20)15+ C2	+ H	1.69E-06	2.00E-07	.50	0.00
338	H1105+ + 03-	= (H20)15+ C3	+ H	1.69E-06	2.00E-07	.50	0.00
339	H1105+ + 04-	= (H20)15+ C4	+ H	1.69E-06	2.00E-07	.50	0.00
340	H1105+ + N02-	= (H20)15+ N02	+ H	1.69E-06	2.00E-07	.50	0.00
341	H1105+ + N03-	= (H20)15+ N03	+ H	1.69E-06	2.00E-07	.50	0.00
342	H1105+ + N03-	= (H20)15+ N0	+ H02	1.69E-06	2.00E-07	.50	0.00
343	H1105+ + C03-	= (H20)15+ C02	+ OH	1.69E-06	2.00E-07	.50	0.00
344	H1105+ + C04-	= (H20)15+ C02	+ H02	1.69E-06	2.00E-07	.50	0.00
345	H402+ + 0-	= H20 + 0	+ H20	1.69E-06	2.00E-07	.50	0.00
346	H402+ + 02-	= H20 + C2	+ H20	1.69E-06	2.00E-07	.50	0.00
347	H402+ + 03-	= H20 + C3	+ H20	1.69E-06	2.00E-07	.50	0.00
348	H402+ + 04-	= H20 + C4	+ H20	1.69E-06	2.00E-07	.50	0.00
349	H402+ + N02-	= H20 + N02	+ H20	1.69E-06	2.00E-07	.50	0.00
350	H402+ + N03-	= H20 + N03	+ H20	1.69E-06	2.00E-07	.50	0.00
351	H402+ + N03-	= (H20)12+ N0	+ G2	1.69E-06	2.00E-07	.50	0.00
352	H402+ + C03-	= (H20)12+ C02	+ G	1.69E-06	2.00E-07	.50	0.00
353	H402+ + C04-	= (H20)12+ C02	+ G2	1.69E-06	2.00E-07	.50	0.00
354	N02+ + 0-	= N2 + N0	+ G	1.69E-06	2.00E-07	.50	0.00
355	N02+ + 02-	= N2 + N0	+ C2	1.69E-06	2.00E-07	.50	0.00
356	N02+ + 03-	= N2 + N0	+ C3	1.69E-06	2.00E-07	.50	0.00
357	N02+ + 04-	= N2 + N0	+ C4	1.69E-06	2.00E-07	.50	0.00
358	N02+ + N02-	= N2 + N0	+ N02	1.69E-06	2.00E-07	.50	0.00
359	N02+ + N03-	= N2 + N0	+ N03	1.69E-06	2.00E-07	.50	0.00
360	N02+ + N03-	= N2 + N202	+ C2	1.69E-06	2.00E-07	.50	0.00
361	N02+ + C03-	= N2 + N02	+ C02	1.69E-06	2.00E-07	.50	0.00
362	N02+ + C04-	= N2 + N03	+ C02	1.69E-06	2.00E-07	.50	0.00
363	N0202+ + 0-	= C02 + N0	+ G	1.69E-06	2.00E-07	.50	0.00
364	N0202+ + 02-	= C02 + N0	+ C2	1.69E-06	2.00E-07	.50	0.00
365	N0202+ + 03-	= C02 + N0	+ C3	1.69E-06	2.00E-07	.50	0.00
366	N0202+ + 04-	= C02 + N0	+ C4	1.69E-06	2.00E-07	.50	0.00
367	N0202+ + N02-	= C02 + N0	+ N02	1.69E-06	2.00E-07	.50	0.00
368	N0202+ + N03-	= C02 + N0	+ N03	1.69E-06	2.00E-07	.50	0.00
369	N0202+ + N03-	= C02 + N202	+ C2	1.69E-06	2.00E-07	.50	0.00
370	N0202+ + C03-	= C02 + C02	+ N02	1.69E-06	2.00E-07	.50	0.00
371	N0202+ + C04-	= C02 + C02	+ N03	1.69E-06	2.00E-07	.50	0.00

