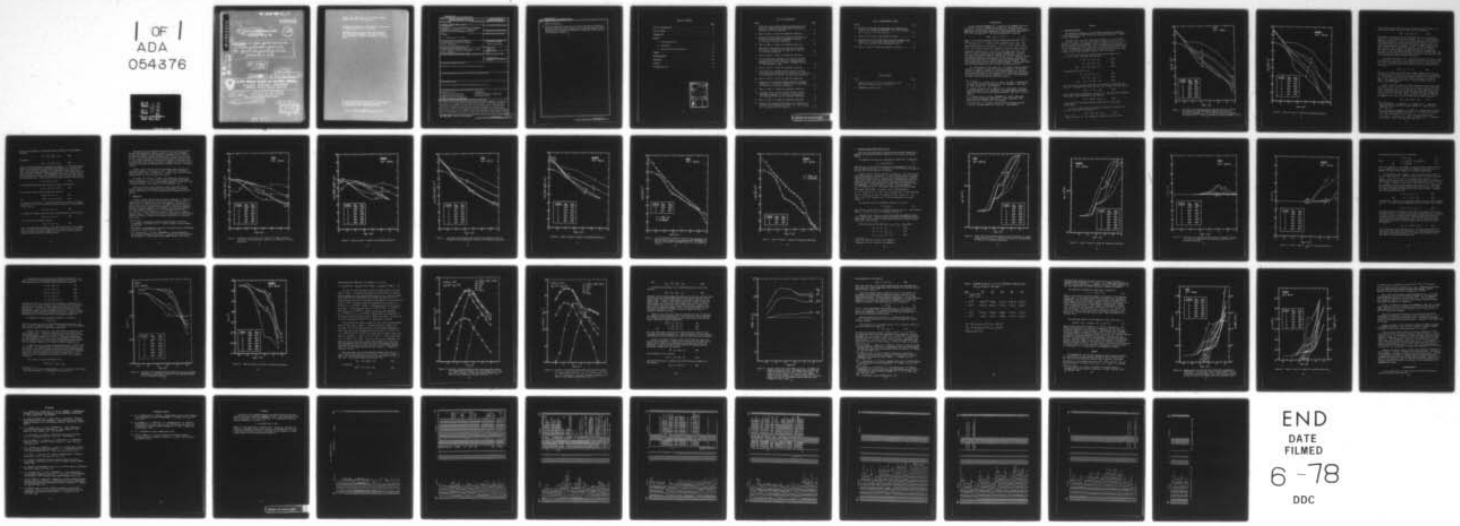
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BENCHMARK-76 Code
Effective Rate Coefficients
Computed Electron Densities
Computed Positive-ion Densities
Computed Negative-ion Densities
AIRCHEM Code
Disturbed Atmospheric Conditions
Multispecies Code

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Electron, positive and negative ion densities have been computed as a function of time at an altitude of 60 km under conditions where the prompt ionization parameter was assigned the values ten to the eighth, tenth or eleventh power per cubic centimeter and the delayed ionization parameter was assigned the values ten to the sixth, eighth or tenth power ion pairs per cubic centimeter per second, subject to the condition that the magnitude of the former be greater than the magnitude of the latter. Model times extend to 10,000 seconds in most

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cases and computations were made for daytime and nighttime conditions. Selected results and limited comparisons are reported together with the variations of the computed equivalent rate coefficients with time and with ionization conditions.

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INTRODUCTION

We have employed BENCHMARK-76, a version of the AIRCHEM[1] code with a 64 species set and a nominal 496 reaction set, to obtain species densities as a function of time at an altitude of 60 km for the following conditions. For the prompt ionization, N_o was assigned the values 10^{11}, 10^{10} or 10^{8} ion-pairs cm^{-3}. The delayed ionization is given by

$$Q(t) = Q_o\ (1 + t)^{-1.2}, \qquad (1)$$

where t is the time in seconds, and Q_o assigned the values 10^{6}, 10^{8} or 10^{10} ion-pairs $cm^{-3}\ s^{-1}$, subject to the constraint $|Q_o| < |N_o|$. The relative distribution of the species: N_2^+, O_2^+, N^+, O^+, $N(^4S)$, $N(^2D)$, $O(^3P)$, $O(^1D)$ $O_2(a^1\Delta)$ and $O_2(b^1\Sigma)$ produced by ionization under disturbed conditions is taken to be: 0.64, 0.16, 0.14, 0.06, 0.45, 0.61, 1.28, 0.10, 0.24 and 0.05 particles per ion pair, respectively. This distribution closely follows that of Gilmore,[2,3] except that $N_2(A^3\Sigma)$ is not carried, $[O_2(^1\Delta)]$ is taken as 0.24 and [O] is 1.28. Cases for daytime and nighttime conditions are reported; the calculations correspond to about a three hour interval centered around noon and midnight. Appropriate neutral densities have been outlined elsewhere.[4] The program coding and fixed input parameters have also been discussed previously.[3]

It is the purpose of this report to: (1) display selected computed results as a function of time and ionization conditions, (2) show the results of comparison studies of a very limited nature, and (3) report the computed variations of the equivalent rate coefficients (ERC's) as a function of time and ionization conditions. (A copy of these BENCHMARK-76 results may be obtained by writing the authors.)

---

[1] E. L. Lortie, M. D. Kregel and F. E. Niles, "AIRCHEM: A Computational Technique for Modeling the Chemistry of the Atmosphere," BRL Report No. 1913, August 1976. (AD# A030157)

[2] F. Gilmore as quoted by B. F. Myers and M. R. Schoonover, "Electron Energy Degradation in the Atmosphere: Consequent Species and Energy Densities, Electron Flux, and Radiation Spectra," DNA 3513T, 3 Jan 75, Table 6.

[3] J. M. Heimerl and F. E. Niles, "BENCHMARK-76: Model Computations for Disturbed Atmospheric Conditions I. Input Parameters," BRL Report No. 2022, October 1977. (AD #A050355)

[4] F. E. Niles and J. M. Heimerl, "Selected Neutral Species Profiles 0-100 km," BRL Memo Report 2767, July 1977. (AD# A042620)

RESULTS

A. Selected Densities

The daytime and nighttime electron density computed as a function of time after burst is shown for the six ionization conditions in Figures 1 and 2, respectively.

We might expect that the larger the disturbance, i.e., the larger the value of N_o for a given Q_o, the longer it would take for the electron density to return to its quiescent value. In Figure 1 curves 4 and 6 (also 2 and 3) at the latest times ($t \geq 10^3$ s) show that the computed value of the electron density, [e], for curve 4 (2) falls below that for curve 6 (3). To examine why our expectations are not borne out by these computations, let us focus attention on curves 4 and 6 of Figure 1.

For both of these curves the main charge flow is found to be $Q \rightarrow e \rightarrow O_2^- \rightarrow CO_3^-$. The major reactions are

$$e + O_2 + O_2 \rightarrow O_2^- + O_2 \qquad \text{R125*}$$

$$O_2^- + O_3 \rightarrow O_3^- + O_2 \qquad \text{R246}$$

$$\text{and} \quad O_3^- + CO_2 \rightarrow CO_3^- + O_2. \qquad \text{R269}$$

A secondary path exists; to wit,

$$O_2^- + O_2 + M \rightarrow O_4^- + M \qquad \text{R285}$$

$$O_4^- + CO_2 \rightarrow CO_4^- + M \qquad \text{R273}$$

$$\text{and} \quad CO_4^- + O \rightarrow CO_3^- + O_2. \qquad \text{R255}$$

In any event the charge at this point in the sequence resides upon the CO_3^- ion. The major loss process for this ion is found to be the reaction

$$CO_3^- + O \rightarrow O_2^- + CO_2. \qquad \text{R252}$$

which simply cycles charge back to the O_2^- ion. The major loss of process for the O_2^- ion in both cases is the reaction

$$O_2^- + O_2(^1\Delta) \rightarrow 2\ O_2 + e, \qquad \text{R137}$$

whose product is an electron and the entire cycle $e \rightleftarrows O_2^- \rightleftarrows CO_3^-$ begins again.

For curve 4 there exists an important secondary loss process for the CO_3^- ion; namely, the reaction,

$$CO_3^- + NO \rightarrow NO_2^- + CO_2. \qquad \text{R250}$$

*Read as reaction 125, see Appendix for complete reaction listing.

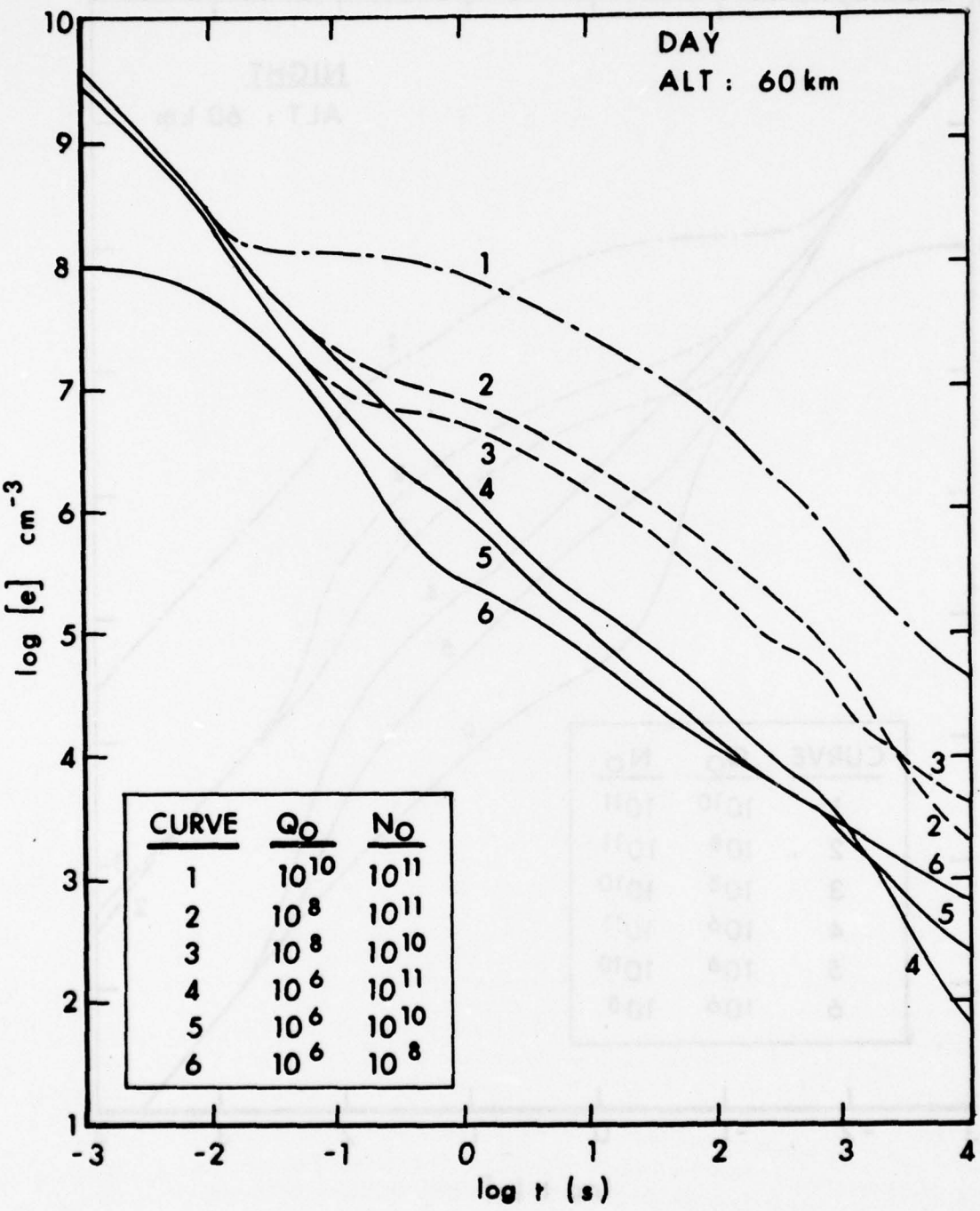


Figure 1. Logarithm of the computed daytime electron density at 60 km as a function of the logarithm of time for six different excitation conditions. Q_o is the delayed ionization parameter in ion-pairs $cm^{-3}s^{-1}$ and N_o the prompt ionization parameter in cm^{-3}.

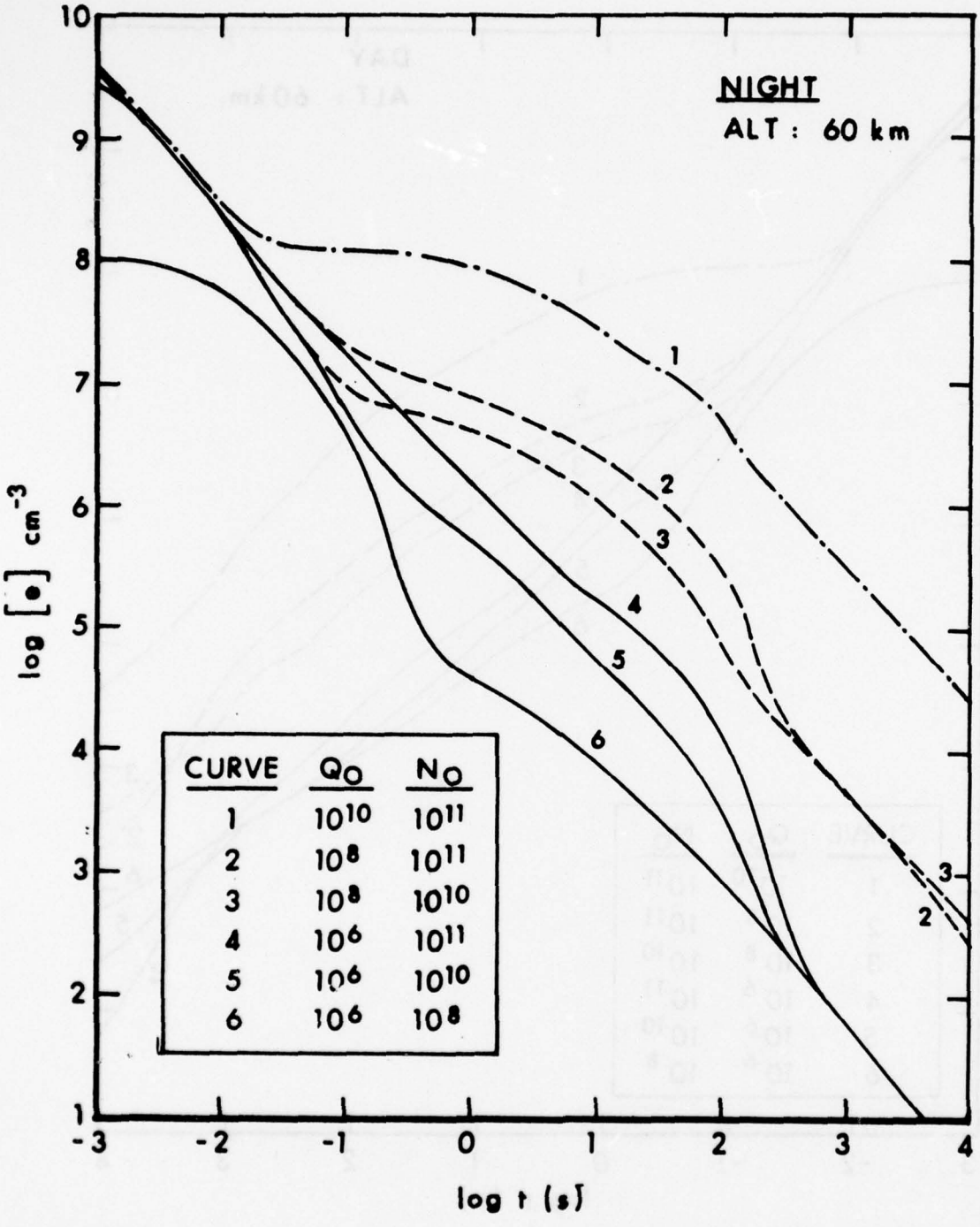


Figure 2. Same as Figure 1, except for nighttime conditions.

This reaction allows about 10% of the charge to flow to the NO_2^- ion which reacts rapidly to form the NO_3^- ion by the reaction

$$NO_2^- + O_3 \rightarrow NO_3^- + O_2. \qquad \text{R 260}$$

By contrast, reaction 250 for the conditions of curve 6 allows only about 0.1% of the charge to flow to the NO_3^- ion. It is the relative importance of the CO_3^- ion loss via reaction 250 that accounts for the calculated difference in the late time electron densities. For case 4 the charge that flows to the NO_3^- ion tends to remain bound to it. (The electron affinity of the NO_3^- ion (EA = 3.9 eV)[5] is greater than that of the O_2^- ion (0.440 eV)[6] or the CO_3^- ion (EA = 2.69 eV)[7].) This process tends to deplete the number density of free electrons. For curve 6, the path forming the NO_3^- ion is about a hundred times less effective than for curve 4 and the number density of free electrons tends to be maintained through the recycling process.

To find why reaction 250 is so pivotal a reaction the values of [NO] are examined at late times. It is found that the value of [NO] for curve 4 is about one hundred times larger than for curve 6. The reason for this lies in the formation of the NO molecule at the earliest times by the reaction

$$N(^2D) + O_2 \rightarrow NO + O. \qquad \text{R86}$$

The value of $[N(^2D)]$, hence the value of [NO] through reaction 86, is determined in large part by the value of the prompt ionization parameter, N_o. To summarize we find that for the same value of Q, the greater the value of N_o, the larger the value of [NO], the larger the value of $[NO_3^-]$, the smaller the value of [e]. Similar arguments apply for curves 2 and 3 of Figure 1.

Figure 2 explicitly shows a similar phenomenon at the latest times for curves 2 and 3. Curves 4 and 6 also cross as in Figure 1 but their values are so similar to case 5 that they are indistinguishable on this scale. Arguments similar to the daytime case apply here, except that the details of the reactions change. As before, the main charge flow is given by $Q \rightarrow e \rightarrow O_2 \rightarrow CO_3^-$ by reactions 125, 246 and 269. But here the major loss for the CO_3^- ion at late times at night is given by

$$CO_3^- + NO_2 \rightarrow NO_3^- + CO_2. \qquad \text{R 251}$$

---

[5] See for example E. E. Ferguson, D. B. Dunkin and F. C. Fehsenfeld, "Reactions of NO_2^- and NO_3^- with HCl and HBr," J. Chem. Phys. 57, 1459-1463, 1972.

[6] R. J. Celotta, R. A. Bennett, J. L. Hall, M. W. Siegel and J. Levine, "Molecular Photodetachment Spectrometry. II. The Electron Affinity of O_2 and the Structure of O_2^-," Phys. Rev. A6, 631-642, 1972.

[7] S. P. Hong, S. B. Woo and E. M. Helmy, "Photodetachment of Thermally Relaxed CO_3^-," Phys. Rev. A15, 1563-1569, 1977.

The NO_3^- ion formation is aided among other reactions by the secondary reactions

$$O_2^- + NO_2 \rightarrow NO_2^- + O_2 \qquad \text{R244}$$

followed by

$$NO_2^- + O_3 \rightarrow NO_3^- + O_2. \qquad \text{R260}$$

There are two differences for nighttime conditions. 1) The NO_2 molecule rather than the NO molecule determines the charge flow to the NO_3^- ion and 2) the recycling of charge is not important at late times. This last difference comes about because reaction 252 is not an important loss process for CO_3^- at night. The fundamental reason for this lies in the fact that the value of [O] falls markedly at late times at night relative to the daytime case. Atomic oxygen is converted to ozone by the reaction

$$O + O_2 + M \rightarrow O_3 + M; \qquad \text{R117}$$

but the dominant daytime loss process for ozone, the reaction

$$O_3 + h\nu \rightarrow O(^1D) + O_2(^1\Delta), \qquad \text{R47}$$

which returns atomic oxygen through the reactions

$$O(^1O) + M \rightarrow O + M \qquad \text{R97}$$

and

$$O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma), \qquad \text{R99}$$

is unavailable at night. A similar photon reaction explains the NO/NO_2 difference. To wit, at late times the primary source of the NO_2 molecule is the reaction

$$NO + O_3 \rightarrow NO + O_2. \qquad \text{R88}$$

In daytime the primary loss process for the NO_2 molecule is the reaction

$$NO_2 + h\nu \rightarrow NO + O \qquad \text{R40}$$

with aid from the secondary reaction

$$NO_2 + O \rightarrow NO + O_2. \qquad \text{R92}$$

Again, at night when no photons are available reaction 40 is not significant. Reaction 92 does not compensate for the loss because as we have alluded to above the atomic oxygen density also falls at late times at night with the result that the $[NO_2]$ builds.

The dominant electron depopulating process at late times for both day and night conditions (Figures 1 and 2) is three body attachment. At night the dominant electron production mechanism at late times is the delayed ionization source term whose value is given by Q (see equation 1). Thus at the later times the electron densities tend to track Q. For daytime conditions the recycling of charge, as discussed above, may permit the rates of other reactions to compete with the source rate with the result that the daytime electron densities need not, in general, track Q.

Figures 3 and 4 show the sum of the negative ions (exclusive of electrons) computed as a function of time. Conditions correspond to those in Figures 1 and 2, respectively. Figures 5 and 6 show the corresponding plots for the sum of the positive ions.

For times less than 10^{-2} seconds, the electron and positive ion curves (Figures 1, 2, 5 and 6) tend to group according to the prompt ionization parameter, N_o. For times greater than 10^{-1} seconds they tend to group according to the delayed ionization parameter, Q_o.

Some of the curves cease abruptly in these (and other) figures because computations are automatically halted whenever the electron density falls below 10 cm^{-3}, the assumed quiescent background electron density.

B. Comparison

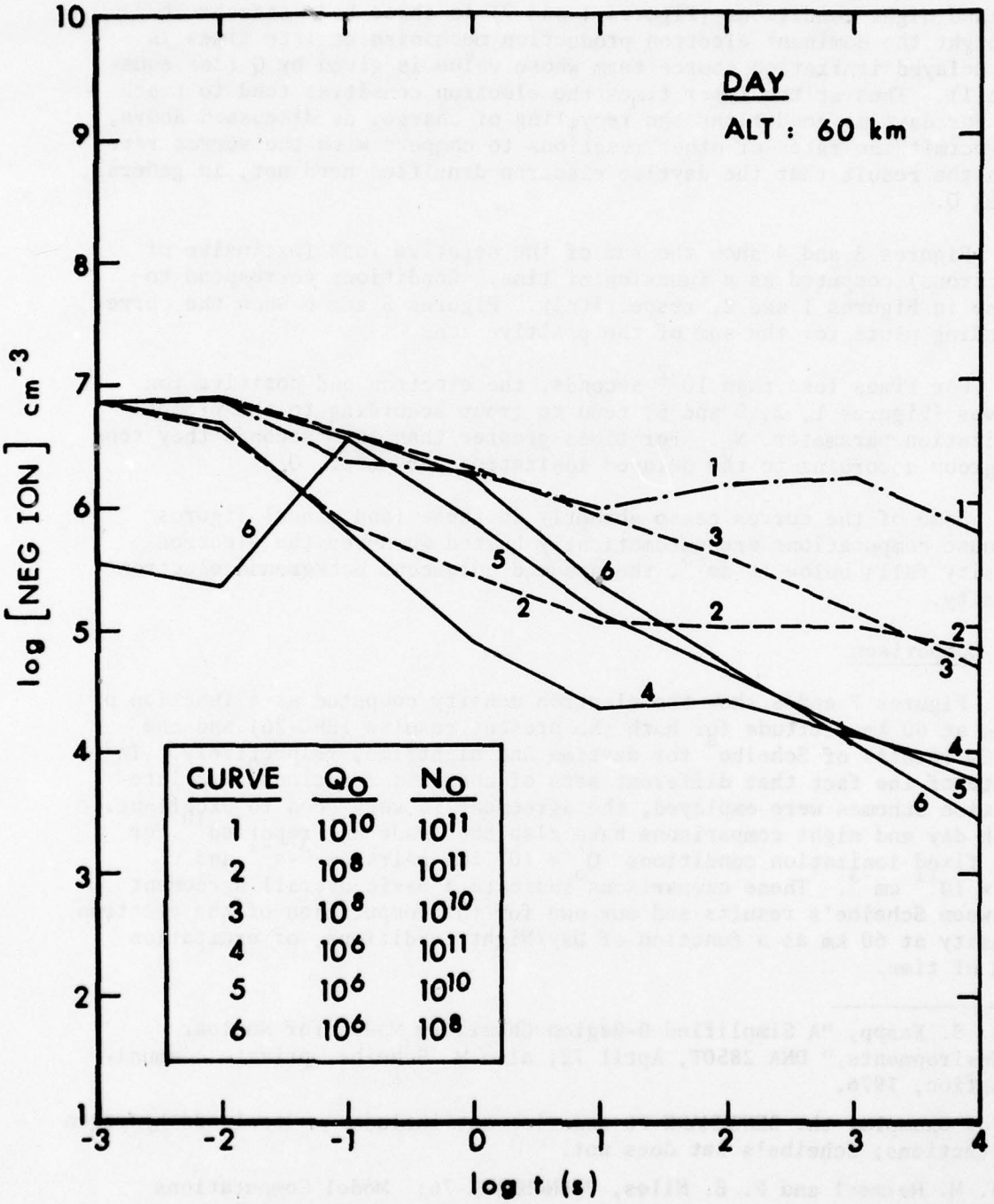
Figures 7 and 8 show the electron density computed as a function of time at 60 km altitude for both the present results (BRL-76) and the DCHEM results of Scheibe[8] for daytime and nighttime, respectively. In spite of the fact that different sets of chemical reactions[9] and integration schemes were employed, the agreement is very good to excellent. Both day and night comparisons have also been made and reported[10] for the fixed ionization conditions $Q_o = 10^8$ ion-pairs-cm^{-3}-s^{-1} and $N_o = 10^{11}$ cm^{-3}. These comparisons indicate a basic overall agreement between Scheibe's results and our own for the computation of the electron density at 60 km as a function of Day/Night conditions, of excitation and of time.

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[8] W. S. Knapp, "A Simplified D-Region Chemistry Model for Nuclear Environments," DNA 2850T, April 72; also M. Scheibe, private communication, 1976.

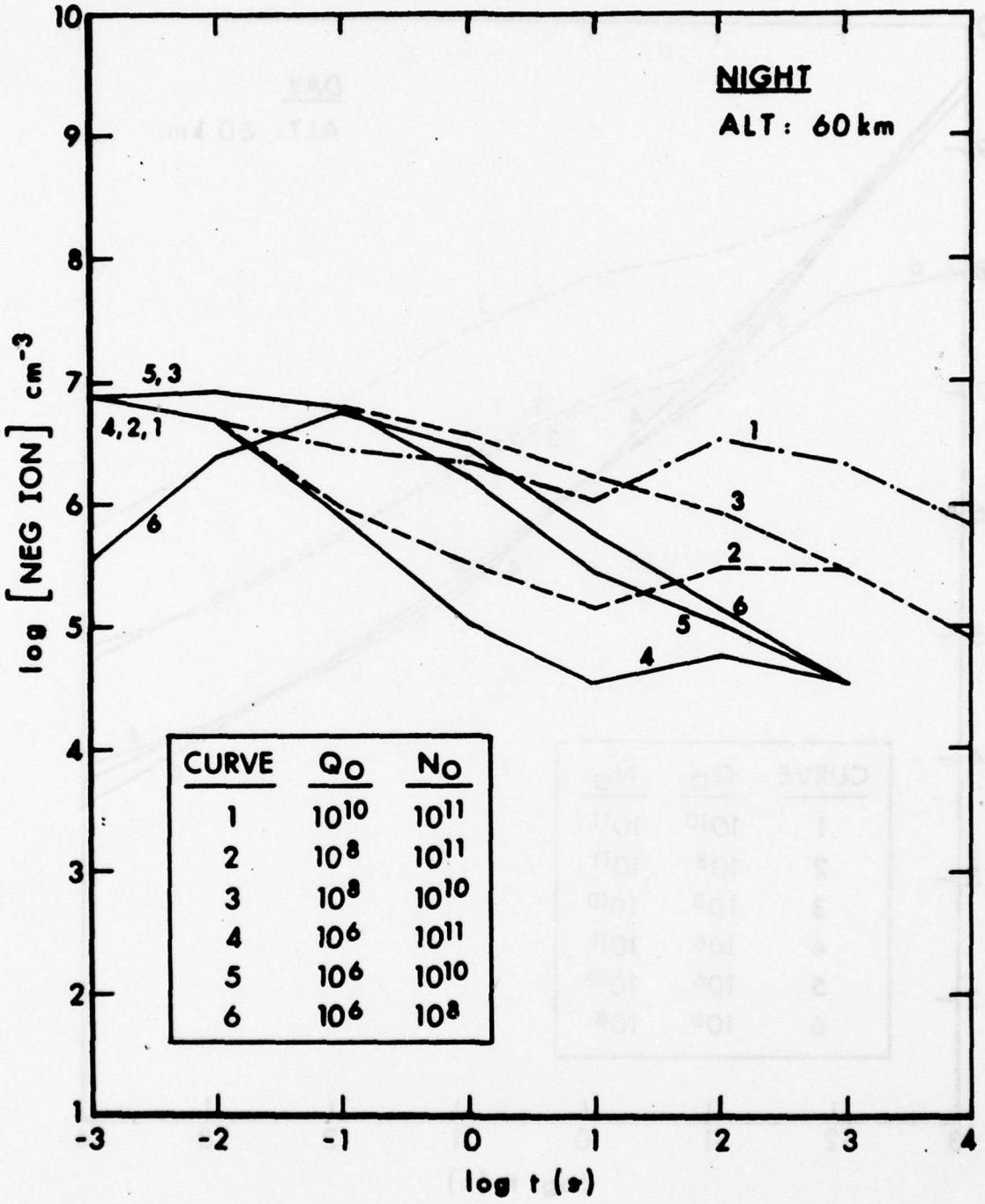
[9] For example, the BENCHMARK-76 reaction set includes neutral odd-hydrogen reactions; Scheibe's set does not.

[10] J. M. Heimerl and F. E. Niles, "BENCHMARK-76: Model Computations for Disturbed Atmospheric Conditions II. Results for the Stratosphere and Mesosphere," BRL Technical Report ARBRL-TR-02050, March 1978.



CURVE	Q_O	N_O
1	10^{10}	10^{11}
2	10^{8}	10^{11}
3	10^{8}	10^{10}
4	10^{6}	10^{11}
5	10^{6}	10^{10}
6	10^{6}	10^{8}

Figure 3. Logarithm of the daytime total negative ion density 60 km as a function of the logarithm of time for six different ionization conditions.



CURVE	Q_O	N_O
1	10^{10}	10^{11}
2	10^{8}	10^{11}
3	10^{8}	10^{10}
4	10^{6}	10^{11}
5	10^{6}	10^{10}
6	10^{6}	10^{8}

Figure 4. Same as Figure 3, except for nighttime conditions.

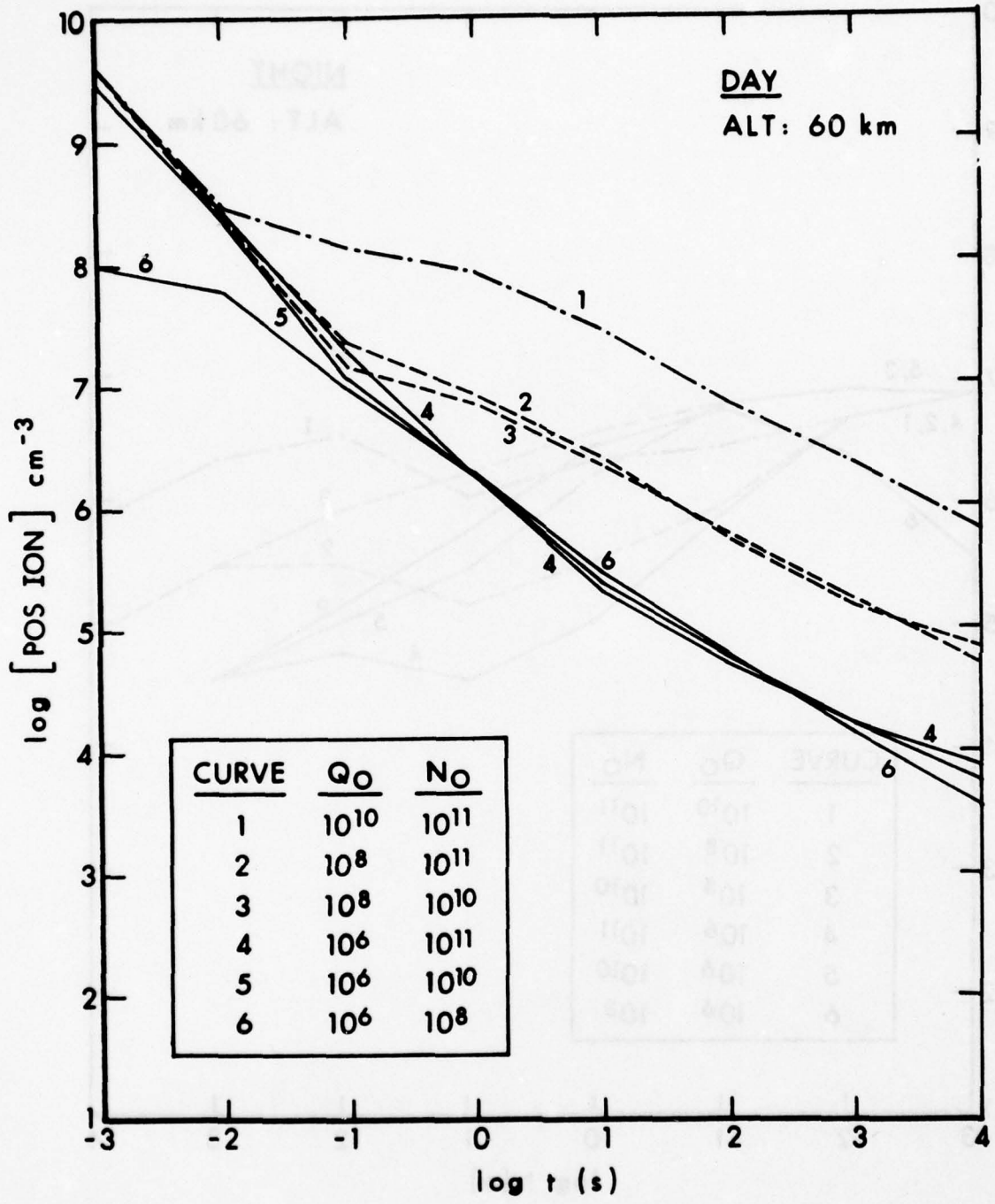


Figure 5. Logarithm of the daytime total positive ion density at 60 km as a function of the logarithm of time for six ionization conditions.

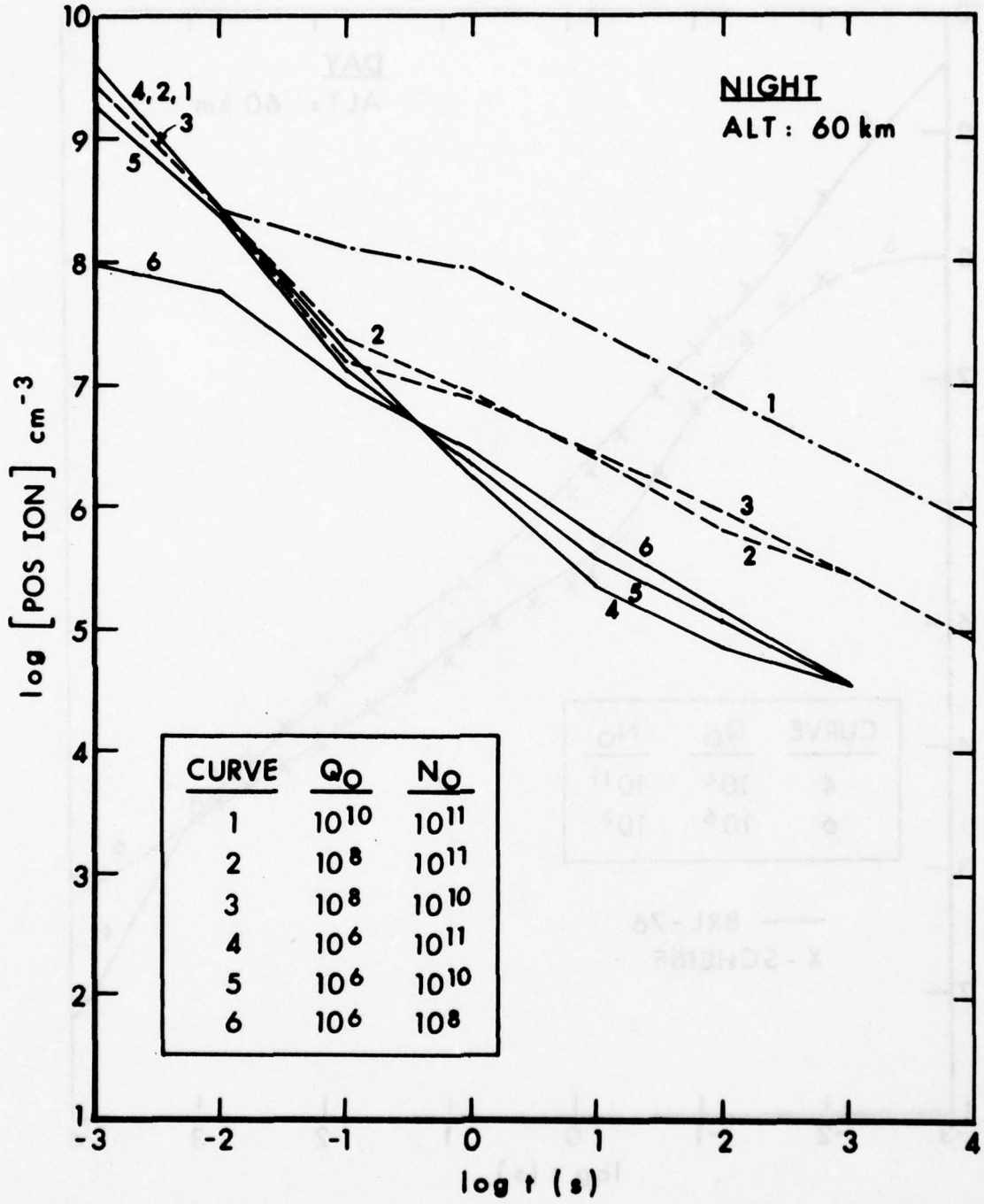


Figure 6. Same as Figure 5, except for nighttime conditions.

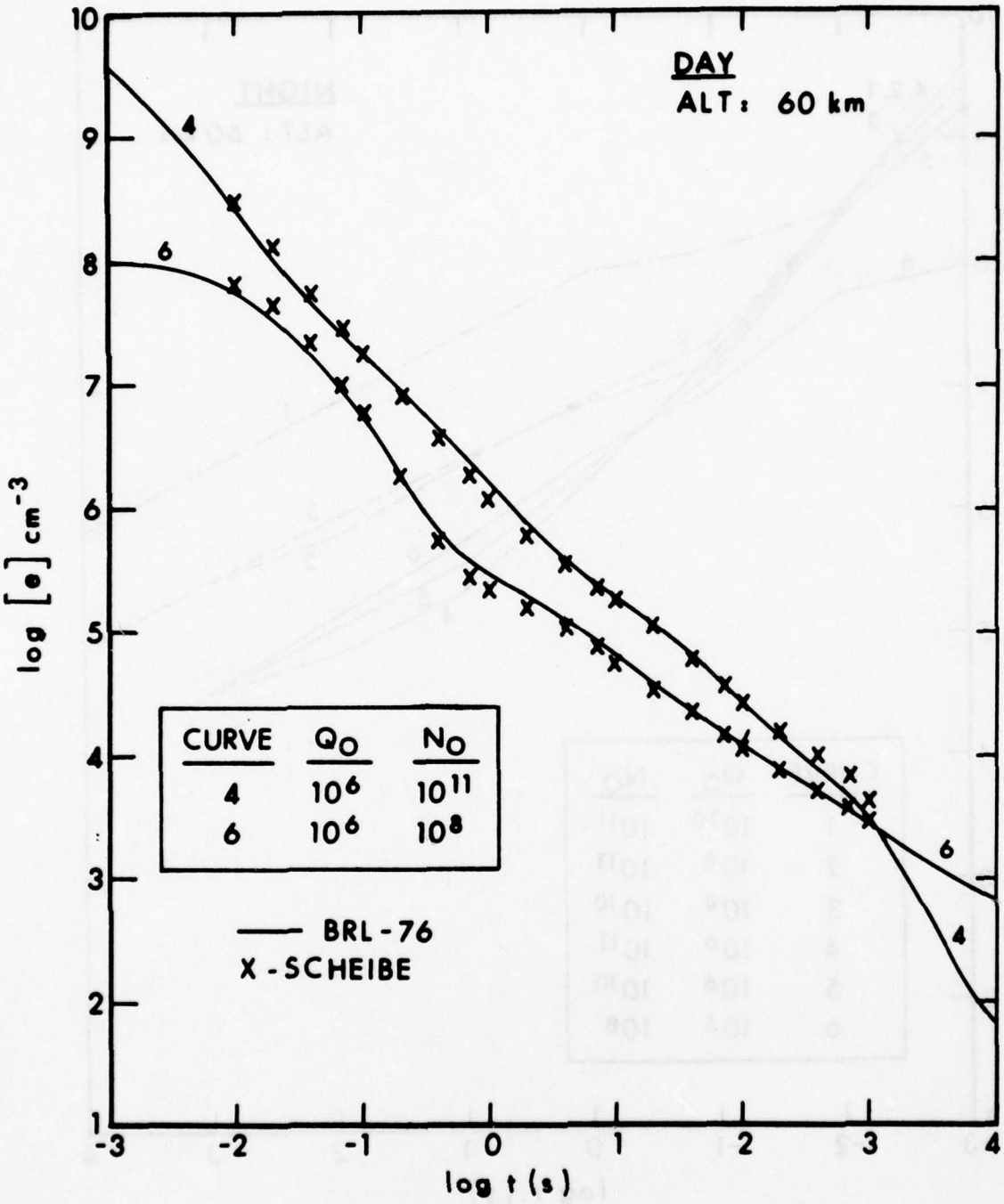


Figure 7. For two excitation conditions at 60 km the logarithm of the daytime electron density as computed by BRL's BENCHMARK-76 code (—) and Schiebe's DAIRCHEM code (X) vs. the logarithm of time.

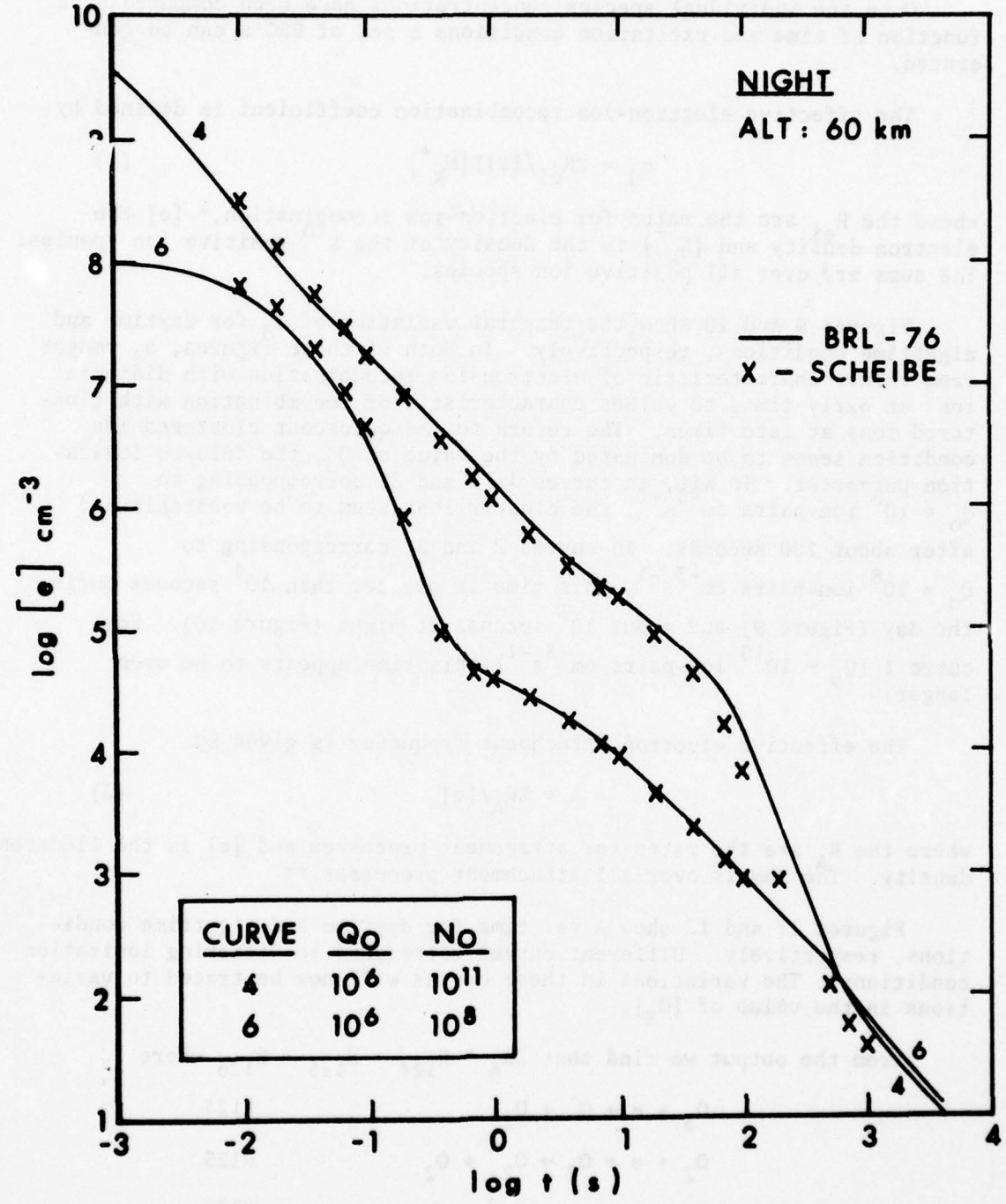


Figure 8. Same as Figure 7, except for nighttime conditions.

C. Equivalent Rate Coefficients (ERC's)

Once the individual species concentrations have been computed as a function of time and excitation conditions a set of ERC's can be generated.

The effective electron-ion recombination coefficient is defined by

$$\alpha_d = \Sigma R_{ei}/[e]\Sigma[N_k^+] \qquad (2)$$

where the R_{ei} are the rates for electron-ion recombination,* [e] the electron density and $[N_k^+]$ is the density of the k^{th} positive ion species. The sums are over all positive ion species.

Figures 9 and 10 show the temporal variation of α_d for daytime and nighttime conditions, respectively. In both of these figures, α_d ranges from values characteristic of electron-ion recombination with diatomic ions at early times to values characteristic of recombination with clustered ions at late times. The return to the quiescent clustered ion condition seems to be dominated by the value of Q_o, the delayed ionization parameter. To wit, in curves 4, 5 and 6, corresponding to $Q_o = 10^6$ ion-pairs $cm^{-3}s^{-1}$, the cluster ions seem to be reestablished after about 100 seconds. In curves 2 and 3, corresponding to $Q_o = 10^8$ ion-pairs $cm^{-3}s^{-1}$, this time is greater than 10^4 seconds during the day (Figure 9) and about 10^3 seconds at night (Figure 10). For curve 1 ($Q_o = 10^{10}$ ion-pairs $cm^{-3}s^{-1}$) this time appears to be even longer.

The effective electron attachment frequency is given by

$$A = \Sigma R_A/[e] \qquad (3)$$

where the R_A are the rates for attachment processes and [e] is the electron density. The sum is over all attachment processes.**

Figures 11 and 12 show A vs. time for daytime and nighttime conditions, respectively. Different curves correspond to differing ionization conditions. The variations in these curves will now be traced to variations in the value of $[O_3]$.

From the output we find that $\Sigma R_A \simeq R_{124} + R_{125} + R_{126}$ where

$$O_3 + e \rightarrow O^- + O_2 \qquad \text{R124}$$

$$O_2 + e + O_2 \rightarrow O_2^- + O_2 \qquad \text{R125}$$

$$O_2 + e + N_2 \rightarrow O_2^- + N_2 \qquad \text{R126}$$

*Reactions 138-162, inclusive (see Appendix)

**Reactions 122-126, inclusive (see Appendix)

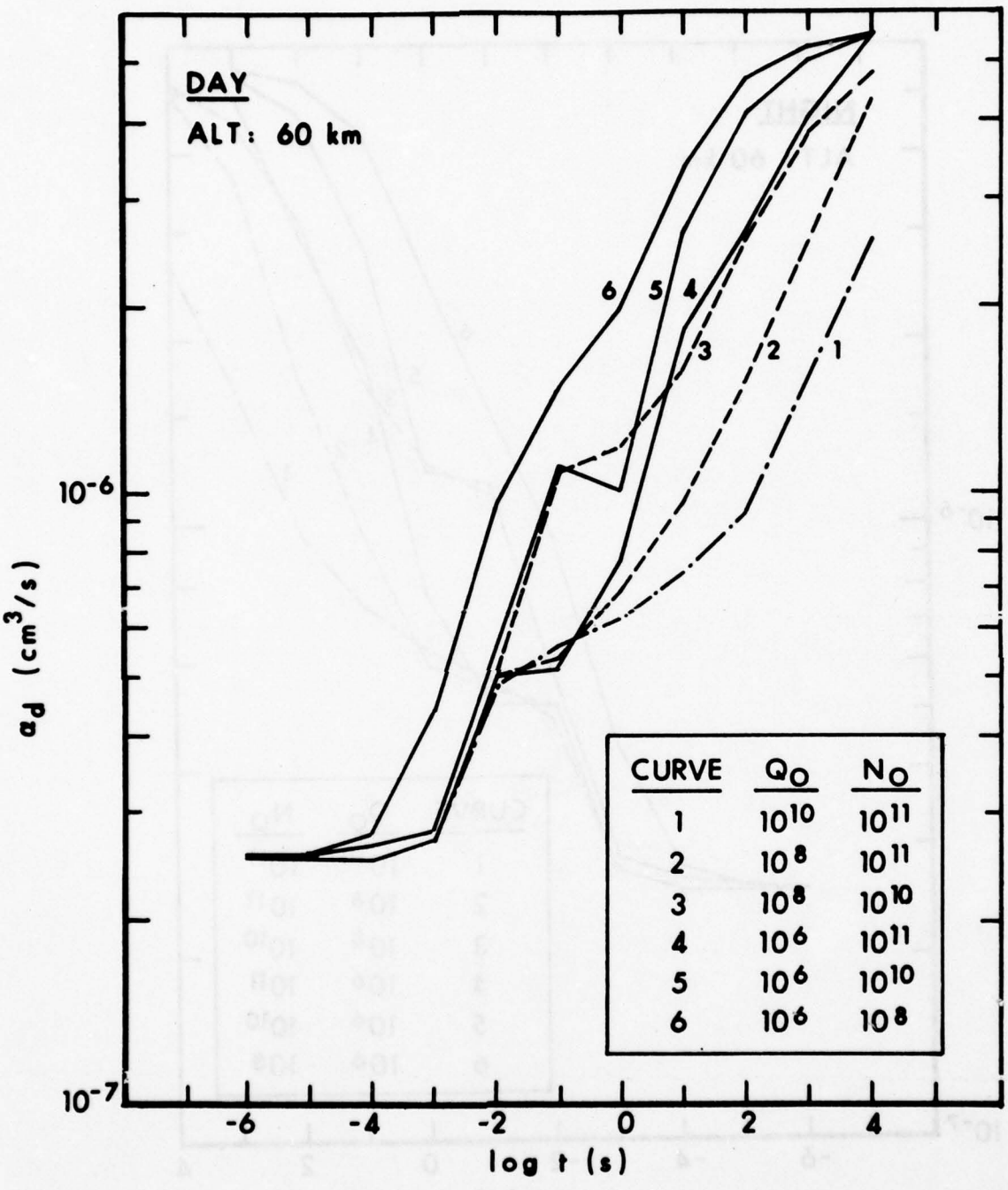


Figure 9. Logarithm of the computed daytime effective electron-ion recombination coefficient, α_d, at 60 km as a function of the logarithm of time for six ionization conditions.

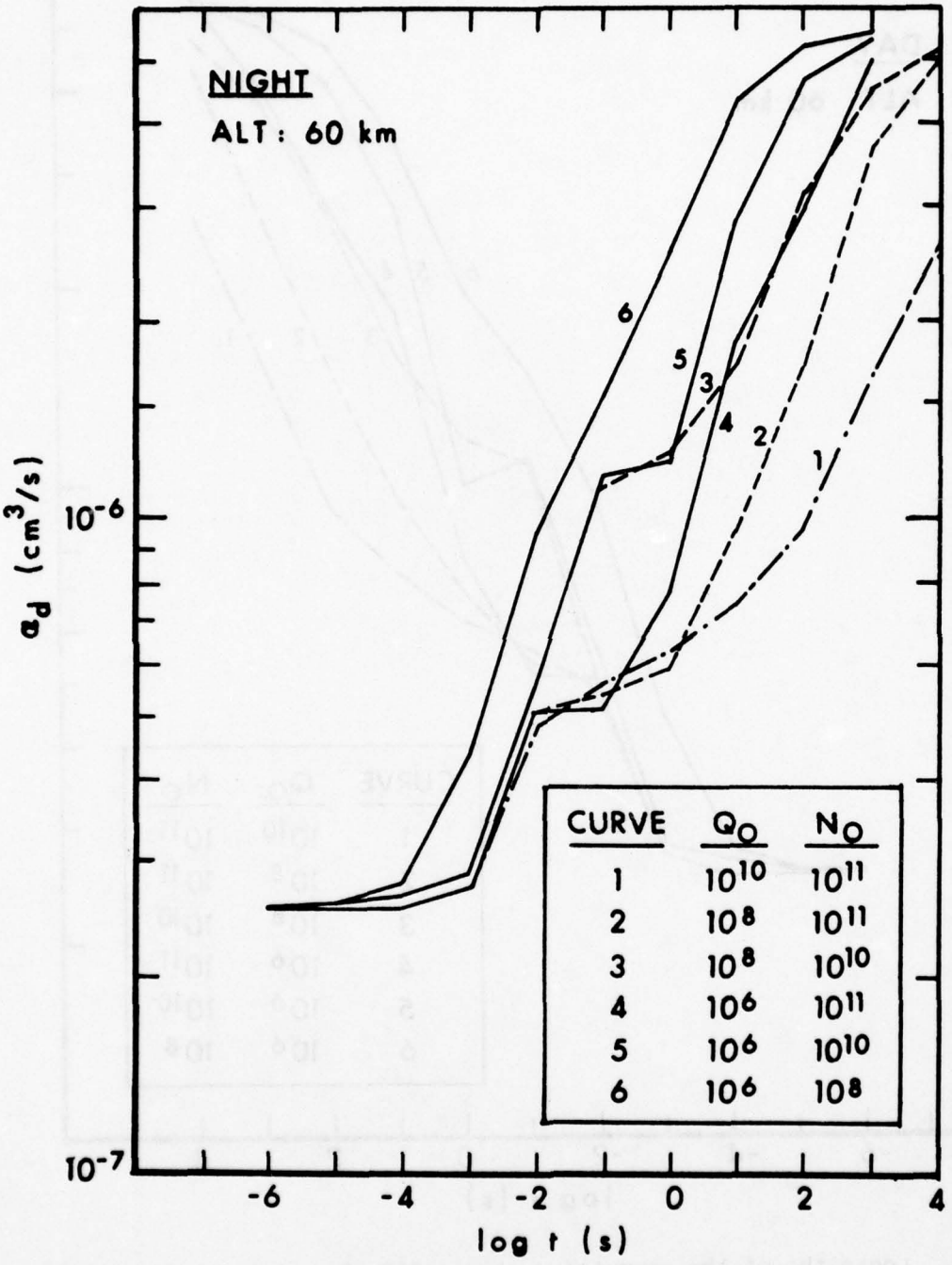


Figure 10. Same as Figure 9, except for nighttime conditions.

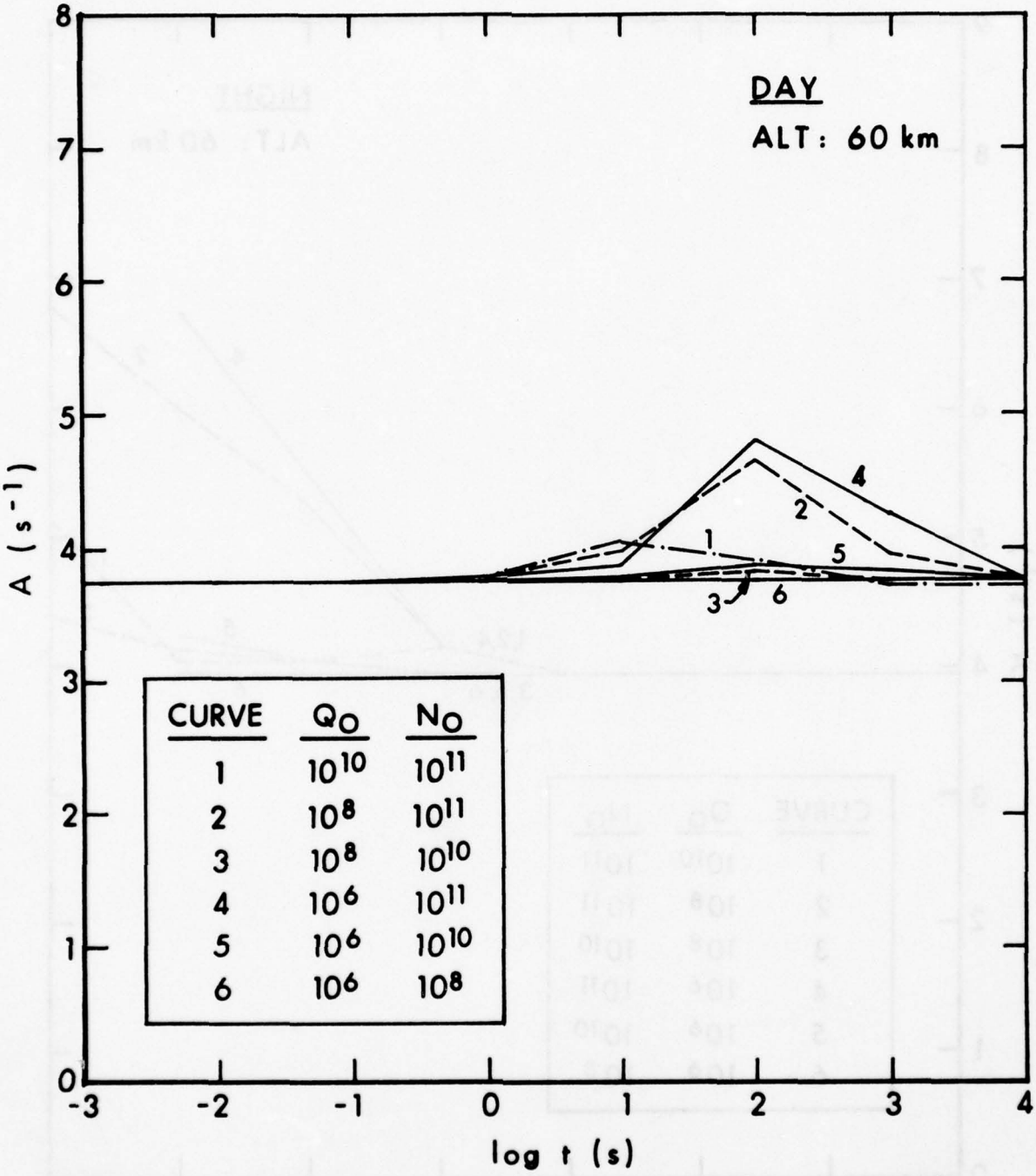


Figure 11. Logarithm of the computed daytime effective attachment frequency, A, at 60 km as a function of the logarithm of time for six ionization conditions.

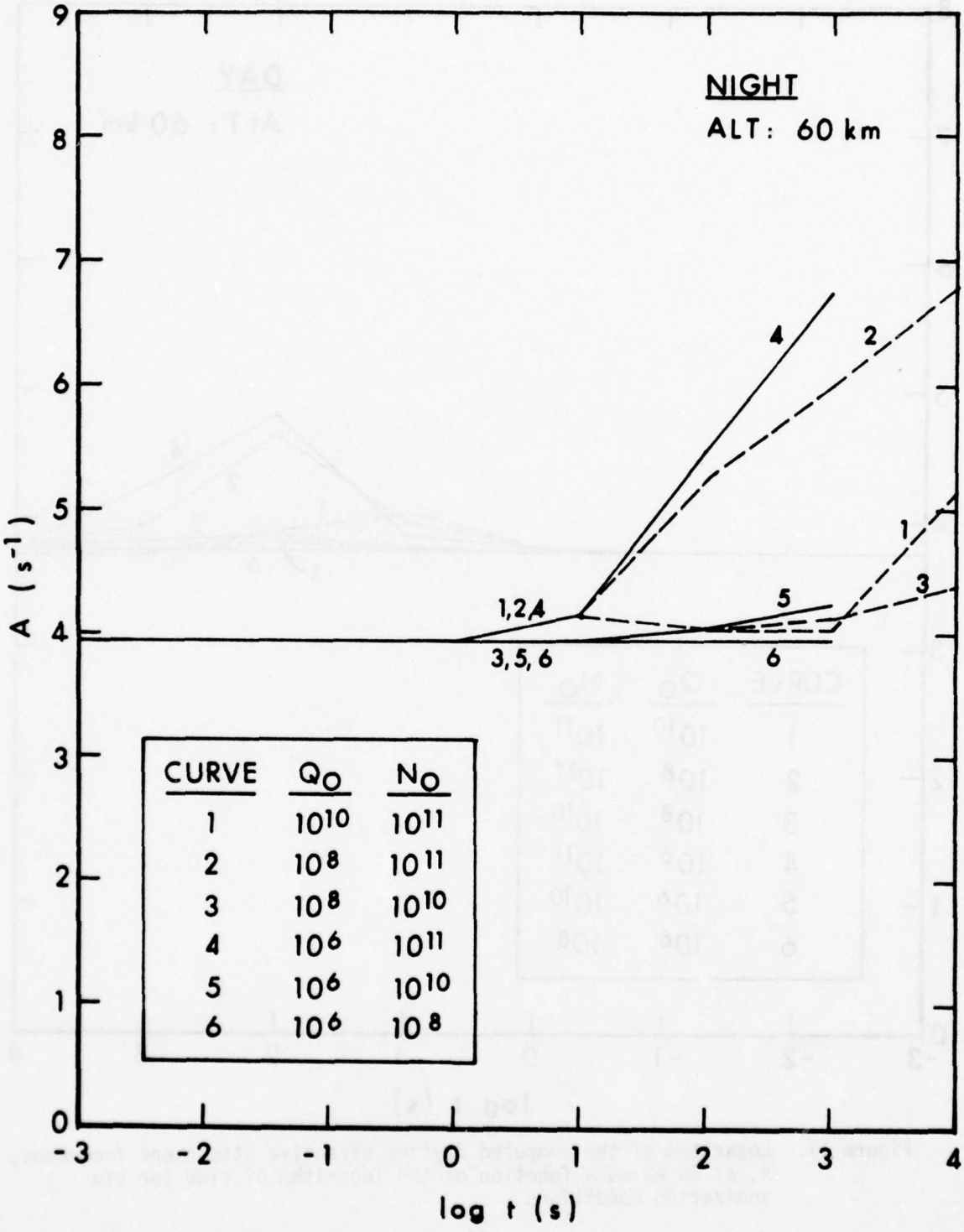


Figure 12. Same as Figure 11, except for nighttime conditions.

Substituting into equation (3) we find that

$$A \simeq C(1 + B) \tag{4}$$

where

$$C = k_{125}[O_2]^2 + k_{126}[O_2][N_2] \tag{5}$$

and

$$B = k_{124}[O_3]/C. \tag{6}$$

Since C in Equation (5) is constant to several decimal places and since k_{124} in Equation (6) is held fixed, the changes in the value of A in Equation (4) must reflect changes in the ozone concentration.

For the daytime case, Figure 11, let us consider curve 4 since it has the largest excursion. Figure 11 shows three easily determined time domains. For $10^{-3} \leq t \leq 10^{-1}$s A is observed to be constant. It is found that B of Equation (6) is 0.01 in this time period. [B of Equation (6) is simply a measure of the relative importance of $R_{124}/(R_{125} + R_{126})$.] Thus Equations (4) and (5) show that at early times $A \approx C$. The reason that the value of $[O_3]$ remains constant over this interval lies in the near balance between the production and loss rates of ozone. The major reactions populating ozone are

$$O + O_2 + M \rightarrow O_3 + M \qquad \text{R117}$$

and

$$O_4^+ + O \rightarrow O_2^+ + O_3. \qquad \text{R204}$$

Reaction 204 is found to be an important source of O_3 up to and including $t = 10^{-2}$s. The major reaction depopulating ozone over this time interval is

$$O_2(^1\Sigma) + O_3 \rightarrow 2\ O_2 + O. \qquad \text{R104}$$

The overall effect of reactions 117 and 104 is to convert $O_2(^1\Sigma)$ to O_2. Eventually $[O_2(^1\Sigma)]$ is depleted and for times greater than 10^{-1}s the value of $[(O_2(^1\Sigma)]$ falls to such an extent that the production rate (now due almost exclusively to Reaction 117) exceeds the loss rate with the result that the ozone concentration rises. By 10^2 seconds the ozone concentration has risen to such an extent that the rate of O_3 loss by the reaction

$$O_3 + h\nu \rightarrow O(^1D) + O_2(^1\Delta) \qquad \text{R49}$$

tends to balance the O_3 production rate. For times greater than 10^3s the value of $[O_3]$ tracks the value of [O] (in fact their densities are about equal) and since the value of the atomic oxygen begins to fall, the value of the ozone density does also.

At night only two time domains are observed in Figure 12. For times less than 10^0s the daytime arguments apply for A constant. For times greater than 10^0 seconds the loss rates which are due to

$$H + O_3 \rightarrow HO + O_2 \qquad R70$$

$$N + O_3 \rightarrow NO + O_2 \qquad R85$$

$$NO + O_3 \rightarrow NO_2 + O_2 \qquad R88$$

$$O + O_3 \rightarrow O_2 + O_2 \qquad R93$$

$$O + O_3 \rightarrow O_2(^1\Delta) + O_2 \qquad R94$$

and Reaction (104) fall relative to the production by Reaction (117) and again the rise in the value of $[O_3]$ is reflected by an increase in the value of A in Figure 12. The ozone density, $[O_3]$, will not rise indefinitely. In fact at 10^3s the major loss rate, which is due to Reaction 88, greatly exceeds the production rate to 117 thus we would anticipate the value of $[O_3]$ (hence the value of A) to fall as in the daytime case but at times later than those graphed in Figure 12.

The effective electron detachment frequency is defined by

$$D = \Sigma R_D / \Sigma [N_k^-], \qquad (7)$$

where the R_D are the rates for individual detachment processes* and $[N_k^-]$ is the k^{th} negative ion density. The sums are over all detachment rates and all negative ion densities, respectively.

Figures 13 and 14 show D vs. time for daytime and nighttime conditions, respectively. Ionization conditions are listed nearby their corresponding curves. The most notable feature in both Figures 13 and 14 is the apparent grouping of the curves. There are three groups, the first composed of curves 1, 2 and 4; the second of curves 3 and 5 and the third of curve 6. From the key on these figures we find that they are grouped according to the prompt ionization parameter, N_o.

In Figure 13 curve 6 attains the approximate limit of $10^0 s^{-1}$ after 10^0 seconds. This limiting value is typical of daytime quiescent conditions and is the value the other five daytime curves should approach, but do not. We shall now address (1) why curve 6 attains its limiting value and (2) why the others do not attain a similar limit. To be specific we shall concentrate our attention on curve 4 as a contrast to curve 6.

It is found to a good approximation that

$$\Sigma R_D \approx R_{137} + R_{135} + R_{129},$$

*Reactions 1-5 and 11 for photodetachment; 127-137 inclusive for two body collisional detachment. See Appendix for reaction list.

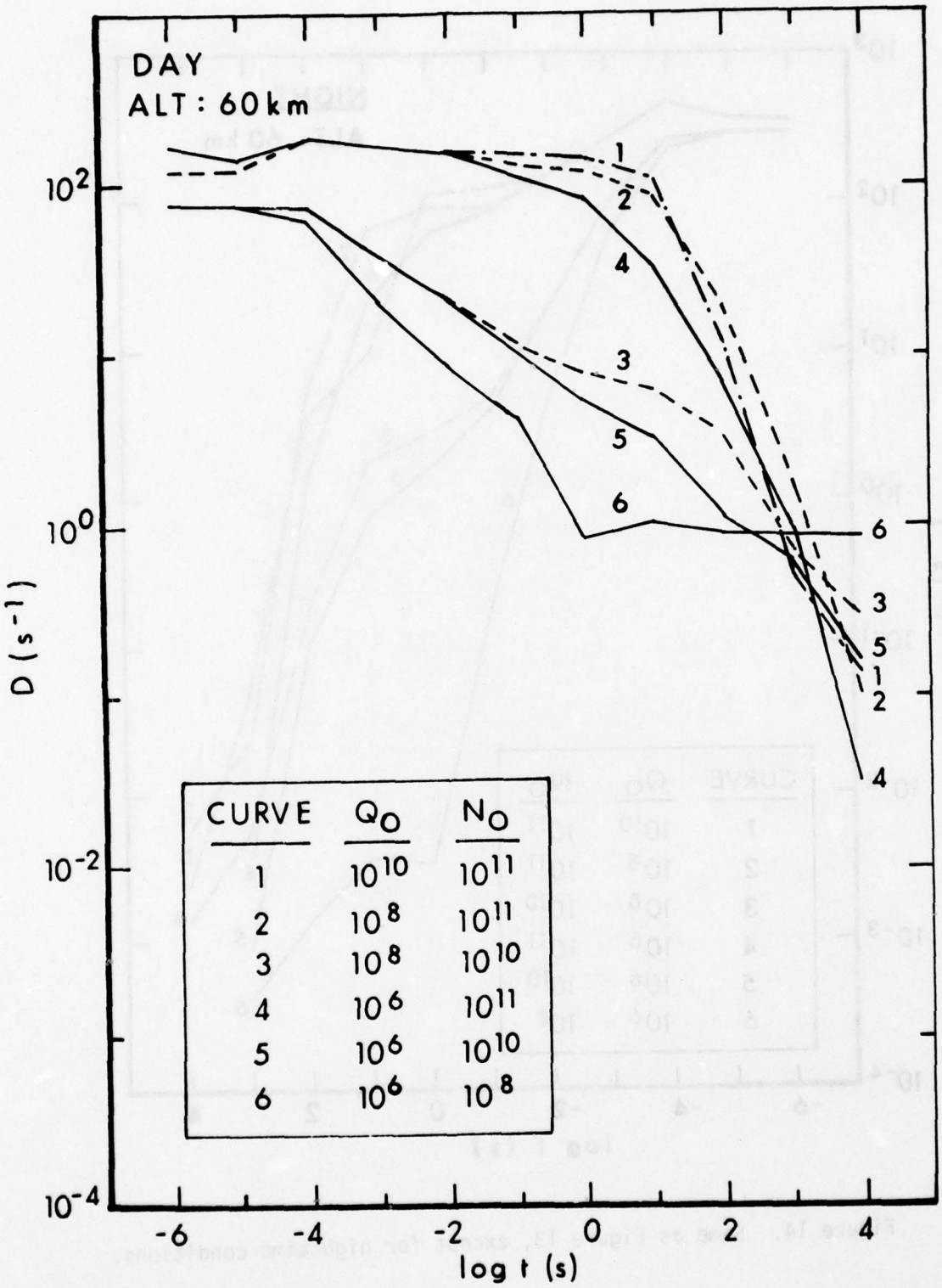


Figure 13. Logarithm of the computed daytime effective electron detachment frequency, D, at 60 km as a function of the logarithm of time for six ionization conditions.

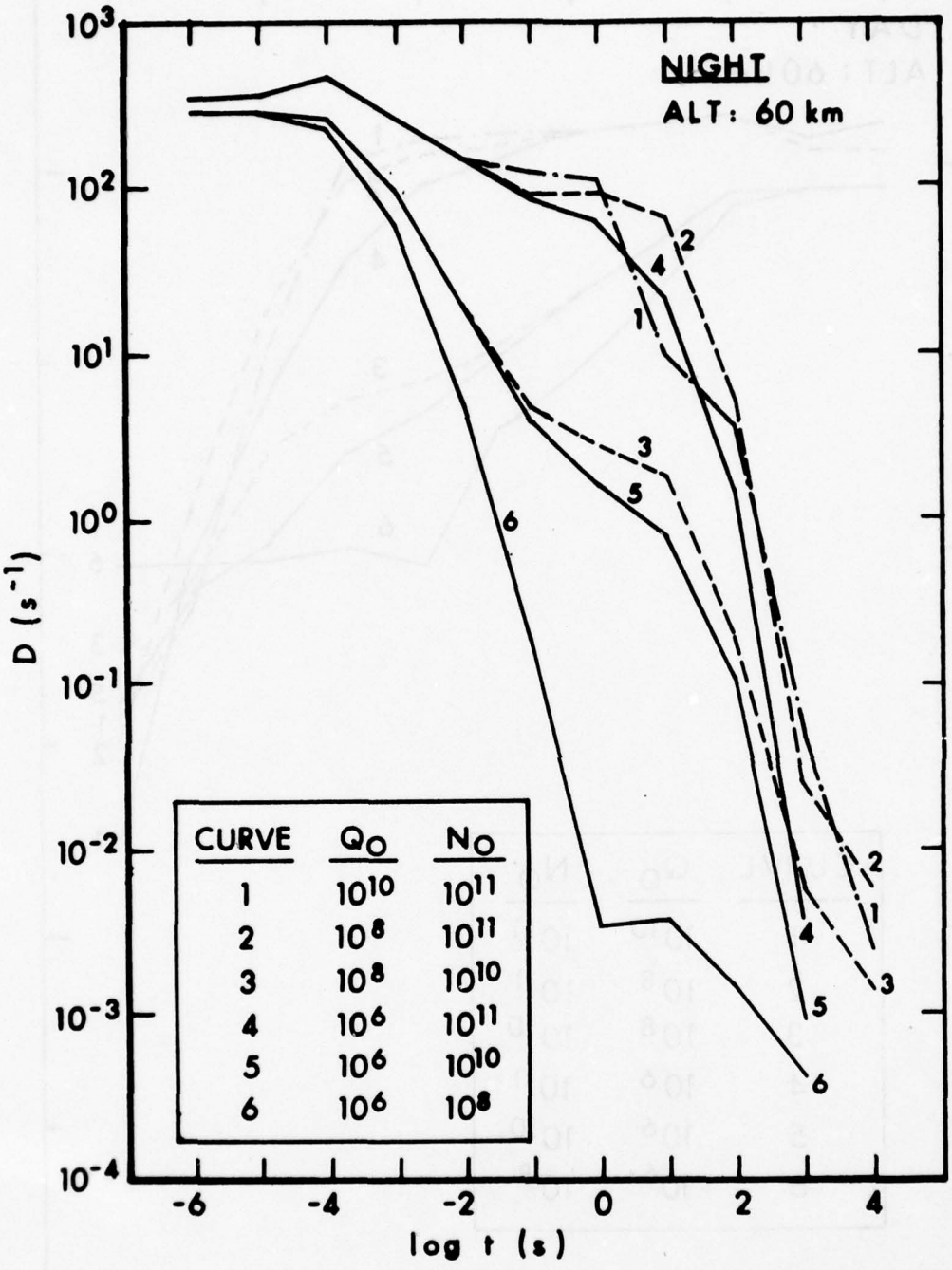


Figure 14. Same as Figure 13, except for nighttime conditions.

substituting this expression into Equation (7) we have

$$D \approx (k_{137}[O_2(^1\Delta)] + k_{135}[O])\ ([O_2^-]/\Sigma[N_k^-]) + k_{129}[N_2][O^-]/\Sigma[N_k^-]. \quad (8)$$

For case 6 we see from Figure 15 that for times greater than 10^0s $\Sigma[N_k^-] \approx [CO_3^-]$. In addition $[O_2^-]/[CO_3^-]$ and $[O^-]/[CO_3^-]$ are approximately constant over this time interval (see Fig. 15). Since the value of $[N_2]$ and the rate coefficients are constant the behavior of the $O_2(^1\Delta)$ molecule and of the O atom needs to be examined. Over the interval $10^1 \leq t \leq 10^4$s, the value of $[O_2(^1\Delta)]$ monotomically rises from 1.5 x 10^{10}cm^3 to 3.4 x 10^{10}cm^{-3}. There is no dramatic change in the value of [O] either. It first declines from 1.4 x 10^{10}cm^{-3} to 1.1 x 10^{10}cm^{-3}, then rises to 1.3 x 10^{10}cm^{-3}. Since k_{137} and k_{135} are comparable (2 x 10^{-10}cm^3/s vs. 1.5 x 10^{-10}cm^3/s, respectively) the variations in the values of $[O_2(^1\Delta)]$ and [O] tend to offset each other. Thus for case 6 and for times greater than 10^0s D is approximately constant.

On the other hand, Figure 16 shows for case 4 and for times greater than 10^1s that $\Sigma[N_k^-] \approx [NO_3^-]$. In addition both $[O_2^-]/[NO_3^-]$ and $[O^-]/[NO_3^-]$ can be seen from the figure to be declining functions of time. The value of [O] monotomically declines from 4.4 x 10^{11}cm^{-3} to 1.0 x 10^{10}cm^{-3} ($10^1 \leq t \leq 10^4$s), while the value of $[O_2(^1\Delta)]$ first rises from 4.0 x 10^{10}cm^3 ($t = 10^1$s) to 3.4 x 10^{11}cm^{-3} ($t = 10^3$s), then falls to 2.7 x 10^{10}cm^{-3} ($t = 10^4$s). Since k_{137} and k_{135} are comparable, the declining value of [O] tends to offset the rising value of $[O_2(^1\Delta)]$. Thus D in Equation (8) will follow the ratio of the negative ion densities and the net result is that D for case 4 and for times greater than 10^1s is a decreasing function of time. Cases 1, 2, 3 and 5 are similar to case 4.

One can ask why the late time dominant negative ion is NO_3^- in case 4 (and in other cases) but not in case 6. The answer to this is found to be in the production of the NO_3^- ion from either the CO_3^- or CO_4^- ions. The specific reactions are found to be

$$CO_4^- + NO \rightarrow OONO^- + CO_2 \qquad \text{R254}$$

followed by

$$OONO^- + NO \rightarrow NO_2^- + NO_2 \qquad \text{R262}$$

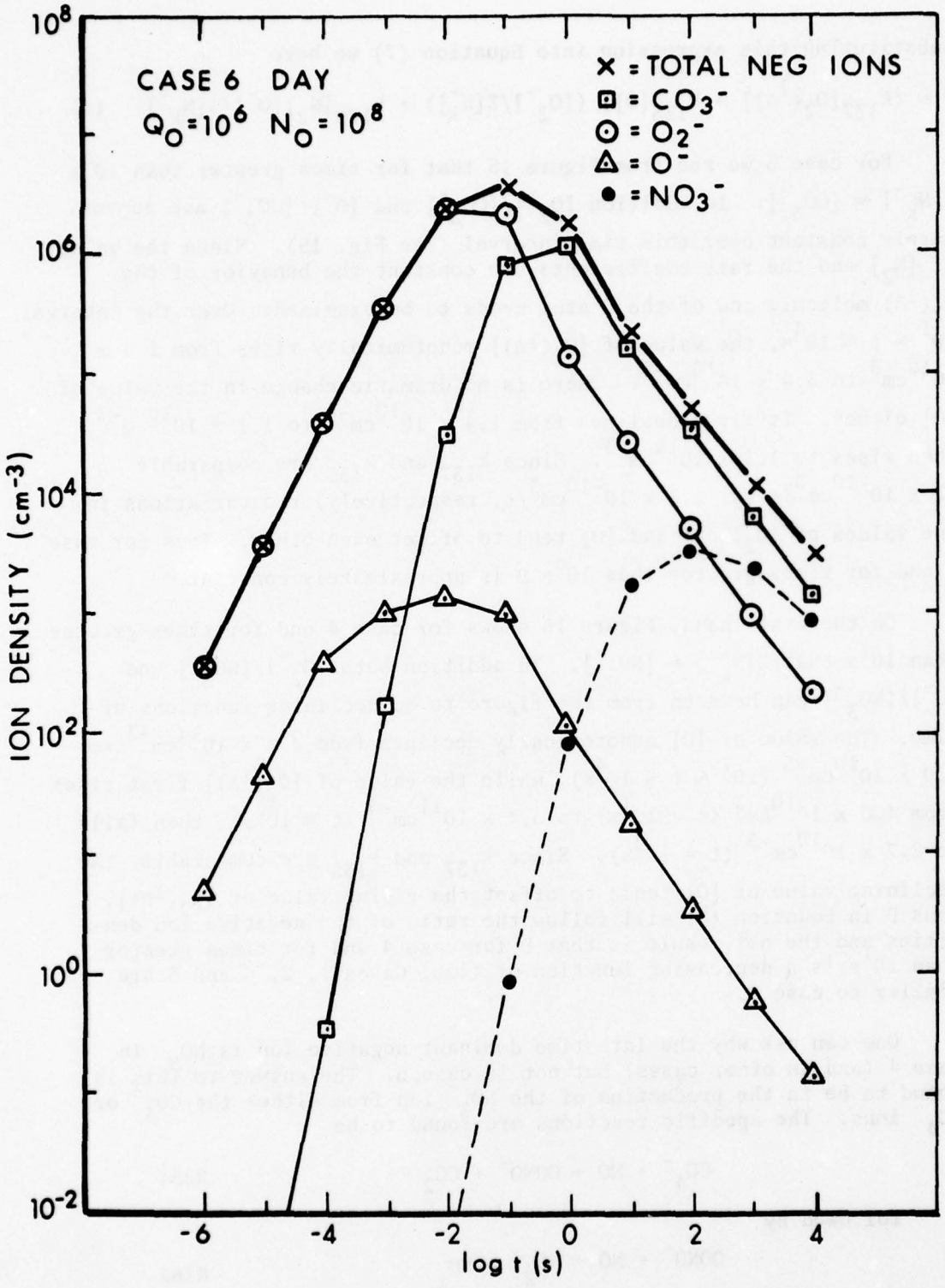


Figure 15. Histories of selected daytime negative ion densities at 60 km for the excitation conditions: $Q_o = 10^6$ ion-pairs $cm^{-3}s^{-1}$ and $N_o = 10^8 cm^{-3}$ (Case 6). The NO_3^- ion density, dashed line, is shown for easy comparison with Case 4, Fig. 16.

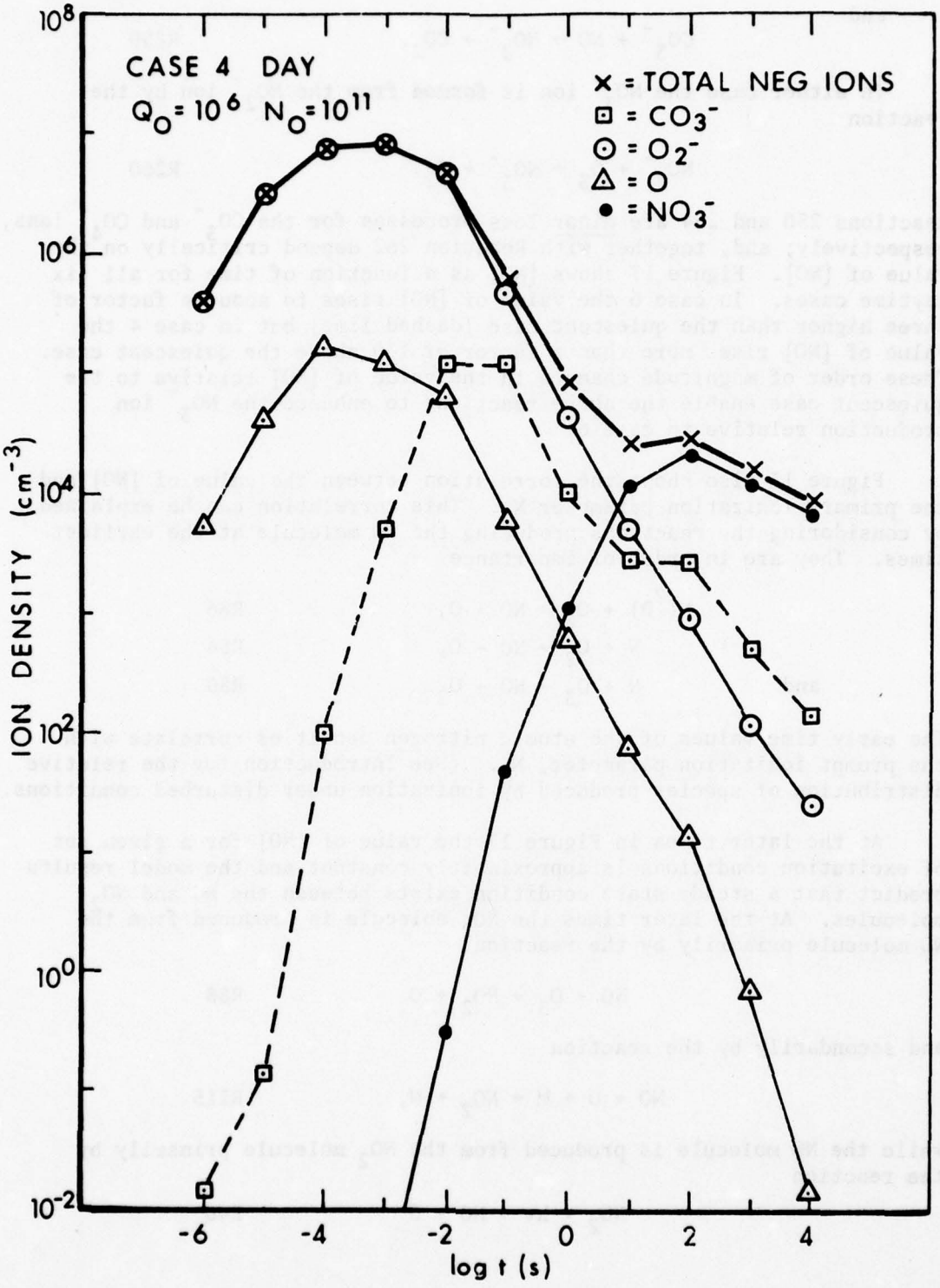


Figure 16. Histories of selected daytime negative ion densities at 60 km for the excitation conditions: $Q_o = 10^6$ ion-pairs $cm^{-3}s^{-1}$ and $N_o = 10^{11}$ cm^3 (Case 4). The CO_3^- ion density, dashed line, is shown for easy comparison with Case 6, Fig. 15.

and

$$CO_3^- + NO \rightarrow NO_2^- + CO_2. \qquad R250$$

In either case the NO_3^- ion is formed from the NO_2^- ion by the reaction

$$NO_2^- + O_3 \rightarrow NO_3^- + O_2. \qquad R260$$

Reactions 250 and 254 are minor loss processes for the CO_3^- and CO_4^- ions, respectively; and, together with Reaction 262 depend critically on the value of [NO]. Figure 17 shows [NO] as a function of time for all six daytime cases. In case 6 the value of [NO] rises to about a factor of three higher than the quiescent case (dashed line) but in case 4 the value of [NO] rises more than a factor of 100 above the quiescent case. These order of magnitude changes in the value of [NO] relative to the quiescent case enable the above reactions to enhance the NO_3^- ion production relative to case 6.

Figure 17 also shows the correlation between the value of [NO] and the primary ionization parameter N_o. This correlation can be explained by considering the reactions producing the NO molecule at the earliest times. They are in order of importance

$$N(^2D) + O_2 \rightarrow NO + O, \qquad R86$$

$$N + O_2 \rightarrow NO + O, \qquad R84$$

and

$$N + O_3 \rightarrow NO + O_2. \qquad R85$$

The early time values of the atomic nitrogen densities correlate with the prompt ionization parameter, N_o. (See Introduction for the relative distribution of species produced by ionization under disturbed conditions.)

At the later times in Figure 17 the value of [NO] for a given set of excitation conditions is approximately constant and the model results predict that a steady state condition exists between the NO and NO_2 molecules. At the later times the NO_2 molecule is produced from the NO molecule primarily by the reaction

$$NO + O_3 \rightarrow NO_2 + O_2 \qquad R88$$

and secondarily by the reaction

$$NO + O + M \rightarrow NO_2 + M, \qquad R115$$

while the NO molecule is produced from the NO_2 molecule primarily by the reaction

$$NO_2 + h\nu \rightarrow NO + O \qquad R40$$

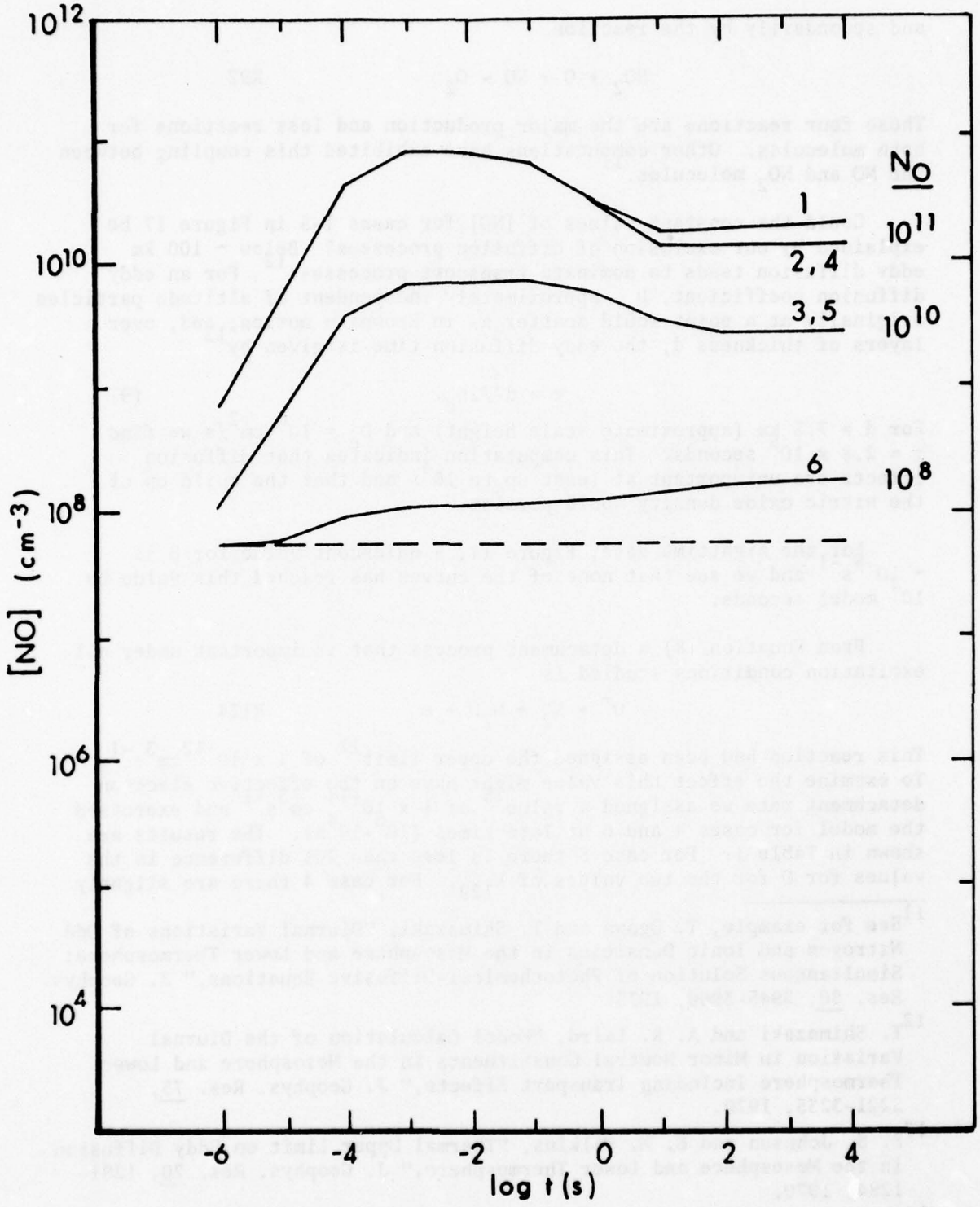


Figure 17. History of the nitric oxide density at 60 km. The dashed line denotes the quiescent value. The numbers refer to excitation conditions whose key may be found listed in the figures. The column to the far right of the curves lists the values of prompt ionization parameter, N_o, clearly showing the correlation between the value of this parameter and the late time value computed for nitric oxide.

and secondarily by the reaction

$$NO_2 + O \rightarrow NO + O_2. \qquad R92$$

These four reactions are the major production and loss reactions for both molecules. Other computations have exhibited this coupling between the NO and NO_2 molecules.[11]

Could the constant values of [NO] for cases 1-5 in Figure 17 be explained by our exclusion of diffusion processes? Below ~ 100 km eddy diffusion tends to dominate transport processes.[12] For an eddy diffusion coefficient, D_e, approximately independent of altitude particles originally at a point would scatter as in Brownian motion; and, over layers of thickness d, the eddy diffusion time is given by[13]

$$\tau = d^2/2D_e. \qquad (9)$$

For d = 7.5 km (approximate scale height) and $D_e = 10^6$ cm^2/s we find $\tau = 2.8 \times 10^5$ seconds. This computation indicates that diffusion effects are unimportant at least up to 10^4 s and that the build up of the nitric oxide density would persist.

For the nighttime case, Figure 14, a quiescent value for D is ~ 10^{-8} s^{-1} and we see that none of the curves has reached this value by 10^4 model seconds.

From Equation (8) a detachment process that is important under all excitation conditions studied is

$$O^- + N_2 \rightarrow N_2O + e \qquad R124$$

This reaction had been assigned the upper limit[14] of 1×10^{-12} cm^3s^{-1}. To examine the effect this value might have on the effective electron detachment rate we assigned a value[15] of 1×10^{-14} cm^3s^{-1} and exercised the model for cases 4 and 6 at late times (10^0-10^4 s). The results are shown in Table 1. For case 6 there is less than 20% difference in the values for D for the two values of k_{129}. For case 4 there are slightly

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[11] See for example, T. Ogawa and T. Shimazaki, "Diurnal Variations of Odd Nitrogen and Ionic Densities in the Mesosphere and Lower Thermosphere: Simultaneous Solution of Photochemical-Diffusive Equations," J. Geophys. Res. 80, 3945-3960, 1975.

[12] T. Shimazaki and A. R. Laird, "Model Calculation of the Diurnal Variation in Minor Neutral Constituents in the Mesosphere and Lower Thermosphere Including Transport Effects," J. Geophys. Res. 75, 3221-3235, 1970.

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[14] W. Lindinger, D. C. Albritton, F. C. Fehsenfeld and E. E. Ferguson, "Reactions of O^- with N_2, N_2O, SO_2, NH_3, CH_4 and C_2H_4 and $C_2H_2^-$ with O from 300°K to Relative Kinetic Energies of ~ 2 eV," J. Chem. Phys. 63, 3238-3242, 1975.

[15] F. C. Fehsenfeld, private communication, 1977.

TABLE 1. COMPUTED VALUES OF D (s^{-1}) AS A FUNCTION OF TIME AND VALUE OF k_{129} FOR CASE 6[†] AND CASE 4[*]

CASE	k_{129} (cc/s) \ time (s)	10^0	10^1	10^2	10^3	10^4
6	10^{-12}	8.89(-1)[**]	1.06(0)	9.17(-1)	8.60(-1)	8.97(-1)
6	10^{-14}	7.58(-1)	8.95(-1)	7.77(-1)	7.50(-1)	7.84(-1)
4	10^{-12}	8.14(+1)	3.38(+1)	4.98(0)	9.77(-1)	3.23(-2)
4	10^{-14}	5.58(+1)	2.27(+1)	2.88(0)	7.61(-1)	2.92(-2)

[†] $Q_o = 10^6$ ion pairs $cm^{-3}s^{-1}$, $N_o = 10^8$ cm^{-3}

[*] $Q_o = 10^6$ ion pairs $cm^{-3}s^{-1}$, $N_o = 10^{11} cm^{-3}$

[**] Read as 8.89×10^{-1}.

differing rates of decline for the two values of k_{129} resulting in a maximum of 53% difference at 10^2 seconds. As we have found previously,[10] with the smaller value for k_{129}, reaction 129 was no longer dominant, but was still significant ($\geq$ 10%) and could not in general be ignored.

The effective recombination coefficient is defined by

$$\psi = (1 + \lambda)(\alpha_d + \lambda\alpha_i), \qquad (9)$$

where λ is the ratio of the total negative ion density to the electron density and α_i is the effective positive ion-negative ion recombination coefficient.[1] In the steady state, a criterion many times employed in hybrid models,[16] ψ (solid lines in Figures 18 and 19), should equal the source term divided by the electron density squared, $Q/[e]^2$ (dashed lines in Figures 18 and 19). This equality is approximately reached (i.e., within 20%) in both Figures 18 and 19 by 10^{-1} s for curve 1, by 10^0 s for curves 2 and 3 and by 10^2 s for curves 4, 5 and 6 (by 10^3 s for curve 6 at night). These curves tend to be grouped according to the value of Q_o. We have not been able to find a simple explanation as to why this is so.

The governing equation for the approach to the steady state is

$$d[e]/dt = Q(t) - \psi\{\alpha_d(Q), \lambda(Q), \alpha_i(t)\}[e]^2 , \qquad (10)$$

where Q and ψ are given by equations (1) and (9), respectively. The explicit dependencies are written out to emphasize the fact that ψ is an implicit function of time through Q. From equation (10), one might expect the tendency to group the time at which a steady state condition is reached with Q_o, as observed in Figures 18 and 19. But, the non-linearity and implicit functional dependencies upon time in equation (10) have prevented any simple qualitative understanding of the observed grouping with Q_o. Several attempts to solve simpler formulations of equation (10) indicate that these simpler solutions would not reproduce the computed results of Figures 18 and 19. In other words to attain the results observed in Figures 18 and 19, we have found that equation (10) should be solved in its entirety, as is accomplished by the BENCHMARK-76 program.

SUMMARY

The BENCHMARK-76 code has been employed to obtain species densities as a function of time and excitation conditions for an altitude of 60 km. The excitation conditions employed were as follows. The prompt ionization, N_o, was assigned the values 10^{11}, 10^{10} or 10^8 cm^{-3}, and the delayed ionization is given by $Q(t) = Q_o(1 + t)^{-1.2}$ where t is the time

[16] See for example, A. P. Mitra, "D-Region in Disturbed Condition, Including Flares and Energetic Particles," J. Atmos. and Terr. Phys. 37, 895-913, 1975.

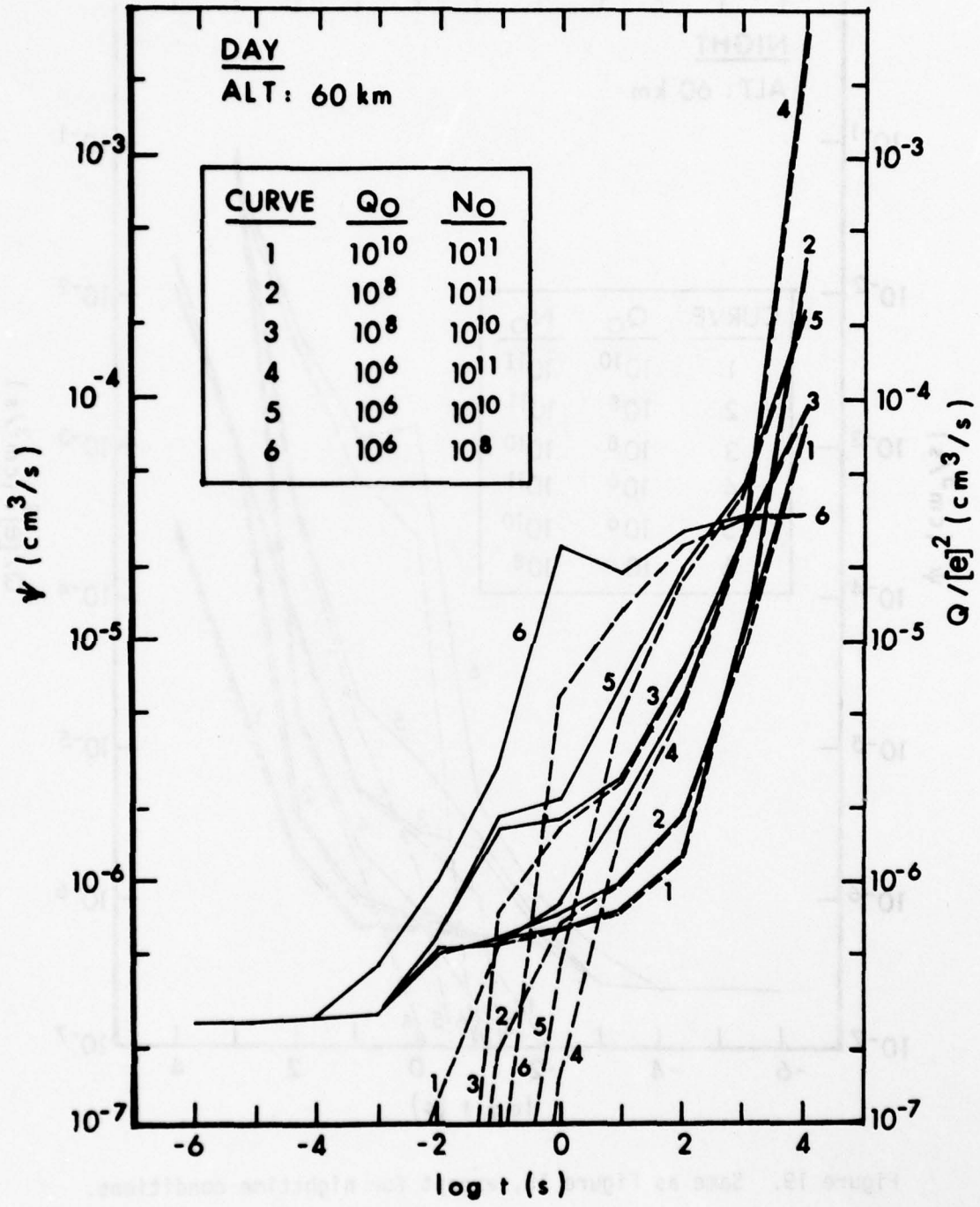


Figure 18. Composite plot of the logarithm of the total recombination coefficient, ψ (solid line), and of $Q/[e]^2$ (dashed line), as a function of the logarithm of time. Conditions are daytime at 60 km for the six different excitation parameters shown.

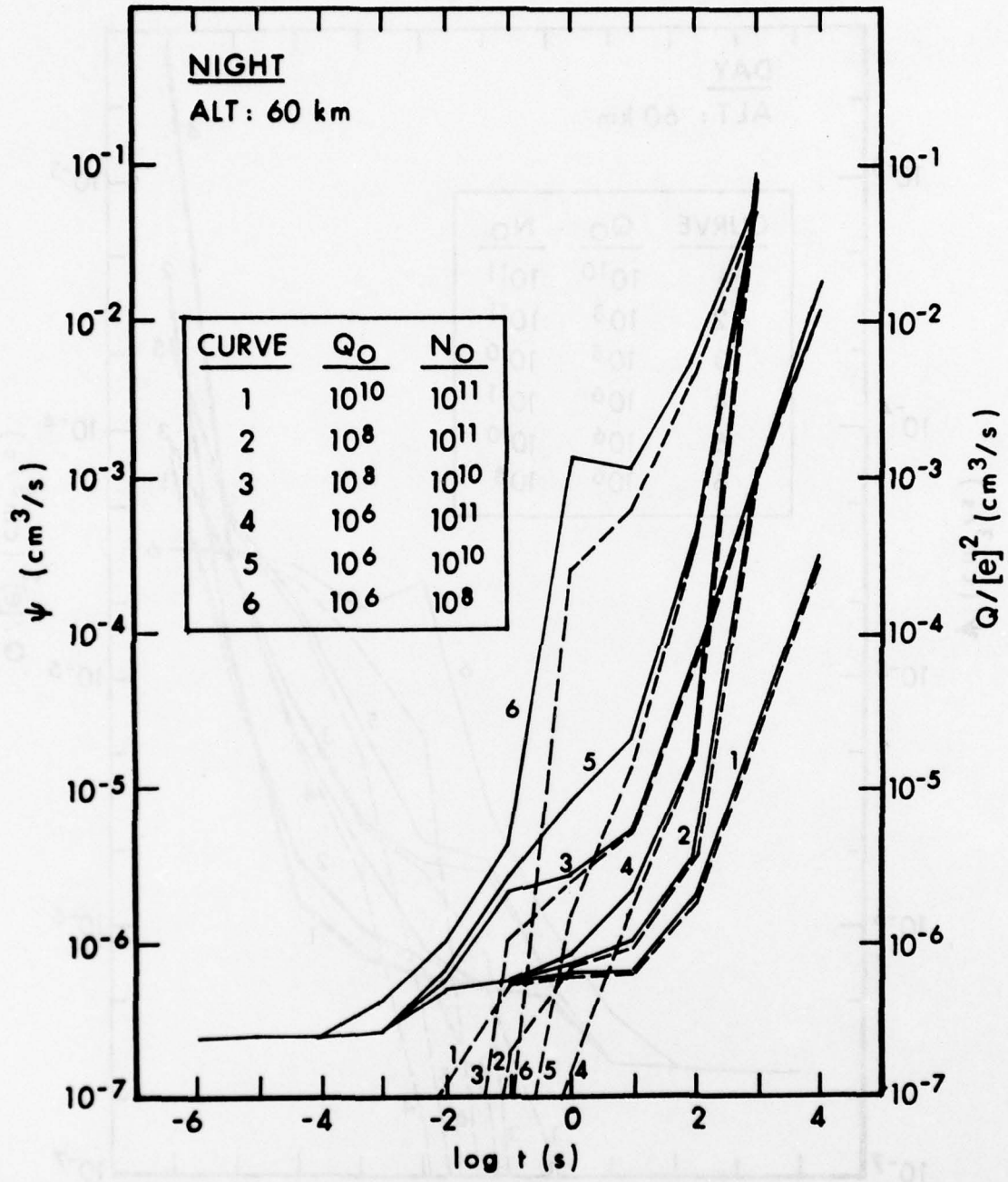


Figure 19. Same as Figure 15, except for nighttime conditions.

in seconds and Q_o assigned the values of 10^6, 10^8 or 10^{10} ion-pairs $cm^{-3}s^{-1}$, subject to the constraint $|Q_o| < |N_o|$. Computations were made for three hour intervals around noon (DAY) and midnight (NIGHT). Analysis of these calculations is summarized as follows.

First, for a given delayed ionization parameter, Q_o, it is found that the greater the initial ionization parameter, N_o, the sooner the electron density relaxes to its quiescent value. This inversion of one's intuitive feeling is traced to severe neutral chemistry changes that affect the negative ion chemistry.

Second, the comparison between the BENCHMARK-76 (BRL) and the DCHEM (MRC) calculations of the electron densities at 60 km for both day and night conditions and for $Q_o = 10^6$ ion-pairs $cm^{-3}s^{-1}$ and $N_o = 10^8$ or 10^{11} cm^{-3} are good to excellent.

Third, the calculated relaxation of the effective electron-ion recombination coefficient to quiescent values is dominated by Q_o, i.e., the larger Q_o the longer the relaxation time. The return to quiescent values for the higher excitation conditions is computed to take longer than 10^4 seconds.

Fourth, variations in the effective electron attachment frequency, A, amounting to almost a factor of two at night, are traced in detail and found to result from ozone enhancement at late times.

Fifth, only the daytime effective electron recombination coefficient for the mildest excitation studied is found to relax to a typical quiescent value. In the daytime, all other, stronger excitation cases indicate a relaxation to values much below that expected for quiescent conditions. This phenomenon is traced to the greater build up in the nitric oxide density with the larger value of N_o. In the nighttime cases, no curves approach their quiescent values even after 10^3 or 10^4 s. We have found that the reaction $O^- + N_2 \rightarrow N_2O + e$ is non-negligible, even when its rate coefficient is reduced one hundredfold to 10^{-14} cm^3/s.

Finally, the time to attain a steady state condition as measured by the criterion $\psi = Q/[e]^2$, is found to be a function of Q_o. The smaller this parameter, the longer it takes to reach the steady state. Attempts to understand this behavior by simplifying the governing non-linear differential equation for the electron density were not successful, but, led us to the conclusion that, in order to obtain these results, this equation ought to be solved in its entirety, as is accomplished by the BENCHMARK-76 program.

ACKNOWLEDGEMENT

To M. G. Heaps and G. E. Keller goes our thanks for reading an earlier version of this manuscript.

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5. See for example E. E. Ferguson, D. B. Dunkin and F. C. Fehsenfeld, "Reactions of NO_2^- and NO_3^- with HCl and Hbr," J. Chem. Phys. 57, 1459-1463, 1972.

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9. For example, the BENCHMARK-76 reaction set includes neutral odd-hydrogen reactions; Scheibe's set does not.

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11. See for example, T. Ogawa and T. Shimazaki, "Diurnal Variations of Odd Nitrogen and Ionic Densities in the Mesosphere and Lower Thermosphere: Simultaneous Solution of Photochemical-Diffusive Equations," J. Geophys. Res. 80, 3945-3960, 1975.

12. T. Shimazaki and A. R. Laird, "Model Calculation of the Diurnal Variation in Minor Neutral Constituents in the Mesosphere and Lower Thermosphere Including Transport Effects," J. Geophys. Res. 75, 3221-3235, 1970.

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15. F. C. Fehsenfeld, private communication, 1977.

16. See for example, A. P. Mitra, "D-Region in Disturbed Condition, Including Flares and Energetic Particles," J. Atmos. and Terr. Phys. 37, 895-913, 1975.

APPENDIX

The table in this Appendix displays the nominal 496 reactions that link the 64 species within the BENCHMARK-76 code. Reactions proceed from left to right only. Each rate coefficient, k, is constructed from the reaction parameters A, B and C, i.e.

$$k = A(T/300)^{B} \exp(-C/T) ,$$

where T is the temperature in degrees Kelvin. Except for the first 60 reactions, involving a photon as a reactant, the reference for the value of the rate coefficient is given to the right of the parameter C column. Further details can be obtained from Reference 3.

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TABLE A. BENCHMARK-76 REACTION SET

REAC. NO.	REACTION	WAVELENGTH REGION	REFERENCE	REF. NO.
1	NO2- + HV = NO2 + E			1
2	O- + HV = O + E			2
3	O- + HV = O1D + E			3
4	O2- + HV = O2 + E			4
5	O3- + HV = O3 + E			5
6	CO3- + HV = CO2 + O-			6
7	78- + HV = CO3- + H2O			7
8	CO4- + HV = O2- + CO2			8
9	94- + HV = CO4- + H2O			9
10	64- + HV = NO2- + H2O			10
11	NO3- + HV = O + NO2 + E			11
12	62- + HV = NO + O2-			12
13	80- + HV = NO3- + H2O			13
14	125- + HV = NO3- + HNO3			14
15	O2-W + HV = O2- + H2O			15
16	O3- + HV = O- + O2			16
17	O4- + HV = O2- + O2			17
18	NO74 + HV = NO+ + CO2			18
19	NO48 + HV = NO+ + H2O			19
20	NO58 + HV = NO+ + N2			20
21	NO92 + HV = NO48 + CO2			21
22	NO66 + HV = H3O+ + HNO2			22
23	NO66 + HV = NO48 + H2O			23
24	NO76 + HV = NO48 + N2			24
25	N110 + HV = NO66 + CO2			25
26	NO84 + HV = NO66 + H2O			26
27	NO94 + HV = NO66 + N2			27
28	64+ + HV = NO2+ + H2O			28
29	82+ + HV = 64+ + H2O			29
30	O250 + HV = O2+ + H2O			30
31	O260 + HV = O2+ + N2			31
32	O4+ + HV = O2+ + O2			32
33	H2 + HV = H + H			33
34	H2O + HV = H + HO			34
35	H2O2 + HV = HO + HO			35
36	HNO2 + HV = HO + NO			36
37	HNO3 + HV = HO + NO2			37
38	HO2 + HV = HO + O			38
39	NO + HV = N + O			39
40	NO2 + HV = NO + O			40
41	N2 + HV = N2D + N			41
42	N2O + HV = N2 + O1D			42
43	O2 + HV = O + O			43
44	O2 + HV = O + O1D			44
45	O2 + HV = O21D			45
46	O2 + HV = O21S			46
47	O3 + HV = O + J2			47
48	O3 + HV = O + J21D			48
49	O3 + HV = O1D + O21D			49
50	N + HV = N+ + E			50
51	NO + HV = NO+ + E			51
52	NO2 + HV = NO2+ + E			52
53	N2 + HV = N + J+ + E			53
54	N2 + HV = N2D + N+ + E			54
55	N2 + HV = N2+ + E			55
56	O + HV = O+ + E			56
57	O2 + HV = O2+ + E			57
58	O2 + HV = O + J+ + E			58
59	O2 + HV = O1D + O+ + E			59
60	O21D + HV = O2+ + E			60

REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
61	H + H2O2 = HO + H2O	5.3E-10	.0	4500	BAULCH ETAL HI TEMP REAC RATE DATA,LEEDS NO3 69	61
62	H + H2O2 = H2 + HO2	2.8E-12	.0	1900	HAMPSON,ED NBSIR-73-207 AUG 73	62
63	H + HO = H2 + O	4.2E-12	1.0	3500	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	63
64	H + HO2 = H2 + O2	4.2E-11	.0	350	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	64
65	H + HO2 = HO + HO	4.2E-10	.0	950	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	65
66	H + HO2 = H2O + O	8.3E-11	.0	500	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	66
67	H + NO2 = NO + HO	5.8E-10	.0	740	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	67
68	H + N2O = N2 + HO	1.3E-10	.0	7600	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	68
69	H + O2 = O + HO	3.7E-10	.0	8450	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	69
70	H + O3 = HO + O2	2.6E-11	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	70
71	HO + H2 = H + H2O	3.6E-11	.0	2590	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	71
72	HO + H2O2 = H2O + HO2	1.7E-11	.0	910	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	72
73	HO + HNO2 = NO2 + H2O	2.1E-12	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 INDIRECT	73
74	HO + HNO3 = H2O + NO2 + O	1.3E-13	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 DIF PROD	74
75	HO + HO = O + H2O	1.0E-11	.0	550	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	75
76	HO + HO2 = H2O + O2	6.0E-11	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 ESTIMATE	76
77	HO + O3 = O2 + HO2	1.6E-12	.0	1000	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	77
78	HO2 + HO2 = H2O2 + O2	3.0E-11	.0	500	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	78
79	HO2 + O3 = HO + O2 + O2	1.0E-13	.0	1250	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	79
80	N + HO = H + NO	5.3E-11	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	80
81	N + NO = N2 + O	1.4E-11	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 .5 B/R	81
82	N + NO = O1D + N2	1.4E-11	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 .5 B/R	82
83	N + NO2 = N2O + O	1.4E-12	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 TENATIVE	83
84	N + O2 = NO + O	3.3E-12	1.0	3150	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	84
85	N + O3 = NO + O2	5.7E-13	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	85
86	N2D + O2 = NO + O	7.5E-12	.5	0	SLANGER,WOOD + BLACK JGR 76, 8430 71	86
87	NO + HO2 = HO + NO2	2.0E-13	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	87
88	NO + O3 = NO2 + O2	9.0E-13	.0	1200	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	88
89	O + H2O2 = HO + HO2	2.8E-12	.0	2125	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 ONE CHAN	89
90	O + HO = O2 + H	4.2E-11	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	90
91	O + HO2 = HO + O2	8.0E-11	.0	500	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 ESTIMATE	91
92	O + NO2 = NO + O2	9.1E-12	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	92
93	O + O3 = O2 + O2	1.0E-11	.0	2300	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 .5 B/R	93
94	O + O3 = O21D + O2	1.0E-11	.0	2300	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 .5 B/R	94
95	O1D + H2 = HO + H	2.9E-10	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	95
96	O1D + H2O = HO + HO	3.5E-10	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	96
97	O1D + M = O + M	5.5E-11	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	97
98	O1D + N2O = NO + NO	1.1E-10	.0	0	GARVIN,ED NBSIR 73-206 MAY 73	98
99	O1D + O2 = O + O21S	7.4E-11	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	99
100	O1D + O3 = O2 + O2	2.5E-10	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	100
101	O21D + O2 = O2 + O2	2.2E-18	.8	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	101
102	O21D + O21D = O21S + O2	2.0E-18	.0	0	ARNOLD + OGRYZLO, CAN J PHYS 45, 2053 67	102
103	O21S + M = O2 + M	2.0E-15	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	103
104	O21S + O3 = O + O2 + O2	2.5E-11	.0	0	GILPIN,SCHIFF + WELGE, J CHEM PHYS 55, 1087 71	104
105	H + H + M = H2 + M	8.3E-33	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 M=H2	105
106	H + HO + M = H2O + M	6.8E-31	-2.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 HI TEMP	106
107	H + O + M = HO + M	2.0E-32	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 M=AR HIT	107
108	H + O2 + M = HO2 + M	2.1E-32	.0	-290	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	108
109	HO + HO + M = H2O2 + M	2.5E-33	.0	-2550	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 HI TEMP	109
110	HO + NO2 + M = HNO3 + M	2.2E-30	-2.5	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 M=N2	110
111	HO + O + M = HO2 + M	1.0E-31	.0	0	ESTIMATED	111
112	N + N + M = N2 + M	8.3E-34	.0	-500	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	112
113	N + O + M = NO + M	1.0E-32	-.5	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	113
114	NO + O2 + NO = NO2 + NO2	3.3E-39	.0	-526	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	114
115	O + NO + M = NO2 + M	4.0E-33	.0	-940	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	115
116	O + O + M = O2 + M	1.3E-32	-1.0	170	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 HI TEMP	116
117	O + O2 + M = O3 + M	1.1E-34	.0	-510	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75 *	117
118	O1D + N2 + M = N2O + M	2.8E-36	.0	0	HAMPSON + GARVIN,ED NBS-TN-866 JUNE 75	118
119	O1D = O + HV	6.8E-03	.0	0	DNA HANDBOOK 1968H REV3 TABLE 24 REACTION XXX-1	119
120	O21D = O2 + HV	2.6E-04	.0	0	DNA HANDBOOK 1968H REV3 TABLE 24 REACTION XXX-5	120

REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
121	O21S = O2 + HV	8.3E-02	.0	0	DNA HANDBOOK 1948H REV3 TABLE 24 REACTION XXX-6	121
122	NO2 + E = NO2-	4.0E-11	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION IX-7 SAT 38	122
123	HNO3 + E = NO2- + HO	5.0E-08	.0	0	FERGUSON ET AL DNA 3722F, AUG 75	123
124	O3 + E = O- + O2	9.0E-12	1.5	0	DNA HANDBOOK REV3 TABLE 24 REACTION IX-1 1 CHAN	124
125	O2 + E + O2 = O2- + O2	1.4E-29	-1.0	600	DNA HANDBOOK REV3 TABLE 24 REACTION IX-2	125
126	O2 + E + N2 = O2- + N2	1.0E-31	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION IX-3	126
127	O- + H2 = H2O + E	6.0E-10	-.2	0	MCFARLAND ETAL J CHEM PHYS 59,6629 73	127
128	O- + N = NO + E	2.2E-10	.0	0	DNA HANDBOOK TABLE 24	128
129	O- + N2 = N2O + E	1.0E-12	.0	0	LINDINGER ETAL J CHEM PHYS 63,3238,75 UP LIM	129
130	O- + NO = NO2 + E	2.5E-10	-.8	0	MCFARLAND ETAL J CHEM PHYS 59,6629 73	130
131	O- + O = O2 + E	2.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XII-1	131
132	O- + O21D = O3 + E	3.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XII-3	132
133	O2- + N = NO2 + E	3.0E-10	.0	0	FEHSENFELD, PRIVATE COMMUNICATION	133
134	O2- + N2 = O2 + E + N2	1.9E-12	1.5	4990	DNA HANDBOOK REV3 TABLE 24 REACTION X-4	134
135	O2- + O = O3 + E	1.5E-10	.0	0	F. C. FEHSENFELD, PRIVATE COMMUNICATION 75,	135
136	O2- + O2 = O2 + E + O2	2.7E-10	.5	5590	DNA HANDBOOK REV3 TABLE 24 REACTION X-5	136
137	O2- + O21D = O2 + E + O2	2.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION X-6	137
138	H3O+ + E = H + H2O	1.3E-06	-.2	0	DNA HANDBOOK REV4 TABLE 16-1	138
139	H+37 + E = H + H2O + H2O	2.8E-06	-.2	0	DNA HANDBOOK REV4 TABLE 16-1	139
140	H+36 + E = H2O + H + HO	3.0E-06	-1.0	0	DNA HANDBOOK TABLE 24 EST	140
141	H+47 + E = H + H2O + N2	1.0E-06	-.2	0	ESTIMATED	141
142	H+55 + E = H + H2O + H2O + H2O	5.1E-06	-.2	0	DNA HANDBOOK REV4 TABLE 16-1	142
143	H+73 + E = H + H2O + H2O + H2O + H2O	6.1E-06	-.2	0	DNA HANDBOOK REV4 TABLE 16-1	143
144	H+91 + E = H + H2O + H2O + H2O + H2O + H2O	7.4E-06	-.2	0	DNA HANDBOOK REV4 TABLE 16-1	144
145	NO+ + E = O + N	1.0E-07	-1.0	0	DNA HBK REV4 TABLE 16-1 KLEY ETAL JCP 66,4157,7	145
146	NO+ + E = O + N2D	3.0E-07	-1.0	0	DNA HBK REV4 TABLE 16-1 KLEY ETAL JCP 66,4157,7	146
147	NO74 + E = NO + CO2	1.0E-06	-.2	0	DNA HANDBOOK, EST.	147
148	NO48 + E = NO + H2O	1.0E-06	-.2	0	DNA HANDBOOK TABLE 24	148
149	NO58 + E = NO + N2	1.0E-06	-.2	0	DNA HANDBOOK, EST.	149
150	NO92 + E = NO + H2O + CO2	1.0E-06	-.2	0	DNA HANDBOOK, EST.	150
151	NO66 + E = NO + H2O + H2O	2.0E-06	-.2	0	DNA HANDBOOK TABLE 24	151
152	NO76 + E = NO + H2O + N2	1.0E-06	-.2	0	DNA HANDBOOK, EST.	152
153	N110 + E = NO + H2O + H2O + CO2	1.0E-06	-.2	0	DNA HANDBOOK, EST.	153
154	NO84 + E = NO + H2O + H2O + H2O	3.0E-06	-.2	0	DNA HANDBOOK REV3 TABLE 24 REACTION IV-10	154
155	NO94 + E = NO + H2O + H2O + N2	1.0E-06	-.2	0	DNA HANDBOOK, EST.	155
156	NO2+ + E = NO + O	3.0E-07	-.5	0	DNA HANDBOOK REV3 TABLE 24 REACTION IV-6 EST	156
157	64+ + E = NO2 + H2O	1.0E-06	-.5	0	DNA HANDBOOK, EST.	157
158	82+ + E = NO2 + H2O + H2O	2.0E-06	-.5	0	DNA HANDBOOK, EST.	158
159	N2+ + E = N + N2D	2.7E-07	.0	0	DNA HANDBOOK REV4 FIGURE 16-1 ESTIMATED PRODUCT	159
160	O2+ + E = O + O1D	2.1E-07	-.7	0	DNA HANDBOOK, TABLE 24-1.	160
161	O2S0 + E = O2 + H2O	1.5E-06	-.2	0	DNA HANDBOOK, EST.	161
162	O4+ + E = O2 + O2	2.0E-06	-1.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION IV-11	162
163	N+ + O2 = N + O2+	2.8E-10	.0	0	MCFARLAND ETAL J C P 59,6620 73 T<4600,B/R=.5	163
164	N2+ + O2 = N2 + O2+	5.0E-11	-.8	0	MCFARLAND ETAL J CHEM PHYS 59,6620 73 T<3560	164
165	NO2+ + NO = NO2 + NO+	2.9E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIII-27	165
166	64+ + NO = NO48 + NO2	1.0E-10	.0	0	DNA HANDBOOK, EST.	166
167	82+ + NO = NO66 + NO2	1.0E-10	.0	0	DNA HANDBOOK, EST.	167
168	O+ + O2 = O + O2+	2.0E-11	-.4	0	MCFARLAND ETAL J CHEM PHYS 59,6620 73 T<1800	168
169	O2+ + NO = O2 + NO+	4.4E-10	.0	0	LINDINGER ETAL JGR 80,3725 75	169
170	O2+ + NO2 = O2 + NO2+	6.6E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIII-16	170
171	O2S0 + NO = NO+ + O2 + H2O	1.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-26 EST	171
172	O2S0 + NO2 = O2 + H2O + NO2+	1.0E-10	.0	0	ESTIMATED	172
173	O4+ + NO = O2 + O2 + NO+	5.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-23 EST	173
174	O4+ + NO2 = O2 + O2 + NO2+	5.0E-10	.0	0	ESTIMATED	174
175	H3O+ + HNO3 = 64+ + H2O	1.6E-09	.0	0	FEHSENFELD ETAL J CHEM PHYS 63,2835 75	175
176	H+36 + H2O = H+37 + HO	1.4E-09	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-33	176
177	H+47 + H2O = H+37 + N2	1.0E-09	.0	0	ESTIMATED	177
178	N+ + O2 = NO+ + O	2.8E-10	.0	0	MCFARLAND ETAL J C P 59,6620,73 T<4600,B/R=.5	178
179	NO74 + H2O = NO48 + CO2	1.0E-09	.0	0	ESTIMATED	179
180	NO48 + HO2 = H3O+ + NO + O2	5.0E-10	.0	0	ESTIMATED, ANALOGY WITH NO48 + H2O2	180

REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
181	NO48 + HO = H3O+ + NO2	6.0E-11	.0	0	FEHSENFELD + FERGUSON RAD SCI 7.113 72 UP-LIM	181
182	NO48 + H2O2 = H3O+ + NO2 + HO	3.0E-11	.0	0	ESTIMATED	182
183	NO48 + H2O2 = NO2+ + H2O + H2O	3.0E-11	.0	0	ESTIMATED	183
184	NO48 + H2O2 = 64+ + H2O	3.0E-11	.0	0	ESTIMATED	184
185	NO58 + CO2 = NO74 + N2	1.0E-09	.0	0	ESTIMATED	185
186	NO58 + H2O = NO48 + N2	1.0E-09	.0	0	ESTIMATED	186
187	NO92 + H2O = NO66 + CO2	1.0E-09	.0	0	ESTIMATED	187
188	NO76 + CO2 = NO92 + N2	1.0E-09	.0	0	ESTIMATED	188
189	N110 + H2O = NO84 + CO2	1.0E-09	.0	0	ESTIMATED	189
190	NO84 + H2O = H+55 + HNO2	7.0E-11	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-30	190
191	NO94 + CO2 = N110 + N2	1.0E-09	.0	0	ESTIMATED	191
192	64+ + NO = NO48 + NO2	3.1E-11	.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75	192
193	82+ + H2O = H+37 + HNO3	1.0E-10	.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75 LOW LIM	193
194	N2+ + O = N2D + NO+	1.0E-11	-.2	0	MCFARLAND ETAL JGR 79.2925 74 B/R EST.	194
195	N2+ + O = NO+ + N	1.3E-10	-.4	0	MCFARLAND ETAL JGR 79.2925 74 B/R EST.	195
196	O+ + N2 = NO+ + N	1.2E-12	-1.0	0	MCFARLAND ETAL J CHEM PHYS 59.6620 73 T<750	196
197	O2+ + N = NO+ + O	1.8E-10	.0	0	DNA HANDBOOK TABLE 24	197
198	O2+ + N2 = NO+ + NO	1.0E-16	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-9 EST	198
199	O2S0 + H2O = H3O+ + HO + O2	2.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-27A	199
200	O2S0 + H2O = H+36 + O2	1.0E-09	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-27B	200
201	O2S0 + O2 = O4+ + H2O	2.0E-10	.0	2300	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-25 EST	201
202	O2S0 + O2 = O4+ + N2	1.0E-09	.0	0	ESTIMATED	202
203	O4+ + H2O = O2S0 + O2	1.5E-09	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-24	203
204	O4+ + O = O2+ + O3	3.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-22	204
205	H3O+ + H2O + M = H+37 + M	3.4E-27	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-13B	205
206	H3O+ + N2 + M = H+47 + M	1.4E-30	-2.0	0	ESTIMATED	206
207	H+37 + H2O + M = H+55 + M	2.3E-27	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-14B	207
208	H+55 + H2O + M = H+73 + M	2.4E-27	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-15B	208
209	H+73 + H2O + M = H+91 + M	9.0E-28	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-16	209
210	NO+ + CO2 + M = NO74 + M	2.4E-29	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-10B	210
211	NO+ + H2O + M = NO48 + M	1.5E-28	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-9	211
212	NO+ + N2 + M = NO58 + M	2.0E-31	-4.4	0	JOHNSEN ETAL J CHEM PHYS 63.3374 75	212
213	NO48 + CO2 + M = NO92 + M	2.0E-29	-2.0	0	ESTIMATED	213
214	NO48 + H2O + M = NO66 + M	1.1E-27	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-11	214
215	NO48 + N2 + M = NO76 + M	2.0E-31	-4.4	0	ESTIMATED	215
216	NO66 + CO2 + M = N110 + M	2.0E-29	-2.0	0	ESTIMATED	216
217	NO66 + H2O + M = NO84 + M	1.6E-27	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-12	217
218	NO66 + N2 + M = NO94 + M	2.0E-31	-4.4	0	ESTIMATED	218
219	NO2+ + H2O + M = 64+ + M	5.0E-28	-2.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75 TEMP EST	219
220	64+ + H2O + M = 82+ + M	2.0E-27	-2.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75 TEMP EST	220
221	O+ + N2 + M = NO+ + N + M	6.0E-29	-2.0	0	DNA HANDBOOK TABLE 18A-5 TAKE (T/82)**-2.X3.8	221
222	O2+ + H2O + M = O2S0 + M	2.8E-28	-2.0	0	FEHSENFELD ETAL J CHEM PHYS 55.2115 71 M=N2	222
223	O2+ + O2 + M = O4+ + M	3.9E-30	-3.2	0	PAYZANT ETAL J CHEM PHYS 59.5615 73 X1.5	223
224	O2+ + N2 + M = O260 + M	9.0E-31	-2.0	0	DNA HANDBOOK TABLE 18A-5 TAKE (T/200)**-2.X3.8	224
225	H+36 + M = H3O+ + HO + M	3.0E-03	-2.0	12000	ESTIMATED	225
226	H+37 + M = H3O+ + H2O + M	1.6E 01	-2.0	18200	ESTIMATED	226
227	H+47 + M = H3O+ + N2 + M	1.1E-08	-2.0	1900	ESTIMATED	227
228	H+55 + M = H+37 + H2O + M	1.6E-01	-2.0	11300	ESTIMATED	228
229	H+73 + M = H+55 + H2O + M	1.0E-01	-2.0	8600	ESTIMATED	229
230	H+91 + M = H+73 + H2O + M	1.3E 00	-2.0	7700	ESTIMATED	230
231	NO74 + M = NO+ + CO2 + M	7.8E-09	-2.0	5600	ESTIMATED	231
232	NO58 + M = NO+ + N2 + M	1.1E-08	-4.4	1900	J CHEM PHY 60. 4362. 74 + JCP 63. 3374. 75	232
233	NO92 + M = NO48 + CO2 + M	4.0E-09	-2.0	5600	ESTIMATED	233
234	NO66 + M = NO48 + H2O + M	5.9E-02	-2.0	8700	ESTIMATED	234
235	NO76 + M = NO48 + N2 + M	1.1E-08	-4.4	1900	ESTIMATED	235
236	N110 + M = NO66 + CO2 + M	4.0E-09	-2.0	5600	ESTIMATED	236
237	NO84 + M = NO66 + H2O + M	2.2E-02	-2.0	7000	ESTIMATED	237
238	NO94 + M = NO66 + N2 + M	1.1E-08	-4.4	1900	ESTIMATED	238
239	O2S0 + O21D = O2+ + O2 + H2O	1.0E-10	.0	0	ESTIMATED	239
240	O4+ + M = O2+ + O2 + M	1.2E-05	-3.2	5300	PAYZANT ETAL J CHEM PHYS 59. 5615. 73	240

REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
241	CO4- + O3 = O3- + CO2 + O2	1.3E-10	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61,3181 74	241
242	O- + NO2 = O + NO2-	1.2E-09	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XV-2	242
243	O- + O3 = O + O3-	5.3E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XV-3	243
244	O2- + NO2 = O2 + NO2-	1.2E-09	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61,3181 74	244
245	O2- + O = O2 + O-	1.5E-10	.0	0	F. C. FEHSENFELD, PRIVATE COMMUNICATION 75.	245
246	O2- + O3 = O2 + O3-	4.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XV-5	246
247	O2-W + O3 = O3- + O2 + H2O	2.3E-10	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61,3181 74	247
248	O4- + O3 = O3- + O2 + O2	5.0E-10	.0	0	ESTIMATED	248
249	CO3- + HNO3 = NO3- + HO + CO2	8.0E-10	.0	0	FEHSENFELD ETAL J CHEM PHYS 63,2835 75	249
250	CO3- + NO = NO2- + CO2	9.0E-12	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-23	250
251	CO3- + NO2 = NO3- + CO2	2.0E-10	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61,3181 74	251
252	CO3- + O = O2- + CO2	8.0E-11	.0	0	DNA HANDBOOK TABLE 24	252
253	78- + NO = 64- + CO2	7.0E-12	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61,3181 74	253
254	CO4- + NO = 62- + CO2	4.8E-11	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-27	254
255	CO4- + O = CO3- + O2	1.5E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-25	255
256	CO4- + O2 = O4- + CO2	4.3E-10	.0	3000	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-26 EST	256
257	94- + NO = 80- + CO2	5.0E-10	.0	0	ESTIMATED	257
258	NO2- + HNO3 = NO3- + HNO2	1.6E-09	.0	0	FEHSENFELD ETAL J CHEM PHYS 63,2835 75	258
259	NO2- + NO2 = NO3- + NO	2.0E-13	.0	0	FEHSENFELD ETAL J CHEM PHYS 63,2835 75 UP LIM	259
260	NO2- + O3 = NO3- + O2	1.8E-11	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-10	260
261	64- + O3 = 80- + O2	5.0E-10	.0	0	ESTIMATED	261
262	62- + NO = NO2- + NO2	1.5E-11	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-15	262
263	80- + HNO3 = 125- + H2O	5.0E-10	.0	0	FEHSENFELD ETAL J CHEM PHYS 63,2835 75 LOW LIM	263
264	O- + HNO3 = NO3- + HO	3.0E-09	.0	0	FEHSENFELD ETAL J CHEM PHYS 63,2835 75	264
265	O2- + HNO3 = NO3- + HO2	2.8E-09	.0	0	FEHSENFELD ETAL J CHEM PHYS 63,2835 75	265
266	O2- + N = O- + NO	1.0E-10	.0	0	FEHSENFELD, PRIVATE COMMUNICATION	266
267	O2-W + CO2 = CO4- + H2O	5.8E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-21	267
268	O2-W + NO = 62- + H2O	3.1E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-20	268
269	O3- + CO2 = CO3- + O2	5.5E-10	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61,3181 74	269
270	O3- + NO = NO2- + O2	2.8E-12	.0	0	F. C. FEHSENFELD, PRIVATE COMMUNICATION 75.	270
271	O3- + NO2 = NO3- + O2	2.8E-10	.0	0	DUNKIN ETAL CHEM PHYS LET 15,257 72	271
272	O3- + O = O2- + O2	3.2E-10	.0	0	F. C. FEHSENFELD, PRIVATE COMMUNICATION 75.	272
273	O4- + CO2 = CO4- + O2	4.3E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-19	273
274	O4- + H2O = O2-W + O2	1.4E-09	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-18	274
275	O4- + NO = 62- + O2	2.5E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-17	275
276	O4- + O = O3- + O2	4.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-16	276
277	CO3- + H2O + M = 78- + M	1.0E-28	-1.0	0	J CHEM PHYS 61,3181 74 M=O2 TEMP DEP ESTIMATED	277
278	CO4- + H2O + M = 94- + M	5.0E-29	-1.0	0	ESTIMATED	278
279	NO2- + H2O + M = 64- + M	1.3E-28	-1.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XXIII-11	279
280	NO3- + H2O + M = 80- + M	7.5E-29	-1.0	0	PAYZANT, PRIVATE COMMUNICATION 72	280
281	O- + CO2 + M = CO3- + M	3.1E-28	-1.0	0	J CHEM PHYS 61,3181 74 M=O2 TEMP DEP ESTIMATED	281
282	O- + O2 + M = O3- + M	1.1E-30	-1.0	0	PARKES,TRAN FAR SOC 67,711 71 M=O2 TEMP DEP EST	282
283	O2- + CO2 + M = CO4- + M	2.0E-29	-1.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XXIII-9	283
284	O2- + H2O + M = O2-W + M	3.0E-28	-1.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XXIII-8	284
285	O2- + O2 + M = O4- + M	3.5E-31	-1.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XXIII-6	285
286	O4- + M = O2- + O2 + M	2.0E-05	-1.0	6300	DNA HANDBOOK REV3 TABLE 24 REACTION XXIV-1	286
287	H3O+ + CO3- = HO + H2O + CO2	2.0E-07	-.5	0	ESTIMATED	287
288	H3O+ + 78- = CO2 + O + H2O + H2O + H	2.0E-07	-.5	0	ESTIMATED	288
289	H3O+ + CO4- = HO2 + H2O + CO2	2.0E-07	-.5	0	ESTIMATED	289
290	H3O+ + 94- = CO2 + O2 + H2O + H2O + H	2.0E-07	-.5	0	ESTIMATED	290
291	H3O+ + NO2- = HO + H2O + NO	2.0E-07	-.5	0	ESTIMATED	291
292	H3O+ + 64- = H + H2O + NO2 + H2O	2.0E-07	-.5	0	ESTIMATED	292
293	H3O+ + NO3- = H2O + HO + NO2	2.0E-07	-.5	0	ESTIMATED	293
294	H3O+ + 62- = H2O + NO + HO2	2.0E-07	-.5	0	ESTIMATED	294
295	H3O+ + 80- = NO2 + H2O + H + H2O + O	2.0E-07	-.5	0	ESTIMATED	295
296	H3O+ + 125- = HNO3 + HNO3 + H2O	2.0E-07	-.5	0	ESTIMATED	296
297	H3O+ + O- = H2O + HO	2.0E-07	-.5	0	ESTIMATED	297
298	H3O+ + O2- = H + H2O + O2	2.0E-07	-.5	0	ESTIMATED	298
299	H3O+ + O2-W = O2 + H + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	299
300	H3O+ + O3- = HO + H2O + O2	2.0E-07	-.5	0	ESTIMATED	300

REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
301	H3O+ + O4- = HO2 + H2O + O2	2.0E-07	-.5	0	ESTIMATED	301
302	H+37 + CO3- = HO + H2O + CO2 + H2O	2.0E-07	-.5	0	ESTIMATED	302
303	H+37 + 78- = CO2 + O + H2O + H2O + H2O + H	2.0E-07	-.5	0	ESTIMATED	303
304	H+37 + CO4- = HO2 + H2O + H2O + CO2	2.0E-07	-.5	0	ESTIMATED	304
305	H+37 + 94- = CO2 + O2 + H2O + H2O + H2O + H	2.0E-07	-.5	0	ESTIMATED	305
306	H+37 + NO2- = HO + H2O + H2O + NO	2.0E-07	-.5	0	ESTIMATED	306
307	H+37 + 64- = H + H2O + NO2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	307
308	H+37 + NO3- = HO + H2O + H2O + NO2	2.0E-07	-.5	0	ESTIMATED	308
309	H+37 + 62- = H2O + H2O + HO2 + NO	2.0E-07	-.5	0	ESTIMATED	309
310	H+37 + 80- = NO2 + H2O + H + H2O + H2O + O	2.0E-07	-.5	0	ESTIMATED	310
311	H+37 + 125- = HNO3 + HNO3 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	311
312	H+37 + O- = H2O + H2O + HO	2.0E-07	-.5	0	ESTIMATED	312
313	H+37 + O2- = HO2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	313
314	H+37 + O2-W = O2 + H + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	314
315	H+37 + O3- = HO + H2O + H2O + O2	2.0E-07	-.5	0	ESTIMATED	315
316	H+37 + O4- = HO2 + H2O + H2O + O2	2.0E-07	-.5	0	ESTIMATED	316
317	H+55 + CO3- = HO + H2O + CO2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	317
318	H+55 + 78- = CO2 + O + H2O + H2O + H2O + H2O + H	2.0E-07	-.5	0	ESTIMATED	318
319	H+55 + CO4- = HO2 + H2O + H2O + H2O + CO2	2.0E-07	-.5	0	ESTIMATED	319
320	H+55 + 94- = CO2 + O2 + H2O + H2O + H2O + H2O + H	2.0E-07	-.5	0	ESTIMATED	320
321	H+55 + NO2- = HO + H2O + NO + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	321
322	H+55 + 64- = H + H2O + NO2 + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	322
323	H+55 + NO3- = HO + H2O + NO2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	323
324	H+55 + 62- = H2O + H2O + H2O + HO2 + NO	2.0E-07	-.5	0	ESTIMATED	324
325	H+55 + 80- = NO2 + H2O + H + H2O + H2O + H2O + H2O + O	2.0E-07	-.5	0	ESTIMATED	325
326	H+55 + 125- = HNO3 + HNO3 + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	326
327	H+55 + O- = H2O + H2O + H2O + HO	2.0E-07	-.5	0	ESTIMATED	327
328	H+55 + O2- = H2O + HO2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	328
329	H+55 + O2-W = O2 + H + H2O + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	329
330	H+55 + O3- = HO + H2O + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	330
331	H+55 + O4- = HO2 + H2O + H2O + H2O + O2	2.0E-07	-.5	0	ESTIMATED	331
332	H+73 + CO3- = H2O + H2O + H2O + H2O + CO2 + HO	2.0E-07	-.5	0	ESTIMATED	332
333	H+73 + 78- = H + H2O + H2O + H2O + H2O + CO2 + O + H2O	2.0E-07	-.5	0	ESTIMATED	333
334	H+73 + CO4- = H2O + H2O + H2O + H2O + CO2 + HO2	2.0E-07	-.5	0	ESTIMATED	334
335	H+73 + 94- = H + H2O + H2O + H2O + H2O + CO2 + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	335
336	H+73 + NO2- = H2O + H2O + H2O + H2O + HO + NO	2.0E-07	-.5	0	ESTIMATED	336
337	H+73 + 64- = H + H2O + H2O + H2O + H2O + NO2 + H2O	2.0E-07	-.5	0	ESTIMATED	337
338	H+73 + NO3- = H2O + H2O + H2O + H2O + HO + NO2	2.0E-07	-.5	0	ESTIMATED	338
339	H+73 + 62- = H2O + H2O + H2O + H2O + HO2 + NO	2.0E-07	-.5	0	ESTIMATED	339
340	H+73 + 80- = H + H2O + H2O + H2O + H2O + NO2 + O + H2O	2.0E-07	-.5	0	ESTIMATED	340
341	H+73 + 125- = HNO3 + HNO3 + H2O + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	341
342	H+73 + O- = H2O + H2O + H2O + H2O + HO	2.0E-07	-.5	0	ESTIMATED	342
343	H+73 + O2- = H2O + H2O + H2O + H2O + HO2	2.0E-07	-.5	0	ESTIMATED	343
344	H+73 + O2-W = H + H2O + H2O + H2O + H2O + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	344
345	H+73 + O3- = H2O + H2O + H2O + H2O + HO + O2	2.0E-07	-.5	0	ESTIMATED	345
346	H+73 + O4- = H2O + H2O + H2O + H2O + HO2 + O2	2.0E-07	-.5	0	ESTIMATED	346
347	H+91 + CO3- = H2O + H2O + H2O + H2O + H2O + HO + CO2	2.0E-07	-.5	0	ESTIMATED	347
348	H+91 + 78- = H H2O H2O H2O H2O H2O CO2 O H2O	2.0E-07	-.5	0	ESTIMATED	348
349	H+91 + CO4- = H2O + H2O + H2O + H2O + H2O + HO2 + CO2	2.0E-07	-.5	0	ESTIMATED	349
350	H+91 + 94- = H H2O H2O H2O H2O H2O CO2 O2 H2O	2.0E-07	-.5	0	ESTIMATED	350
351	H+91 + NO2- = H2O + H2O + H2O + H2O + H2O + HO + NO	2.0E-07	-.5	0	ESTIMATED	351
352	H+91 + 64- = H H2O H2O H2O H2O H2O NO2 H2O	2.0E-07	-.5	0	ESTIMATED	352
353	H+91 + NO3- = H2O + H2O + H2O + H2O + H2O + HO + NO2	2.0E-07	-.5	0	ESTIMATED	353
354	H+91 + 62- = H2O + H2O + H2O + H2O + H2O + HO2 + NO	2.0E-07	-.5	0	ESTIMATED	354
355	H+91 + 80- = H H2O H2O H2O H2O H2O NO2 O H2O	2.0E-07	-.5	0	ESTIMATED	355
356	H+91 + 125- = HNO3 + HNO3 + H2O + H2O + H2O + H2O H2O	2.0E-07	-.5	0	ESTIMATED	356
357	H+91 + O- = H2O + H2O + H2O + H2O + H2O + HO	2.0E-07	-.5	0	ESTIMATED	357
358	H+91 + O2- = H2O + H2O + H2O + H2O + H2O + HO2	2.0E-07	-.5	0	ESTIMATED	358
359	H+91 O2-W = H H2O H2O H2O H2O H2O O2 H2O	2.0E-07	-.5	0	ESTIMATED	359
360	H+91 + O3- = H2O + H2O + H2O + H2O + H2O + HO + O2	2.0E-07	-.5	0	ESTIMATED	360

REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
361	H+91 + O4- = H2O + H2O + H2O + H2O + H2O + HO2 + O2	2.0E-07	-.5	0	ESTIMATED	361
362	NO+ + CO3- = NO + O + CO2	2.0E-07	-.5	0	ESTIMATED	362
363	NO+ + 78- = CO2 + O + H2O + NO	2.0E-07	-.5	0	ESTIMATED	363
364	NO+ + CO4- = CO2 + O2 + NO	2.0E-07	-.5	0	ESTIMATED	364
365	NO+ + 94- = CO2 + O2 + H2O + NO	2.0E-07	-.5	0	ESTIMATED	365
366	NO+ + NO2- = NO2 + NO	3.5E-07	-.5	0	DNA HANDBOOK REV3 TABLE 24 REACTION V-8	366
367	NO+ + 64- = NO2 + H2O + NO	2.0E-07	-.5	0	ESTIMATED	367
368	NO+ + NO3- = NO + NO2 + O	4.0E-07	-.5	0	DNA HANDBOOK REV3 TABLE 24 REACTION V-9	368
369	NO+ + 62- = O2 + NO + NO	2.0E-07	-.5	0	ESTIMATED	369
370	NO+ + 80- = NO2 + H2O + NO + O	2.0E-07	-.5	0	ESTIMATED	370
371	NO+ + 125- = HNO3 + NO2 + NO2	2.0E-07	-.5	0	ESTIMATED	371
372	NO+ + O- = O + NO	4.9E-07	-.5	0	DNA HANDBOOK REV3 TABLE 24 REACTION V-7	372
373	NO+ + O2- = O2 + NO	5.8E-07	-.5	0	MOSELEY ETAL CASE STUDIES ATOMIC PHYS 5.1 75	373
374	NO+ + O2-W = O2 + H2O + NO	2.0E-07	-.5	0	ESTIMATED	374
375	NO+ + O3- = O3 + NO	2.0E-07	-.5	0	ESTIMATED	375
376	NO+ + O4- = O2 + O2 + NO	2.0E-07	-.5	0	ESTIMATED	376
377	NO48 + CO3- = NO + H2O + CO2 + O	2.0E-07	-.5	0	ESTIMATED	377
378	NO48 + 78- = CO2 + O + H2O + H2O + NO	2.0E-07	-.5	0	ESTIMATED	378
379	NO48 + CO4- = CO2 + NO + H2O + O2	2.0E-07	-.5	0	ESTIMATED	379
380	NO48 + 94- = CO2 + O2 + H2O + H2O + NO	2.0E-07	-.5	0	ESTIMATED	380
381	NO48 + NO2- = NO + H2O + NO2	2.0E-07	-.5	0	ESTIMATED	381
382	NO48 + 64- = NO2 + H2O + NO + H2O	2.0E-07	-.5	0	ESTIMATED	382
383	NO48 + NO3- = NO + H2O + NO2 + O	2.0E-07	-.5	0	ESTIMATED	383
384	NO48 + 62- = O2 + NO + NO + H2O	2.0E-07	-.5	0	ESTIMATED	384
385	NO48 + 80- = NO2 + H2O + NO + H2O + O	2.0E-07	-.5	0	ESTIMATED	385
386	NO48 + 125- = HNO3 + NO2 + NO2 + H2O	2.0E-07	-.5	0	ESTIMATED	386
387	NO48 + O- = O + NO + H2O	2.0E-07	-.5	0	ESTIMATED	387
388	NO48 + O2- = NO + H2O + O2	2.0E-07	-.5	0	ESTIMATED	388
389	NO48 + O2-W = O2 + NO + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	389
390	NO48 + O3- = NO + H2O + O3	2.0E-07	-.5	0	ESTIMATED	390
391	NO48 + O4- = O2 + NO + H2O + O2	2.0E-07	-.5	0	ESTIMATED	391
392	NO66 + CO3- = CO2 + O + NO + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	392
393	NO66 + 78- = CO2 + O + H2O + H2O + H2O + NO	2.0E-07	-.5	0	ESTIMATED	393
394	NO66 + CO4- = CO2 + NO + H2O + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	394
395	NO66 + 94- = CO2 + O2 + H2O + H2O + H2O + NO	2.0E-07	-.5	0	ESTIMATED	395
396	NO66 + NO2- = NO + H2O + H2O + NO2	2.0E-07	-.5	0	ESTIMATED	396
397	NO66 + 64- = NO + NO2 + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	397
398	NO66 + NO3- = NO + H2O + H2O + NO2 + O	2.0E-07	-.5	0	ESTIMATED	398
399	NO66 + 62- = O2 + NO + NO + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	399
400	NO66 + 80- = NO2 + H2O + NO + H2O + H2O + O	2.0E-07	-.5	0	ESTIMATED	400
401	NO66 + 125- = HNO3 + NO2 + NO2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	401
402	NO66 + O- = O + NO + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	402
403	NO66 + O2- = NO + H2O + H2O + O2	2.0E-07	-.5	0	ESTIMATED	403
404	NO66 + O2-W = O2 + NO + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	404
405	NO66 + O3- = NO + H2O + H2O + O3	2.0E-07	-.5	0	ESTIMATED	405
406	NO66 + O4- = O2 + NO + H2O + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	406
407	NO84 + CO3- = NO + H2O + H2O + H2O + CO2 + O	2.0E-07	-.5	0	ESTIMATED	407
408	NO84 + 78- = CO2 + O + H2O + H2O + H2O + H2O + NO	2.0E-07	-.5	0	ESTIMATED	408
409	NO84 + CO4- = CO2 + NO + H2O + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	409
410	NO84 + 94- = CO2 + O2 + H2O + H2O + H2O + NO + H2O	2.0E-07	-.5	0	ESTIMATED	410
411	NO84 + NO2- = NO + H2O + NO2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	411
412	NO84 + 64- = NO + NO2 + H2O + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	412
413	NO84 + NO3- = NO + H2O + NO2 + H2O + H2O + O	2.0E-07	-.5	0	ESTIMATED	413
414	NO84 + 62- = NO + H2O + H2O + H2O + NO + O2	2.0E-07	-.5	0	ESTIMATED	414
415	NO84 + 80- = NO2 + H2O + NO + H2O + H2O + H2O + O	2.0E-07	-.5	0	ESTIMATED	415
416	NO84 + 125- = HNO3 + NO2 + NO2 + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	416
417	NO84 + O- = O + NO + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	417
418	NO84 + O2- = NO + H2O + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	418
419	NO84 + O2-W = O2 + NO + H2O + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	419
420	NO84 + O3- = NO + H2O + O3 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	420

REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
421	NO84 + O4- = O2 + NO + H2O + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	421
422	NO2+ + CO3- = NO + O2 + CO2	2.0E-07	-.5	0	ESTIMATED	422
423	NO2+ + 78- = CO2 + O2 + H2O + NO	2.0E-07	-.5	0	ESTIMATED	423
424	NO2+ + CO4- = CO2 + O2 + NO2	2.0E-07	-.5	0	ESTIMATED	424
425	NO2+ + 94- = CO2 + O2 + H2O + NO + O	2.0E-07	-.5	0	ESTIMATED	425
426	NO2+ + NO2- = NO2 + NO2	2.0E-07	-.5	0	ESTIMATED	426
427	NO2+ + 64- = NO2 + H2O + NO2	2.0E-07	-.5	0	ESTIMATED	427
428	NO2+ + NO3- = NO2 + NO2 + O	2.0E-07	-.5	0	ESTIMATED	428
429	NO2+ + 62- = O2 + NO2 + NO	2.0E-07	-.5	0	ESTIMATED	429
430	NO2+ + 80- = NO2 + H2O + NO + O2	2.0E-07	-.5	0	ESTIMATED	430
431	NO2+ + 125- = HNO3 + NO2 + NO + O2	2.0E-07	-.5	0	ESTIMATED	431
432	NO2+ + O- = O2 + NO	2.0E-07	-.5	0	ESTIMATED	432
433	NO2+ + O2- = O2 + NO + O	2.0E-07	-.5	0	ESTIMATED	433
434	NO2+ + O2-W = O2 + H2O + NO + O	2.0E-07	-.5	0	ESTIMATED	434
435	NO2+ + O3- = O2 + O2 + NO	2.0E-07	-.5	0	ESTIMATED	435
436	NO2+ + O4- = O2 + O2 + NO + O	2.0E-07	-.5	0	ESTIMATED	436
437	64+ + CO3- = NO + H2O + CO2 + O2	2.0E-07	-.5	0	ESTIMATED	437
438	64+ + 78- = NO + CO2 + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	438
439	64+ + CO4- = NO2 + H2O + CO2 + O2	2.0E-07	-.5	0	ESTIMATED	439
440	64+ + 94- = NO2 + H2O + CO2 + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	440
441	64+ + NO2- = NO + NO + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	441
442	64+ + 64- = NO + NO + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	442
443	64+ + NO3- = NO2 + NO + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	443
444	64+ + 62- = NO2 + NO + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	444
445	64+ + 80- = NO2 + NO + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	445
446	64+ + 125- = NO2 + NO + O2 + H2O + HNO3	2.0E-07	-.5	0	ESTIMATED	446
447	64+ + O- = NO + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	447
448	64+ + O2- = NO + O + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	448
449	64+ + O2-W = NO + O + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	449
450	64+ + O3- = NO + O2 + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	450
451	64+ + O4- = NO + O + O2 + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	451
452	82+ + CO3- = NO + H2O + CO2 + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	452
453	82+ + 78- = NO + CO2 + O2 + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	453
454	82+ + CO4- = NO2 + H2O + CO2 + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	454
455	82+ + 94- = NO2 + H2O + CO2 + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	455
456	82+ + NO2- = NO + NO + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	456
457	82+ + 64- = NO + NO + O2 + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	457
458	82+ + NO3- = NO2 + NO + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	458
459	82+ + 62- = NO2 + NO + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	459
460	82+ + 80- = NO2 + NO + O2 + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	460
461	82+ + 125- = NO2 + NO + O2 + H2O + HNO3 + H2O	2.0E-07	-.5	0	ESTIMATED	461
462	82+ + O- = NO + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	462
463	82+ + O2- = NO + O + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	463
464	82+ + O2-W = NO + O + O2 + H2O + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	464
465	82+ + O3- = NO + O2 + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	465
466	82+ + O4- = NO + O + O2 + O2 + H2O + H2O	2.0E-07	-.5	0	ESTIMATED	466
467	O2+ + CO3- = O2 + O + CO2	2.0E-07	-.5	0	ESTIMATED	467
468	O2+ + 78- = CO2 + O + H2O + O2	2.0E-07	-.5	0	ESTIMATED	468
469	O2+ + CO4- = CO2 + O2 + O2	2.0E-07	-.5	0	ESTIMATED	469
470	O2+ + 94- = CO2 + O2 + H2O + O2	2.0E-07	-.5	0	ESTIMATED	470
471	O2+ + NO2- = NO2 + O2	4.1E-07	-.5	0	DNA HANDBOOK REV3 TABLE 24 REACTION V-4	471
472	O2+ + 64- = NO2 + H2O + O2	2.0E-07	-.5	0	ESTIMATED	472
473	O2+ + NO3- = NO2 + O + O2	1.3E-07	-.5	0	DNA HANDBOOK REV3 TABLE 24 REACTION V-5	473
474	O2+ + 62- = O2 + NO + O2	2.0E-07	-.5	0	ESTIMATED	474
475	O2+ + 80- = NO2 + H2O + O2 + O	2.0E-07	-.5	0	ESTIMATED	475
476	O2+ + 125- = HNO3 + NO2 + O + O2	2.0E-07	-.5	0	ESTIMATED	476
477	O2+ + O- = O + O2	1.0E-07	-.5	0	MOSELEY ETAL CASE STUDIES ATOMIC PHYS 5:1 75	477
478	O2+ + O2- = O2 + O2	4.2E-07	-.5	0	DNA HANDBOOK REV3 TABLE 24 REACTION V-2	478
479	O2+ + O2-W = O2 + O2 + H2O	2.0E-07	-.5	0	ESTIMATED	479
480	O2+ + O3- = O3 + O2	2.0E-07	-.5	0	ESTIMATED	480

REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
481	02+ + 04- = 02 + 02 + 02	2.0E-07	-.5	0	ESTIMATED	481
482	0250 + C03- = 02 + H20 + C02 + 0	2.0E-07	-.5	0	ESTIMATED	482
483	0250 + 78- = C02 + 0 + H20 + H20 + 02	2.0E-07	-.5	0	ESTIMATED	483
484	0250 + C04- = C02 + H20 + 02 + 02	2.0E-07	-.5	0	ESTIMATED	484
485	0250 + 94- = C02 + 02 + H20 + H20 + 02	2.0E-07	-.5	0	ESTIMATED	485
486	0250 + N02- = 02 + H20 + N02	2.0E-07	-.5	0	ESTIMATED	486
487	0250 + 64- = 02 + H20 + N02 + H20	2.0E-07	-.5	0	ESTIMATED	487
488	0250 + N03- = 02 + H20 + N02 + 0	2.0E-07	-.5	0	ESTIMATED	488
489	0250 + 62- = 02 + H20 + 02 + NO	2.0E-07	-.5	0	ESTIMATED	489
490	0250 + 80- = N02 + H20 + H20 + 02 + 0	2.0E-07	-.5	0	ESTIMATED	490
491	0250 + 125- = HN03 + N02 + 02 + H20 + 0	2.0E-07	-.5	0	ESTIMATED	491
492	0250 + 0- = 02 + H20 + 0	2.0E-07	-.5	0	ESTIMATED	492
493	0250 + 02- = 02 + H20 + 02	2.0E-07	-.5	0	ESTIMATED	493
494	0250 + 02-w = 02 + 02 + H20 + H20	2.0E-07	-.5	0	ESTIMATED	494
495	0250 + 03- = 02 + H20 + 03	2.0E-07	-.5	0	ESTIMATED	495
496	0250 + 04- = 02 + 02 + H20 + 02	2.0E-07	-.5	0	ESTIMATED	496

DATE OF LAST REACTION CHANGE IS JUNE 26, 1976

DATE OF LAST REFERENCE CHANGE IS JUNE 16, 1977