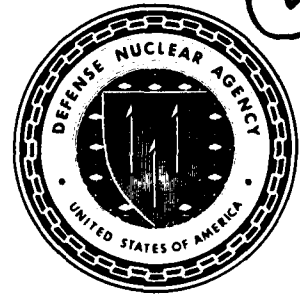




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**NLTE Optical Emission From Major Air Species
A Delta Model for the Visible/UV**

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Santa Barbara, CA 93102-0719

February 1991

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SUMMARY

This report develops models for determining collision-limiting, or "delta" factors for certain electronic states of N_2 , N_2^+ , O_2 , NO and NO^+ molecules. These factors, when multiplied by the Boltzmann populations of the respective states, yield the steady-state populations as they exist under the influence of electron and heavy-particle collisions and a radiation field. With one exception, only electric-dipole-allowed transitions are included. The resulting radiation lies mainly in the visible and ultraviolet (UV) regions. Since the volume-emission rate is proportional to the population of the emitting state, the delta factors can also be used to convert, directly, thermal radiation, calculated under conditions of local thermodynamic equilibrium (LTE) at the neutral gas temperature, to that existing under conditions of non-local thermodynamic equilibrium (NLTE).

For each molecule, and for each state of each molecule considered, a steady-state population is determined from a balance between its rate of population and depopulation by collisional and radiative processes. Separate electron and neutral-gas temperatures are provided for. Radiative and collisional coupling among the states of a given species, where significant, necessitates the solution of simultaneous linear equations for the state populations involved. For radiative absorption, only sunlight is included in our models.

The number and type of states for which delta factors are determined, and the radiative band systems involved, are as follows. For N_2 , there are 11 electronic states including the ground. The band systems are the Vegard-Kaplan, First Positive, Second Positive, Birge-Hopfield 1, Birge-Hopfield 2 and five different Rydberg series. For N_2^+ , there are 4 electronic states including the ground. The bands are the Meinel, First Negative and Second Negative Systems. For O_2 , besides the ground state, we include 21 vibrational states of a single electronic state. Transitions from these states to the ground-vibrational states give rise to bands of the Schumann-Runge System. For NO , there are 7 electronic states including the ground. The band systems are the gamma, beta, delta, Heath, epsilon, Feast 1, Feast 2, beta prime, gamma prime, Feast-Heath and $E^2\Sigma^+ - C^2\Pi$. Finally, for NO^+ , deltas are determined for the ground state and for 10 vibrational states of a single electronically-excited state. Transitions from these states to the ground-vibrational states give rise to bands of the Baer-Miescher System in the vacuum UV.

The models have been computerized with a main driver program DELTAVU and a separate subroutine for each of the 5 molecules involved. Sample calculations are shown giving delta factors computed for three different nuclear-burst conditions as determined by the NORSE code.

Some recommendations are made regarding future improvements and possible expansion of the models to include additional states and species.

PREFACE

The author gratefully acknowledges the contributions of Dr. John DeVore (PRi) to the development of the models described herein. His assistance in providing NORSE-code output, in offering advice through numerous conversations and, indeed, in suggesting the undertaking of this task itself, is greatly appreciated. Thanks also go to Dr. Richard Harris (PRi) for providing information on the states and bands in the AFWL model, and to Dr. Kenneth Schwartz (DNA) for his continuing support of this work.

CONVERSION TABLE

Conversion factors for U.S. Customary to metric (SI) units of measurement

MULTIPLY $\xrightarrow{\hspace{2cm}}$ BY $\xrightarrow{\hspace{2cm}}$ TO GET
 TO GET $\xleftarrow{\hspace{2cm}}$ BY $\xleftarrow{\hspace{2cm}}$ DIVIDE

angstrom	1.000000 $\times$ E -10	meters (m)
atmosphere (normal)	1.01325 $\times$ E +2	kilo pascal (kPa)
bar	1.000000 $\times$ E +2	kilo pascal (kPa)
barn	1.000000 $\times$ E -28	meter ² (m ²)
British thermal unit (thermochemical)	1.054350 $\times$ E +3	joule (J)
calorie (thermochemical)	4.184000	joule (J)
cal (thermochemical) / cm ²	4.184000 $\times$ E -2	mega joule/m ² (MJ/m ²)
curie	3.700000 $\times$ E +1	*giga becquerel (GBq)
degree (angle)	1.745329 $\times$ E -2	radian (rad)
degree Fahrenheit	$t_K = (t_F + 459.67)/1.8$	degree kelvin (K)
electron volt	1.60219 $\times$ E -19	joule (J)
erg	1.000000 $\times$ E -7	joule (J)
erg/second	1.000000 $\times$ E -7	watt (W)
foot	3.048000 $\times$ E -1	meter (m)
foot-pound-force	1.355818	joule (J)
gallon (U.S. liquid)	3.785412 $\times$ E -3	meter ³ (m ³)
inch	2.540000 $\times$ E -2	meter (m)
jerk	1.000000 $\times$ E +9	joule (J)
joule/kilogram (J/kg) (radiation dose absorbed)	1.000000	Gray (Gy)
kilotons	4.183	terajoules
kip (1000 lbf)	4.448222 $\times$ E +3	newton (N)
kip/inch ² (ksi)	6.894757 $\times$ E +3	kilo pascal (kPa)
ktap	1.000000 $\times$ E +2	newton-second/m ² (N-s/m ²)
micron	1.000000 $\times$ E -6	meter (m)
mil	2.540000 $\times$ E -5	meter (m)
mile (international)	1.609344 $\times$ E +3	meter (m)
ounce	2.834952 $\times$ E -2	kilogram (kg)
pound-force (lbs avoirdupois)	4.448222	newton (N)
pound-force inch	1.129848 $\times$ E -1	newton-meter (N-m)
pound-force/inch	1.751268 $\times$ E +2	newton/meter (N/m)
pound-force/foot ²	4.788026 $\times$ E -2	kilo pascal (kPa)
pound-force/inch ² (psi)	6.894757	kilo pascal (kPa)
pound-mass (lbm avoirdupois)	4.535924 $\times$ E -1	kilogram (kg)
pound-mass-foot ² (moment of inertia)	4.214011 $\times$ E -2	kilogram-meter ² (kg m ²)
pound-mass/foot ³	1.601846 $\times$ E +1	kilogram/meter ³ (kg/m ³)
rad (radiation dose absorbed)	1.000000 $\times$ E -2	**Gray (Gy)
roentgen	2.579760 $\times$ E -4	coulomb/kilogram (C/kg)
shake	1.000000 $\times$ E -8	second (s)
slug	1.459390 $\times$ E +1	kilogram (kg)
torr (mm Hg, 0° C)	1.333220 $\times$ E -1	kilo pascal (kPa)

*The becquerel (Bq) is the SI unit of radioactivity; 1 Bq = 1 event/s.

**The Gray (Gy) is the SI unit of absorbed radiation.

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SECTION 1

INTRODUCTION

This report is the visible/ultraviolet (UV) counterpart to References 1.1 and 1.2 that describe a model for computing the non-local thermodynamic equilibrium (NLTE) radiation from selected IR-active molecules. In those reports, we dealt with the determination of non-Boltzmann populations of vibrational states that give rise to the IR radiation. In this report, we are interested in determining the non-Boltzmann populations mainly of electronic states of the air species N_2 , N_2^+ , O_2 , NO and NO^+ that give rise to visible/UV radiation. The object is the construction of NLTE emission models for incorporation in the NORSE code.

The approach taken here, as in References 1.1 and 1.2, is one of providing a collision-limiting, or "delta" factor for each radiating state considered. This factor is defined as one which, when multiplied by the Boltzmann population of the state (or by the LTE emission rate from it), will yield the corresponding non-Boltzmann population (or the NLTE emission rate). The method entails the calculation of the steady-state concentration of each state by equating its population and depopulation rates from collisional and radiative processes.

The electronic states chosen for inclusion in our model are those in the Air Force Weapons Laboratory (AFWL) opacity model (Reference 1.3). Generally, only permitted transitions (i.e. electric-dipole allowed) involving these states are included. This is consistent with the NORSE thermal-emission model that uses absorption cross sections for these same transitions (bands) in determining the LTE volume emission rates for the visible/UV.

Except for the cases of O_2 and NO^+ , for which only one electronically-excited state is significant, a single delta factor is modeled for each electronic state considered. That is, with the above exceptions, the same delta factor is assumed to apply to each vibrational state of a given electronic state. Thus, the same delta factor is used to convert the LTE emission from all bands of a given band system to NLTE emission. This is done for three reasons. First, NORSE cannot presently identify contributions from each band of a given band system to the LTE emission in a specified wavenumber interval. Therefore, it is unable to utilize the increased resolution provided by the availability of separate deltas for each band of a given band system. Second, insufficient data exist on excitation/deexcitation rates for the individual vibrational states to permit development of a reliable delta-factor model for a multitude

of vibrational states of each electronic state. Third, the development of such a model would be quite unwieldy, even if adequate data were available. Consequently, the models developed in this report determine, in some sense, average delta factors for entire band systems and, as such, they provide what can be considered first-order corrections to the LTE emission from each band of a given system.

Coupling between electronic states of different molecules is assumed to be negligibly small and so a separate delta model can be developed for each molecule, independent of that for each of the others. Sections 2 through 6 below describe the delta models for N_2 , N_2^+ , O_2 , NO and NO^+ , respectively. Section 7 shows sample delta-factor results and Section 8 presents some comments and recommendations. The models have been computerized with a main driver program DELTAVU and separate subroutines DELN2, DELN2P, DELO2, DELNO and DELNOP for the molecules N_2 , N_2^+ , O_2 , NO and NO^+ , respectively. The computer listings are given in the Appendix.

SECTION 2

DELTA MODEL FOR N₂

STATES AND BAND SYSTEMS INCLUDED

Table 2.1 shows the electronic states of N₂ included in our Delta model. Also shown are the energy (Ref.2.1) and statistical weight of each state. The energy

Table 2.1. States of N₂ included.

State (v=0)	Energy (cm ⁻¹ /eV)	Statistical Weight g
X ¹ Σ _g ⁺	0.0/0.0	1
A ³ Σ _u ⁺	49,754.78/6.18	3
B ³ Π _g	59,306.81/7.37	6
C ³ Π _u	88,977.84/11.05	6
b ¹ Π _u	100,817.5/12.53	2
b' ¹ Σ _u ⁺	103,670.8/12.86	1
c ₃ ¹ Π _u (c ¹ Π _u)	104,138.2/12.92	2
c' ₄ ¹ Σ _u ⁺ (c' ¹ Σ _u ⁺)	104,323.3/12.95	1
o ₃ ¹ Π _u (o ¹ Π _u)	105,710.4/13.12	2
c ₄ ¹ Π _u (e ¹ Π _u)	115,635.9/14.34	2
c' ₅ ¹ Σ _u ⁺ (e' ¹ Σ _u ⁺)	115,876/14.37	1

values shown are for the ground vibrational states. The statistical weight, g , for Σ states is $2S + 1$ while for other states (Π, Δ, ...) it is $2(2S+1)$ (Ref. 2.2) where S is the total spin quantum number. The first six entries in Table 2.1 are valence states; the last five entries are Rydberg states. For the Rydberg states, quantities in parentheses indicate the older state notation; numerical subscripts refer to the principal quantum number, n . The state $o_3^1\Pi_u$ is the first member ($n=3$) of the Rydberg series $o_n^1\Pi(n=3,4,5,\dots)$ converging on $N_2^+(A^2\Pi_u)$, while the other four Rydbergs are members of series converging on $N_2^+(X^2\Sigma_g^+)$.

Table 2.2 shows the band systems of N_2 included in our model. All are permitted transitions except for the Vegard-Kaplan System that violates the $\Delta S = 0$ rule for electric-dipole radiation. Also shown in Table 2.2 are the (0-0) band-origin wavelengths and wavenumbers of the systems as well as the approximate range of wavelengths over which each band system radiates (Ref. 2.1).

Table 2.2. Band systems of N_2 included.

Band System	λ_{00} ($\text{\AA}$)	$\tilde{\nu}_{00}$ (cm^{-1})	Wavelength Region ($\text{\AA}$)
$A^3\Sigma_u^+ - X^1\Sigma_g^+$ (Vegard-Kaplan)	2,009.9	49,754.8	5325-1250
$B^3\Pi_g - A^3\Sigma_u^+$ (First Positive)	10,469.0	9,552.0	25,310-4780
$C^3\Pi_u - B^3\Pi_g$ (Second Positive)	3,370.3	29,671.0	5460-2680
$b^2\Pi_u - X^1\Sigma_g^+$ (Birge-Hopfield 1)	991.9	100,817.5	1110-850
$b^1\Sigma_u^+ - X^1\Sigma_g^+$ (Birge-Hopfield 2)	964.6	103,670.8	1290-820
$c_3^1\Pi_u - X^1\Sigma_g^+$ (Worley-Jenkins Ryd.)	960.3	104,138.2	960-922
$c_4^1\Sigma_u^+ - X^1\Sigma_g^+$ (Carroll-Yoshino Ryd.)	958.6	104,323.3	960-860
$o_3^1\Pi_u - X^1\Sigma_g^+$ (Worley's Third Ryd.)	946.0	105,710.4	950-880
$c_4^1\Pi_u - X^1\Sigma_g^+$ (Worley-Jenkins Ryd.)	864.8	115,635.9	$\sim$ 865
$c_5^1\Sigma_u^+ - X^1\Sigma_g^+$ (Carroll-Yoshino Ryd.)	863.0	115,876	$\sim$ 863

EXCITATION/DEEXCITATION MECHANISMS

The processes that we include for excitation and deexcitation of the electronic states are electron and heavy-particle collisions, spontaneous radiation and sunlight absorption. The information that we have on the collisional processes is limited. For the singlet states considered here, we have found no data on excitation or quenching by heavy particles and so we include these processes only for electrons. However, this should not be a serious limitation since, for a given temperature, the electron processes usually proceed at much faster rates than do those for heavy particles (Ref. 2.3). For the triplet states, data on heavy-particle collisions is limited to room temperature or to narrow temperature-range measurements.

Many of the high-lying singlet states (valence and Rydberg) are strongly predissociated and their radiation is thus diminished (Refs. 2.1, 2.4). Although sufficient information is available on the predissociation rates to make approximate allowance for them, the reverse process, preassociation, that will tend to partially compensate (Ref. 2.5), cannot be so easily allowed for. For this reason we ignore these processes in our N_2 model. As a consequence, the delta factors predicted by our model for these states, and thus the NLTE emission rates from them, tend to be upper limits to the true values.

Table 2.3 shows the specific reactions or processes included in the N_2 model together with suggested values for the rate coefficients, the Einstein A coefficients and ρB factors ¹ for sunlight. The forward (deexcitation) rate coefficients for the first 19 reactions in Table 2.3 are expressed in the form

$$k = aT^b e^{-c/T} \quad (\text{cm}^3 \text{ sec}^{-1}) \quad (2.1)$$

where the parameters a , b and c are given in Columns 2, 3 and 4, respectively, while the reverse (excitation) rate coefficients are expressed in the form

$$k' = a' e^{-c'/T} k \quad (\text{cm}^3 \text{ sec}^{-1}) \quad (2.2)$$

where a' and c' are given in Columns 5 and 6, respectively. For collisions involving heavy particles, T is the heavy-particle temperature ($^{\circ}\text{K}$) while, for collisions involving electrons, it refers to the electron temperature T_e . Also shown in Table 2.3 are the temperatures, or temperature ranges, for which the rate-coefficient expressions apply and the supporting references.

With respect to Reactions 2-11 through 2-19, we should point out that the products on the right-hand sides are generally uncertain, although there is mounting evidence that the product state of N_2 is usually not the ground state, $X^1\Sigma_g^+$, especially where quenching of the B and C states is concerned. Indeed, the reactions can be chemical in nature with the product species being other than N_2 . Nevertheless, for the sake of simplicity in allowing for the reverse reactions, we assume that the electronically-excited N_2 molecules are quenched to the ground state.

¹ ρ is the energy density of the radiation field at the band frequency and B is the Einstein B coefficient. The product has dimensions sec^{-1} .

Table 2.3. Excitation/deexcitation mechanisms and assumed rates for states of N_2 .

	Reaction	a^*	b	c	a'	d	Temperature (°K)	Reference
(2-1)	$e + N_2(b^1\Pi_u) \longleftrightarrow e + N_2(X^1\Sigma_g^+)$	2.2 (-13)	0.861	385.1	2	145,055	1000-35,000	see text
(2-2)	$e + N_2(b'^1\Sigma_u^+) \longleftrightarrow e + N_2(X^1\Sigma_g^+)$	6.1 (-11)	0.427	6,759.8	1	149,160	1000-35,000	see text
(2-3)	$e + N_2(c_3^1\Pi_u) \longleftrightarrow e + N_2(X^1\Sigma_g^+)$	1.6 (3)	-2.469	97,547.3	2	149,833	1000-35,000	see text
(2-4)	$e + N_2(c_4^1\Sigma_u^+) \longleftrightarrow e + N_2(X^1\Sigma_g^+)$	5.9 (4)	-2.681	101,251.0	1	150,099	1000-35,000	see text
(2-5)	$e + N_2(c_3^1\Pi_u) \longleftrightarrow e + N_2(X^1\Sigma_g^+)$	1.8 (-15)	1.068	-4,454.7	2	152,095	1000-35,000	see text
(2-6)	$e + N_2(c_4^1\Pi_u) \longleftrightarrow e + N_2(X^1\Sigma_g^+)$	5.5 (2)	-2.469	92,502.4	2	166,375	1000-35,000	2.9
(2-7)	$e + N_2(c_6^1\Sigma_u^+) \longleftrightarrow e + N_2(X^1\Sigma_g^+)$	2.6 (4)	-2.681	101,251.6	1	166,721	1000-35,000	2.10
(2-8)	$e + N_2(C^3\Pi_u) \longleftrightarrow e + N_2(X^1\Sigma_g^+)$	6.7 (-9)	-0.102	3,599.9	6	128,020	1000-35,000	see text
(2-9)	$e + N_2(B^3\Pi_g) \longleftrightarrow e + N_2(X^1\Sigma_g^+)$	1.2 (-10)	0.225	2,297.1	6	85,330	1000-35,000	see text
(2-10)	$e + N_2(A^3\Sigma_u^+) \longleftrightarrow e + N_2(X^1\Sigma_g^+)$	1.5 (-13)	0.854	-2,225.5	3	71,587	1000-35,000	see text
(2-11)	$N_2(C^3\Pi_u) + N_2 \longleftrightarrow N_2(X^1\Sigma_g^+) + N_2$	7.1 (-12)	0.	0.	6	128,020	~ 300	2.11,2.12
(2-12)	$N_2(C^3\Pi_u) + O_2 \longleftrightarrow N_2(X^1\Sigma_g^+) + O_2$	2.8 (-10)	0.	0.	6	128,020	~ 300	2.21
(2-13)	$N_2(B^3\Pi_g) + N_2 \longleftrightarrow N_2(X^1\Sigma_g^+) + N_2$	2.7 (-11)	0.	0.	6	85,330	~ 300	2.13,2.22
(2-14)	$N_2(B^3\Pi_g) + O_2 \longleftrightarrow N_2(X^1\Sigma_g^+) + O_2$	1.1 (-10)	0.	0.	6	85,330	~ 300	2.13
(2-15)	$N_2(B^3\Pi_g) + NO \longleftrightarrow N_2(X^1\Sigma_g^+) + NO$	2.4 (-10)	0.	0.	6	85,330	~ 300	2.13
(2-16)	$N_2(A^3\Sigma_u^+) + O_2 \longleftrightarrow N_2(X^1\Sigma_g^+) + O_2$	4.6 (-12)	0.	0.	3	71,587	~ 300	2.16
(2-17)	$N_2(A^3\Sigma_u^+) + NO \longleftrightarrow N_2(X^1\Sigma_g^+) + NO$	6.2 (-11)	0.	0.	3	71,587	~ 300	2.16
(2-18)	$N_2(A^3\Sigma_u^+) + O \longleftrightarrow N_2(X^1\Sigma_g^+) + O$	3.1 (-11)	0.	0.	3	71,587	~ 300	2.18
(2-19)	$N_2(A^3\Sigma_u^+) + N \longleftrightarrow N_2(X^1\Sigma_g^+) + N$	6.3 (-7)	-1.5	0.	3	71,587	7000-16,000	2.19

* Numbers in parentheses mean powers of 10.

Table 2.3. Excitation/deexcitation mechanisms and assumed rates for states of N_2 (Continued).

Reaction	$A(\text{sec}^{-1})^*$	$\rho B(\text{sec}^{-1})^*$	Reference
(2-20) $N_2(b^1\Pi_u) \longleftrightarrow N_2(X^1\Sigma_g^+) + h\nu$	1.0 (8)	3.7 (-8)	2.1, 2.20
(2-21) $N_2(b'^1\Sigma_u^+) \longleftrightarrow N_2(X^1\Sigma_g^+) + h\nu$	1.0 (8)	9.3 (-9)	2.1, 2.20
(2-22) $N_2(c_3^1\Pi_u) \longleftrightarrow N_2(X^1\Sigma_g^+) + h\nu$	1.4 (8)	2.3 (-8)	2.1
(2-23) $N_2(c_4^1\Sigma_u^+) \longleftrightarrow N_2(X^1\Sigma_g^+) + h\nu$	1.0 (9)	7.9 (-8)	2.1
(2-24) $N_2(o_3^1\Pi_u) \longleftrightarrow N_2(X^1\Sigma_g^+) + h\nu$	1.0 (8)	1.1 (-8)	2.20
(2-25) $N_2(c_4^1\Pi_u) \longleftrightarrow N_2(X^1\Sigma_g^+) + h\nu$	6.2 (7)	6.6 (-10)	2.20
(2-26) $N_2(c_5^1\Sigma_u^+) \longleftrightarrow N_2(X^1\Sigma_g^+) + h\nu$	4.5 (7)	2.3 (-10)	2.20
(2-27) $N_2(C^3\Pi_u) \longleftrightarrow N_2(B^3\Pi)g + h\nu$	2.0 (7)	9.0 (-2)	2.15, 2.20
(2-28) $N_2(B^3\Pi_g) \longleftrightarrow N_2(A^3\Sigma_u^+) + h\nu$	1.4 (5)	1.7 (-1)	2.15, 2.20
(2-29) $N_2(A^3\Sigma_u^+) \longleftrightarrow N_2(X^1\Sigma_g^+) + h\nu$	5.0 (-1)	5.5 (-11)	2.15, 2.20

* Numbers in parentheses mean powers of 10.

The rate coefficients for excitation by electron impact (Reactions 2-1 through 2-10 in Table 2.3) were determined from the measured cross sections, $\sigma(E)$, of Cartwright et al. (Ref. 2.6) using the relation (Ref. 2.7)

$$k' = 6.69 \times 10^{-9} T_e^{-3/2} \int_{E_0}^{\infty} \sigma(E) E e^{-E/T_e} dE \quad (2.3)$$

Here, the electron energy, E , the threshold energy for excitation, E_0 , and the electron temperature, T_e , are all in eV units and $\sigma(E)$ is in $\text{\AA}^2$. We performed the integrals in Equation 2.3 numerically for parametric values of T_e ranging from 0.1 to 3.0 eV. The results were fitted to the form 2.1 with T_e in $^{\circ}\text{K}$ and they were then reexpressed in the form 2.2 using the relationship between the excitation and deexcitation rate coefficients:

$$k' = \frac{g_n}{g_m} e^{-(E_n - E_m)/k_b T} k \quad (2.4)$$

where $E_n > E_m$ and k_b is Boltzmann's constant.

Reactions 2-20 through 2-29 in Table 2.3 are the radiation processes included in the model. For these, Columns 2 and 3 give the Einstein A coefficients (sec^{-1}) and the ρB factors (sec^{-1}) for sunlight conditions, respectively. The latter are based on the relation (Ref. 1.1)

$$\rho B = 5.4 \times 10^{-6} \frac{g_n}{g_m} A_{nm} \left(e^{2.391 \times 10^{-4} \tilde{\nu}_{nm}} - 1 \right)^{-1} \quad (2.5)$$

applicable for a 6000 $^{\circ}\text{K}$ sun subtending an angle of 6.8×10^{-5} ster at the earth. The Einstein coefficients in Table 2.3 are "generic" in the sense that no one value corresponds, necessarily, to precisely the value for a specific band of a given band system but, rather, is an average of the values in the referenced data for various bands of the band system.

DELTA-FACTOR EQUATIONS FOR N_2

As shown in Table 2.1, there are eleven states to determine delta factors for. Table 2.4 shows the notation used for these factors.

Table 2.4. Delta-factor notation for states of N₂.

State	Delta	State	Delta	State	Delta
X ¹ Σ _g ⁺	d ₀ ^{N₂}	b ¹ Π _u	d ₄ ^{N₂}	o ₃ ¹ Π _u	d ₈ ^{N₂}
A ³ Σ _u ⁺	d ₁ ^{N₂}	b' ¹ Σ _u ⁺	d ₅ ^{N₂}	e ₄ ¹ Π _u	d ₉ ^{N₂}
B ³ Π _g	d ₂ ^{N₂}	c ₃ ¹ Π _u	d ₆ ^{N₂}	c' ₅ ¹ Σ _u ⁺	d ₁₀ ^{N₂}
C ³ Π _u	d ₃ ^{N₂}	c' ₄ ¹ Σ _u ⁺	d ₇ ^{N₂}		

From the set of 29 reactions in Table 2.3, it is clear that in our model the seven excited singlet states are coupled only to the ground state, whereas the three triplet states are coupled to each other as well as to the ground state. Determination of the NLTE populations and delta factors for the singlet states, therefore, is simpler than that for the triplet states.

Singlet States

As an example, we now illustrate the procedure for determining the delta factor d_4 for the $b^1\Pi_u$ state. Determination of the delta factors for the other singlet states follows in a similar manner.

By reference to the reaction set in Table 2.3, the time rate of change of the concentration of state $b^1\Pi_u$ can be written as

$$\frac{d}{dt}[N_2(b^1\Pi_u)] = (k'_1 N_e + \rho B_{20})[N_2(X^1\Sigma_g^+)] - (k_1 N_e + A_{20})[N_2(b^1\Pi_u)] \quad (2.6)$$

The steady-state solution is

$$[N_2(b^1\Pi_u)]_{ss} = \frac{k'_1 N_2 + \rho B_{20}}{k_1 N_e + A_{20}} [N_2(X^1\Sigma_g^+)]_{ss} \quad (2.7)$$

where N_e is the electron density and subscripts on k , k' , A and ρB correspond to the reaction numbering in Table 2.3. By definition, the delta factor for state $b^1\Pi_u$ is given by the ratio

$$d_4^{N_2} \equiv \frac{[N_2(b^1\Pi_u)]_{ss}}{[N_2(b^1\Pi_u)]_{eq}} \quad (2.8)$$

where the denominator is the Boltzmann population of the state. But the Boltzmann population for state n of an arbitrary species Y can be expressed in the form

$$[Y(n)]_{eq} = [Y] g_n e^{-E_n/kT} / Q_e(T) \quad (2.9)$$

where $[Y]$ is the species concentration, E_n is the state energy and $Q_e(T)$, the electronic partition function, is defined as

$$Q_e(T) = \sum_{n=0}^{\infty} g_n e^{-E_n/kT} \quad (2.10)$$

Alternatively, in terms of the ground-state concentration $[Y(0)]$, Equation 2.9 can be written

$$[Y(n)]_{eq} = \frac{g_n}{g_0} [Y(0)]_{eq} e^{-E_n/kT} = \frac{g_n}{g_0} [Y(0)]_{eq} e^{-1.4388\tilde{\nu}_n/T} \quad (2.11)$$

where $\tilde{\nu}_n$ is the energy (cm^{-1}) of state n . Therefore, given the energy and statistical weight in Table 2.1 for state $b^1\Pi_u$, it follows that

$$[N_2(b^1\Pi_u)]_{eq} = 2[N_2(X^1\Sigma_g^+)]_{eq} e^{-145054.9/T} \quad (2.12)$$

Equations 2.7, 2.8 and 2.12 now lead to the result

$$d_4^{N_2} = \frac{1}{2} \left(\frac{k'_1 N_e + \rho B_{20}}{k_1 N_e + A_{20}} \right) e^{145054.9/T} d_0^{N_2} \quad (2.13)$$

Here, $d_0^{N_2}$ is the delta factor for the ground state:

$$d_0^{N_2} = [N_2(X^1\Sigma_g^+)]_{ss} / [N_2(X^1\Sigma_g^+)]_{eq} \quad (2.14)$$

Determination of $d_0^{N_2}$ will be addressed below.

In a similar fashion, we arrive at the following expressions for the delta factors for the remaining singlet states:

$$d_5^{N_2} = \left(\frac{k'_2 N_e + \rho B_{21}}{k_2 N_e + A_{21}} \right) e^{149180.2/T} d_0^{N_2} \quad (2.15)$$

$$d_6^{N_2} = \frac{1}{2} \left(\frac{k'_3 N_e + \rho B_{22}}{k_3 N_e + A_{22}} \right) e^{149832.7/T} d_0^{N_2} \quad (2.16)$$

$$d_7^{N_2} = \left(\frac{k'_4 N_e + \rho B_{23}}{k_4 N_e + A_{23}} \right) e^{150099.0/T} d_0^{N_2} \quad (2.17)$$

$$d_8^{N_2} = \frac{1}{2} \left(\frac{k'_5 N_e + \rho B_{24}}{k_5 N_e + A_{24}} \right) e^{152094.7/T} d_0^{N_2} \quad (2.18)$$

$$d_9^{N_2} = \frac{1}{2} \left(\frac{k'_6 N_e + \rho B_{25}}{k_6 N_e + A_{25}} \right) e^{166375.4/T} d_0^{N_2} \quad (2.19)$$

$$d_{10}^{N_2} = \left(\frac{k'_7 N_e + \rho B_{26}}{k_7 N_e + A_{26}} \right) e^{166720.9/T} d_0^{N_2} \quad (2.20)$$

Triplet States

As indicated above, the three triplet states are coupled to each other and to the ground state by Reactions 2-8 through 2-19 and 2-27 through 2-29 in Table 2.3. In steady state, the delta factor for each triplet can then be written as a linear combination of the deltas for the other two triplets and for the ground state. In particular, we find that the delta factors $d_1^{N_2}$, $d_2^{N_2}$ and $d_3^{N_2}$ are related to $d_0^{N_2}$, the ground-state delta factor, by means of the equations

$$\begin{aligned} \alpha_2 d_1^{N_2} - \alpha_3 d_2^{N_2} + 0. d_3^{N_2} &= \alpha_1 d_0^{N_2} \\ \beta_2 d_1^{N_2} - \beta_3 d_2^{N_2} + \beta_4 d_3^{N_2} &= -\beta_1 d_0^{N_2} \\ 0. d_1^{N_2} + \gamma_3 d_2^{N_2} - \gamma_4 d_3^{N_2} &= -\gamma_1 d_0^{N_2} \end{aligned} \quad (2.21)$$

where the coefficients are defined in Table 2.5.

Table 2.5. Definition of parameters in Equation 2.1.*.

$\alpha_1 = k_{16,17,18,19}[M] + k_{10}N_e e^{71586.5(\frac{1}{T} - \frac{1}{T_e})}$	$\beta_3 = k_{13,14,15}[M] + k_9 N_e + A_{28}$
$\alpha_2 = k_{16,17,18,19}[M] + k_{10}N_e + A_{29}$	$\beta_4 = A_{27}e^{-42690.2/T}$
$\alpha_3 = 2A_{28}e^{-13743.4/T}$	$\gamma_1 = k_{11,12}[M] + k_8 N_e e^{128020.1(\frac{1}{T} - \frac{1}{T_e})}$
$\beta_1 = k_{13,14,15}[M] + k_9 N_e e^{85329.9(\frac{1}{T} - \frac{1}{T_e})}$	$\gamma_3 = \rho B_{27}e^{42690.2/T}$
$\beta_2 = (\rho B_{28}/2)e^{13743.4/T}$	$\gamma_4 = k_{11,12}[M] + k_8 N_e + A_{27}$
* The notation $k_{16,17,18,19}[M]$ is short for $k_{16}[O_2] + k_{17}[NO] + k_{18}[O] + k_{19}[N]$. Similarly, $k_{13,14,15}[M]$ and $k_{11,12}[M]$ follow from Table 2.3.	

Equations 2.21 are readily solved for $d_1^{N_2}$, $d_2^{N_2}$ and $d_3^{N_2}$ to yield

$$\begin{aligned}
 d_1^{N_2} &= [\alpha_1(\beta_3\gamma_4 - \beta_4\gamma_3) + \alpha_3(\beta_1\gamma_4 + \beta_4\gamma_1)]d_0^{N_2}/D \\
 d_2^{N_2} &= [\alpha_1\beta_2\gamma_4 + \alpha_2(\beta_1\gamma_4 + \beta_4\gamma_1)]d_0^{N_2}/D \\
 d_3^{N_2} &= [\alpha_1\beta_2\gamma_3 + \alpha_2(\beta_3\gamma_1 + \beta_1\gamma_3) - \alpha_3\beta_2\gamma_1]d_0^{N_2}/D
 \end{aligned} \tag{2.22}$$

where

$$D = \alpha_2(\beta_3\gamma_4 - \beta_4\gamma_3) - \alpha_3\beta_2\gamma_4 \quad . \tag{2.23}$$

It remains to determine the ground-state delta factor, $d_0^{N_2}$.

Ground-State Delta Factor, $d_0^{N_2}$

In general, for an arbitrary species Y with electronic states $n = 0, 1, 2, \dots$, we can write

$$[Y(0)] + [Y(1)] + [Y(2)] + \dots = [Y] \quad . \tag{2.24}$$

Dividing both sides of the Equality 2.24 by $[Y(0)]_{eq}$, and recognizing that

$$\frac{[Y(n)]}{[Y(0)]_{eq}} = \frac{[Y(n)]}{[Y(n)]_{eq}} \cdot \frac{[Y(n)]_{eq}}{[Y(0)]_{eq}} = d_n \frac{g_n}{g_0} e^{-E_n/kT} , \quad (2.25)$$

we obtain

$$\sum_{n=0}^{\infty} d_n \frac{g_n}{g_0} e^{-E_n/kT} = \frac{[Y]}{[Y(0)]_{eq}} = \frac{Q_e(T)}{g_0} , \quad (2.26)$$

where use has been made of Equation 2.9. Rearrangement of Equation 2.26 leads to the result

$$d_0 = \frac{Q_e(T)}{g_0} - \sum_{n=1}^{\infty} d_n \frac{g_n}{g_0} e^{-E_n/kT} . \quad (2.27)$$

For N_2 , the lowest electronically-excited state ($A^3\Sigma_u^+$) lies about 6 eV above the ground (see Table 2.1) and so, for temperatures $\lesssim 10,000$ °K, the Boltzmann factors in the summation term on the right side of Equation 2.27 will be very small ($< 10^{-3}$). Moreover, for all cases considered, whether for $T_e = T$ where, it turns out, $d_n \ll 1$ or, for $T_e \gg T$ where $d_n \gg 1$, the Boltzmann factors are sufficiently small to render the summation term in Equation 2.27 small compared to the first term. Therefore, to good approximation,

$$d_0^{N_2} \approx \frac{Q_e^{N_2}(T)}{g_0} \quad (2.28)$$

where, for N_2 , $g_0 = 1$.

Finally, consider the electronic partition function, $Q_e^{N_2}(T)$.

Electronic Partition Function for N_2

We have used, in definition 2.10, the energies and statistical weights for the first 16 states of N_2 (up to and including $b^1\Pi_u$) (Reference 2.23) to compute values for $Q_e^{N_2}(T)$ for temperatures up to 35,000 °K. The results have been fitted, to within 2 percent, by the expression

$$Q_e^{N_2}(T) \approx 1 + 3.256 \times 10^{-4} T^{1.082} e^{-69981.8/T} \quad (2.29)$$

For temperatures up to at least 8000 °K, Equations 2.28 and 2.29 show that $d_0^{N_2} \approx 1$ is a good approximation.

SECTION 3

DELTA MODEL FOR N_2^+

STATES AND BAND SYSTEMS INCLUDED

Table 3.1 shows the electronic states of N_2^+ included in our model as well as their energies (Ref. 2.1) and statistical weights. The energies are given with respect to both the ground state of N_2 and the ground state of N_2^+ .

Table 3.1. States of N_2^+ included.

State ($v=0$)	Energy Relative to $N_2(X^1\Sigma_g^+)$ (cm^{-1}/eV)	Energy Relative to $N_2^+(X^2\Sigma_g^+)$ (cm^{-1}/eV)	Statistical Weight g
$X^2\Sigma_g^+$	12,5667.5/15.58	0.0/0.0	2
$A^2\Pi_u$	13,4683.9/16.70	9016.4/1.12	4
$B^2\Sigma_u^+$	15,1233.5/18.75	25,566.0/3.17	2
$C^2\Sigma_u^+$	19,0209.5/23.58	64,542.0/8.00	2

Table 3.2 shows the three band systems included. Each is a permitted transition. Also shown in Table 3.2 are the (0-0) band-origin wavelengths and wavenumbers of the systems and the approximate wavelength range over which each system radiates (Ref. 2.1).

EXCITATION/DEEXCITATION MECHANISMS

The mechanisms included for excitation and quenching of the electronic states of N_2^+ are electron and heavy-particle collisions, spontaneous radiation and sunlight absorption. Excitation of the excited states of N_2^+ is assumed to occur only by collisions on, and sunlight absorption by, $N_2^+(X^2\Sigma_g^+)$ ions. Excitation by collisions on $N_2(X^1\Sigma_g^+)$ is ignored because, at the temperatures of interest, the excitation rate is very small compared to that by collisions on $N_2^+(X^2\Sigma_g^+)$ ions. For example, even for a

Table 3.2. Band systems of N_2^+ included.

Band System	λ_{00} (Å)	$\tilde{\nu}_{00}$ (cm ⁻¹)	Wavelength Region (Å)
$A^2\Pi_u-X^2\Sigma_g^+$ (Meinel)	11,090.9	9,016.4	17,700-5,500
$B^2\Sigma_u^+-X^2\Sigma_g^+$ (1st Neg.)	3,911.4	25,566.0	5,870-2,860
$C^2\Sigma_u^+-X^2\Sigma_g^+$ (2nd Neg.)	1,549.4	64,542.0	2,230-1,270

temperature as high as 30,000 °K, we estimate that the excitation rate of $N_2^+(A^2\Pi_u)$ by $e + N_2^+(X^2\Sigma_g^+)$ will dominate that by $e + N_2(X^1\Sigma_g^+)$ for N_2 fractional ionization as small as 0.2 percent. The same will be true, to an even greater extent, for excitation of $B^2\Sigma_u^+$ and $C^2\Sigma_u^+$.

Table 3.3 shows the specific reactions included in our N_2^+ model and suggested values for the rate coefficients, the Einstein A coefficients and the ρB factors for sunlight.

Laboratory data on excitation of the electronic states of N_2^+ by electron impact on $N_2^+(X^2\Sigma_g^+)$ appear to be very limited. Most data refer to excitation by impact on $N_2(X^1\Sigma_g^+)$. However, the absolute cross-section measurements of Crandall and Kauppila (Ref. 3.6), for excitation of $N_2^+(B^2\Sigma_u^+)$ by electron impact on $N_2^+(X^2\Sigma_g^+)$, are within a factor of about 2 at threshold (3.17 eV) and within 20 percent at the highest energy (91 eV) of those derived from the Gaunt-factor formula of Seaton (Ref. 3.1) for dipole-allowed transitions. We have, therefore, chosen to use the Seaton formula for the cross sections, σ , to calculate the rate coefficients for Reactions 3-1 to 3-3 in Table 3.3. When the quantity $v\sigma$ is averaged over a Maxwellian velocity (v) distribution, the rate coefficient for excitation of state n from state m ($n > m$) can be written (Ref. 3.2) as

$$k_{mn} = 1.57 \times 10^{-6} \frac{f_{mn}}{T_e^{1/2} E_{ex}} G(E_{ex}/T_e) e^{-E_{ex}/T_e} \quad (\text{cm}^3 \text{ sec}^{-1}) \quad (3.1)$$

where the electron temperature, T_e , and excitation energy, $E_{ex} = E_n - E_m$, are in eV, $G(E_{ex}/T_e)$ is an effective Gaunt factor and f_{mn} is the absorption oscillator strength.

We find that the values for G tabulated in Ref. 3.2 for ionic species can be represented, to good approximation for $T_e \leq 5E_{ex}$, by the formula

Table 3.3. Excitation/deexcitation mechanisms and assumed rates for N_2^+ .

Reaction	a*	b	c	e	h	a'	d	Temperature (°K)	Reference
(3-1) $e + N_2^+(A^2\Pi_u) \longleftrightarrow e + N_2^+(X^2\Sigma_g^+)$	1.68 (-6)	-0.5	37,335.4	0.2	0.356	2.	12,972.7	300-30,000	see text
(3-2) $e + N_2^+(B^2\Sigma_u^+) \longleftrightarrow e + N_2^+(X^2\Sigma_g^+)$	1.72 (-5)	-0.5	105,864.4	0.2	0.356	1.	36,783.9	300-30,000	see text
(3-3) $e + N_2^+(C^2\Sigma_u^+) \longleftrightarrow e + N_2^+(X^2\Sigma_g^+)$	1.52 (-6)	-0.5	267,259.2	0.2	0.356	1.	92,862.7	300-30,000	see text
(3-4) $N_2^+(A^2\Pi_u) + N_2 \longleftrightarrow N_2^+(X^2\Sigma_g^+) + N_2$	7.5 (-10)	0.	0.	0.	1.	2.	12,972.7	~ 300	3.3
(3-5) $+O_2 \longleftrightarrow N_2^+(X^2\Sigma_g^+) + O_2$	6.2 (-10)	0.	0.	0.	1.	2.	12,972.7	~ 300	3.3
(3-6) $+N/O \longleftrightarrow N_2^+(X^2\Sigma_g^+) + N/O$	5.0 (-11)	0.	0.	0.	1.	2.	12,972.7	~ 300	3.4 (He)
(3-7) $N_2^+(B^2\Sigma_u^+) + N_2 \longleftrightarrow N_2^+(X^2\Sigma_g^+) + N_2$	1.0 (-9)	0.	0.	0.	1.	1.	36,783.9	300-500	3.5
(3-8) $+O_2 \longleftrightarrow N_2^+(X^2\Sigma_g^+) + O_2$	1.0 (-9)	0.	0.	0.	1.	1.	36,783.9	300-500	guess
(3-9) $+N/O \longleftrightarrow N_2^+(X^2\Sigma_g^+) + N/O$	1.0 (-10)	0.	0.	0.	1.	1.	36,783.9	300-500	guess
(3-10) $N_2^+(C^2\Sigma_u^+) + N_2/O_2 \longleftrightarrow N_2^+(X^2\Sigma_g^+) + N_2/O_2$	1.0 (-9)	0.	0.	0.	1.	1.	92,862.7	~ 300	guess
(3-11) $+N/O \longleftrightarrow N_2^+(X^2\Sigma_g^+) + N/O$	1.0 (-10)	0.	0.	0.	1.	1.	92,862.7	~ 300	guess
$A \text{ (sec}^{-1}\text{)}^*$									$\rho B \text{ (sec}^{-1}\text{)}^*$
$\longleftrightarrow$									
(3-12) $N_2^+(A^2\Pi_u) \longleftrightarrow N_2^+(X^2\Sigma_g^+) + h\nu$	6.04 (4)**			8.5 (-2)			2.1, 1.1		
(3-13) $N_2^+(B^2\Sigma_u^+) \longleftrightarrow N_2^+(X^2\Sigma_g^+) + h\nu$	1.41 (7)**			1.7 (-1)			2.1, 1.1		
(3-14) $N_2^+(C^2\Sigma_u^+) \longleftrightarrow N_2^+(X^2\Sigma_g^+) + h\nu$	2.0 (7)			2.1 (-5)			2.1, 3.7, 1.1		
* Numbers in parentheses mean powers of 10.									
** Based on $\sum_v A_{0v}$ from Reference 2-1.									

$$G_i(E_{ez}/T_e) = 0.2 + 0.356e^{-2.878E_{ez}/T_e} \quad (3.2)$$

Furthermore, utilizing the relationship between oscillator strength and Einstein A coefficient (Ref. 3.8)

$$f_{mn} = \frac{mc}{8\pi^2 e^2} \frac{g_n}{g_m} \frac{A_{nm}}{\tilde{\nu}_{nm}^2} \quad (3.3)$$

and expressing T_e in $^{\circ}K$, we can write Equation 3.1 as

$$k_{mn} = \frac{2.53 \times 10^{-3}}{T_e^{1/2} E_{ez}} \frac{g_n}{g_m} \frac{A_{nm}}{\tilde{\nu}_{nm}^2} \left(0.2 + 0.356e^{-33397.8E_{ez}/T_e} \right) e^{-11604.5E_{ez}/T_e} \quad (3.4)$$

where E_{ez} is in eV. From detailed balance, the deexcitation rate coefficient, k_{nm} , is given by

$$k_{nm} = \frac{g_m}{g_n} e^{11604.5E_{ez}/T_e} k_{mn} \quad (3.5)$$

so that

$$k_{nm} = \frac{2.53 \times 10^{-3}}{T_e^{1/2} E_{ez}} \frac{A_{nm}}{\tilde{\nu}_{nm}^2} \left(0.2 + 0.356e^{-33397.8E_{ez}/T_e} \right) (\text{cm}^3 \text{ sec}^{-1}) \quad (3.6)$$

Given the form of Expression 3.5, we write the deexcitation rate coefficients 3-1 through 3-3 (Table 3.3) as

$$k = a T_e^b (d + h e^{-c/T_e}) \quad (3.7)$$

and the corresponding excitation rates as

$$k' \equiv \frac{g_n}{g_m} e^{-11604.5E_{ez}/T_e} k = a' e^{-c'/T_e} k \quad (3.8)$$

The parameter values in Equations 3.7 and 3.8, for Reactions 3-1 to 3-3, follow from Equation 3.6 and the energy, wavenumber and Einstein A values shown in Tables 3.1, 3.2 and 3.3.

It is difficult to assign a temperature range for validity of the rate coefficients for the first three reactions in Table 3.3. However, to the extent that the theoretical cross sections are reasonably good, especially for electron energies $\lesssim 15$ eV, the rate coefficients should be valid over a wide temperature range, including the one shown in Table 3.3.

For quenching by heavy particles (Reactions 3-4 through 3-11 in Table 3.3), we have found very little data in the literature. The limited data for the $A^2\Pi_u$ and $B^2\Sigma_u^+$ states, at near room temperatures, is contained in the references shown in Table 3.3. The rate shown for quenching of $A^2\Pi_u$ by N and O atoms is an estimate based on quenching by He atoms. The quenching rates shown for the $C^2\Sigma_u^+$ state are assumed to be the same as those for the $B^2\Sigma_u^+$ state.

The Einstein A coefficients in Table 3.3 for the Meinel and First Negative Bands (Reactions 3-12 and 3-13) are taken to be the sum of those connecting the $v' = 0$ vibrational state to the collection of vibrational states v'' of $X^2\Sigma_g^+$. For the Second Negative Bands, the Einstein values are less certain, but the value adopted should be good to within a factor of about 4. The ρB factors for sunlight are based on Equation 2.5 using the parameter values in Tables 3.1 and 3.2.

DELTA-FACTOR EQUATIONS FOR N_2^+

Table 3.4 shows the delta-factor notation used for the states of N_2^+ .

Table 3.4. Delta-factor notation for states of N_2^+ .

State	$X^2\Sigma_g^+$	$A^2\Pi_u$	$B^2\Sigma_u^+$	$C^2\Sigma_u^+$
Delta	$d_0^{N_2^+}$	$d_1^{N_2^+}$	$d_2^{N_2^+}$	$d_3^{N_2^+}$

From the set of 14 reactions in Table 3.3, we see that each of the three excited states is coupled only to the ground state of N_2^+ . Determination of their delta factors, therefore, is straightforward. It follows a procedure similar to that described

in the previous section for $d_4^{N_2}$ in which we solve the steady-state rate equations for the excited-state populations in terms of the ground-state population. The results are as follows:

$$\begin{aligned}
 d_1^{N_2^+} &= \left(\frac{k_1 N_e e^{12972.7(1/T - 1/T_e)} + k_{4,5,6}[M] + \frac{\rho B_{12}}{2} e^{12972.7/T}}{k_1 N_e + k_{4,5,6}[M] + A_{12}} \right) d_0^{N_2^+} \\
 d_2^{N_2^+} &= \left(\frac{k_2 N_e e^{36783.9(1/T - 1/T_e)} + k_{7,8,9}[M] + \rho B_{13} e^{36783.9/T}}{k_2 N_e + k_{7,8,9}[M] + A_{13}} \right) d_0^{N_2^+} \\
 d_3^{N_2^+} &= \left(\frac{k_3 N_e e^{92862.7(1/T - 1/T_e)} + k_{10,11}[M] + \rho B_{14} e^{92862.7/T}}{k_3 N_e + k_{10,11}[M] + A_{14}} \right) d_0^{N_2^+}
 \end{aligned} \tag{3.9}$$

where, for the ground-state delta factor, we use the approximation (compare Equation 2.28)

$$d_0^{N_2^+} \approx \frac{Q_e^{N_2^+}(T)}{g_{N_2^+}(X)} \tag{3.10}$$

Finally, from the electronic partition-function definition (2.10), using the ground and first four excited states $A^2\Pi_u$, $B^2\Sigma_u^+$, $D^2\Pi$, and $C^2\Sigma_u^+$, we arrive at the result

$$d_0^{N_2^+} \approx 1 + 2e^{-12972.7/T} + e^{-36783.9/T} + 2e^{-75057.9/T} + e^{-92862.7/T} \tag{3.11}$$

From this expression, we can infer that $d_0^{N_2^+}$ begins to depart significantly from unity only above about 5000 °K.

SECTION 4

DELTA MODEL FOR O₂

STATES AND BAND SYSTEMS INCLUDED

The O₂ molecule is a weak light emitter because transitions between most of its low-lying states are strongly forbidden. The exception is the $B^3\Sigma_u^- - X^3\Sigma_g^-$ transition that gives rise to the Schumann-Runge (S.R.) bands that span the region 5350-1750 Å (Ref. 4.1).

These are the only bands considered here. Because only the one electronically-excited state of O₂ is involved, we expand our delta-factor determinations to include vibrational states $v' = 0$ to 20 of the $B^3\Sigma_u^-$ state.

Table 4.1 shows some parameter values for the 0-0 band of the S.R. system. Energies for vibrational states of $B^3\Sigma_u^-$ up to $v' = 20$ and wavenumbers for associated band systems are given in terms of equations cited below.

Table 4.1. State and band-system parameters for O₂.

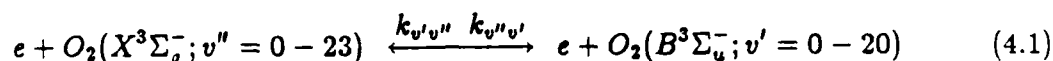
State ($v=0$)	Energy (cm ⁻¹ /eV)	Statistical Weight g	Band System	λ_{00} (Å)	$\tilde{\nu}_{00}$ (cm ⁻¹)	Wavelength Region (Å)
$X^3\Sigma_g^-$	0.0/0.0	3	$B^3\Sigma_u^- - X^3\Sigma_g^-$ (S.R.)	2026.01	49358.15	5350-1750
$B^3\Sigma_u^-$	49358.17/6.12	3				

EXCITATION/DEEXCITATION MECHANISMS

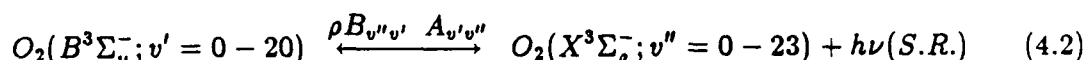
The mechanisms included for excitation and quenching of the $B^3\Sigma_u^-$ state are electron collisions, spontaneous radiation and sunlight absorption. We have found no data in the literature on quenching by heavy particles and so exclude the process from further consideration. However, with a radiative lifetime of typically about 40

ns, one would not expect such collisions to be effective in quenching $B^3\Sigma_u^-$ above about 40 km in the atmosphere.

The electron excitation/deexcitation reactions included in our delta model are



and the radiative processes are



where $k_{v''v'}$ and $k_{v'v''}$ denote rate coefficients for excitation and deexcitation, respectively, and $A_{v'v''}$ and $\rho B_{v'v''}$ are the usual Einstein A coefficients and ρB factors. Note that we include excitation/deexcitation of 21 vibrational states of $B^3\Sigma_u^-$ and 24 vibrational states of the ground state $X^3\Sigma_g^-$. The electron and radiative processes will now be considered separately.

Electron Excitation/Deexcitation Rate Coefficients

There is a dearth of data in the literature on the electron-excitation process 4.1 involving bound vibrational states of the electronic state $B^3\Sigma_u^-$. Most cross-section measurements and calculations (see, for example, References 4.2 and 4.3, respectively) include the absorption continuum which accounts for nearly all the transition probability. For example, the total electronic absorption oscillator strength, f_{el} , for the $X \rightarrow B$ transition is about 0.162 (Ref. 4.4) whereas, for transitions to bound states, $\sum_{v'} f_{0v'} \approx 0.00034$ (Ref. 4.5). The vibrational states of $B^3\Sigma_u^-$ above $v' = 2$ are highly predissociated. The only data on electron-impact cross sections to bound states of $B^3\Sigma_u^-$ we can find are some theoretical results of Garrett et al. (Ref. 4.6) for electron energies up to 25 eV. They calculated cross sections for the transitions $v'' \rightarrow \sum_{v'} v'$ for $v'' = 0, 1$ and 2. We have compared these cross sections with those derived from the Seaton formula (Ref. 3.1) for dipole-allowed transitions and find that the two results agree to within a factor of about 2. For this reason we will use the Seaton cross sections and the excitation rate coefficients for Reactions 4.1 derived from them.

The rate coefficients based on the Seaton cross sections are represented by Equation 3.1. In the present case, the Gaunt factor, G , appearing in Equation 3.1 is

that for neutral species. From the tabulated values for G given in Reference 3.2 we find, to good approximation for $T_e \leq 3.3E_{ez}$, the relation

$$G_n(E_{ez}/T_e) = 0.066(T_e/E_{ez})^{1/2} e^{0.4106(T_e/E_{ez})^{0.548}} \quad (4.3)$$

where T_e and E_{ez} are in eV. Equations 3.1 and 4.3, with T_e in $^{\circ}\text{K}$ and $E_{ez} \equiv \tilde{\nu}_{v',v''}$ in cm^{-1} , lead to the result

$$k_{v',v''} = 0.754 \frac{f_{v''v'}}{\tilde{\nu}_{v',v''}^{3/2}} e^{0.3366(T_e/\tilde{\nu}_{v',v''})^{0.548}} e^{-hc\tilde{\nu}_{v',v''}/k_b T_e} \quad (\text{cm}^3 \text{sec}^{-1}) \quad (4.4)$$

where $\tilde{\nu}_{v',v''}$ are the band-origin wavenumbers of the S.R. bands and, numerically, $hc/k_b = 1.4388 \text{ cm}^{\circ}\text{K}$.

The band wavenumbers are determined from the relation (Ref. 2.2)

$$\tilde{\nu}_{v',v''} = \tilde{\nu}(B^3\Sigma_u^-; v') - \tilde{\nu}(X^3\Sigma_g^-; v'') \quad (4.5)$$

where the energies (cm^{-1}) of the upper and lower states are given, respectively, by

$$\tilde{\nu}(B^3\Sigma_u^-; v') = \tilde{\nu}_e + \omega'_e(v' + 1/2) - \omega'_e x'_e(v' + 1/2)^2 + \omega'_e y'_e(v' + 1/2)^3 \quad (4.6)$$

and

$$\tilde{\nu}(X^3\Sigma_g^-; v'') = \omega''_e(v'' + 1/2) - \omega''_e x''_e(v'' + 1/2)^2 + \omega''_e y''_e(v'' + 1/2)^3 + \omega''_e z''_e(v'' + 1/2)^4 \quad (4.7)$$

Values (cm^{-1}) that we adopt for the electronic and vibrational parameters in Equations 4.6 and 4.7 are (Ref. 2.23):

$$\tilde{\nu}_e = 49793.28; \omega'_e = 709.31; \omega'_e x'_e = 10.65; \omega'_e y'_e = -0.139$$

$$\omega''_e = 1580.193; \omega''_e x''_e = 11.981; \omega''_e y''_e = 0.04747; \omega''_e z''_e = -0.001273$$

As for the absorption oscillator strengths for the S.R. bands in Equation 4.4, we use the relation (Ref. 4.4)

$$f_{v''v'} = 2.36 \times 10^{-8} q_{v''v'} \tilde{\nu}_{v''v'} \quad (4.8)$$

where $q_{v''v'}$ is the Franck-Condon factor connecting the upper and lower states. For these Franck-Condon factors, we adopt the results of Harris et al. (Ref. 4.5) that provide values for v' up to 20 and v'' up to 23.

Einstein A Coefficients and ρB Factors

The Einstein A coefficient connecting vibrational state v' of $B^3\Sigma_u^-$ with vibrational state v'' of $X^3\Sigma_g^-$ is related to the band wavenumber and oscillator strength through Equation 3.3. Numerically, this relationship can be written

$$A_{v''v'} = 0.667 \frac{g_{v''}}{g_{v'}} \tilde{\nu}_{v''v'} f_{v''v'} \quad (4.9)$$

Values of $A_{v''v'}$ for the S.R. bands can be determined from Equations 4.5 through 4.9 given the statistical weight factors in Table 4.1 that yield $g_{v''}/g_{v'} = 1$.

The ρB factors for excitation of the S.R. bands by sunlight absorption are determined from Equation 2.5 using the $A_{v''v'}$ and $\tilde{\nu}_{v''v'}$ values established above.

DELTA-FACTOR EQUATIONS FOR O_2

Given the rate coefficients and optical parameters described above, we are now in a position to formulate steady-state equations to determine delta factors for the states $O_2(B^3\Sigma_u^-; v' = 0 - 20)$. For simplicity of notation, we will hereafter denote the upper states as $O_2(B; v')$ and the lower states as $O_2(X; v'')$.

By equating the production and destruction rates of state $O_2(B; v')$, we arrive at the steady-state population

$$[O_2(B; v')]_{ss} = \frac{\sum_{v''=0}^{\infty} (N_e k_{v''v'} + \rho B_{v''v'}) [O_2(X; v'')]_{ss}}{\sum_{v''=0}^{\infty} (N_e k_{v''v'} + A_{v'v''})} \quad (4.10)$$

Here $k_{v'v''}$, the rate coefficient for electron deexcitation of $O_2(B; v')$, is given in terms of the excitation rate coefficient $k_{v''v'}$ by the detailed-balance relation

$$k_{v'v''} = \frac{g_{v'}}{g_{v''}} e^{(E(B; v') - E(X; v''))/k_b T_e} k_{v''v'} \quad (4.11)$$

where the statistical-weight ratio is unity and the state energies, E , are in ergs.

Next, since the Boltzmann population of $O_2(B; v')$ can be written as

$$[O_2(B; v')]_{eq} = [O_2(X; v'')]_{eq} e^{-(E(B; v') - E(X; v''))/k_b T} \quad (4.12)$$

and since the delta factor for $O_2(B; v')$ is defined as

$$\delta_{O_2(B; v')} \equiv \frac{[O_2(B; v')]_{ss}}{[O_2(B; v')]_{eq}} \quad (4.13)$$

Equations 4.10 through 4.13 can be combined to yield the result

$$\delta_{O_2(B; v')} = \frac{\sum_{v''=0}^{\infty} [(N_e k_{v''v'} + \rho B_{v''v'}) \delta_{O_2(X; v'')} e^{hc\tilde{\nu}_{v'v''}/k_b T}]}{\sum_{v''=0}^{\infty} (N_e k_{v''v'} e^{hc\tilde{\nu}_{v'v''}/k_b T_e} + A_{v'v''})} \quad (4.14)$$

Here, $\delta_{O_2(X; v'')}$, the delta factor for vibrational state v'' of the ground electronic state, is defined by the ratio

$$\delta_{O_2(X; v'')} \equiv \frac{[O_2(X; v'')]_{ss}}{[O_2(X; v'')]_{eq}} \quad (4.15)$$

This ratio can be reduced by writing the $O_2(X;v'')$ population as the product of the total $O_2(X)$ population, $[O_2(X)]$, and the probability, $P(v'')$, that vibrational state v'' is occupied. Thus,

$$\delta_{O_2(X;v'')} = \frac{[O_2(X)]_{ss}}{[O_2(X)]_{eq}} \frac{P_{ss}(v'')}{P_{eq}(v'')} \quad (4.16)$$

We next assume that, in steady state, the vibrational states are Boltzmann populated so that $P_{ss}(v'') = P_{eq}(v'')$. This is a reasonable assumption in view of the fact that O_2 is an infrared-inactive molecule for which radiative transitions between vibrational states of its ground electronic state are forbidden. Equation 4.16 now reduces to

$$\delta_{O_2(X;v'')} \approx \frac{[O_2(X)]_{ss}}{[O_2(X)]_{eq}} \equiv \delta_{O_2(X)} \equiv d_0^{O_2} \quad (4.17)$$

where the notation $d_0^{O_2}$ for the ground-state delta factor conforms with that employed in Sections 2 and 3 for N_2 and N_2^+ , respectively.

For $d_0^{O_2}$, we again invoke the approximation 2.28 even though, for O_2 , it is less valid than it is for N_2 . This is because the first two electronically-excited states of oxygen ($a^1\Delta_g$ and $b^1\Sigma_g^+$) lie only about 1 and 1.6 eV, respectively, above the ground state and so the summation terms in Equation 2.27 are not so negligibly small. Thus, the approximation 2.28 will yield an upper limit to the true value of $d_0^{O_2}$. The key ingredient in Equation 2.28 is the electronic partition function for O_2 that can be calculated from Equation 2.10 given the energy and statistical weights of the states. We have used the first 9 excited states of O_2 (up to $e'^3\Delta_{2u}$ at 9.29 eV), with parameter values given in Reference 2.23, to calculate $Q_e^{O_2}/g_0$ as a function of temperature to 12,000 °K. The results can be fitted, to within about 3 percent, by the expression

$$d_0^{O_2} \approx 1 + 1.336 \times 10^{-2} T^{0.445} e^{-10309.1/T} \quad (4.18)$$

The values for $d_0^{O_2}$ begin to depart significantly from unity only above about 5000 °K.

The deita factors for $O_2(B; v' = 0 - 20)$ can now be determined from Equations 4.14, 4.17 and 4.18 given the parameter expressions in the previous subsection. The summations in Equation 4.14 are performed up to $v'' = 23$ only.

SECTION 5

DELTA MODEL FOR NO

STATES AND BAND SYSTEMS INCLUDED

Table 5.1 shows the electronic states of *NO* included in our model together with their energies (Ref. 2.3) and statistical weights. There is spin-orbit splitting of the $^2\Pi$ states into $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ that have slightly different energies. Similarly, $^2\Delta$ is split into $^2\Delta_{3/2}$ and $^2\Delta_{5/2}$. However, to within the accuracy of the present model, we can ignore these fine-structure splittings. Where distinction is made in Reference 2.23, we have used the energies of the $^2\Pi_{1/2}$ states.

Table 5.1. States of NO included.

State	Energy ($v=0$) (cm^{-1}/eV)	Statistical Weight g
$X^2\Pi$	0.0/0.0	4
$A^2\Sigma^+$	43,965.7/5.45	2
$B^2\Pi$	45,913.6/5.69	4
$C^2\Pi$	52,126/6.46	4
$D^2\Sigma^+$	53,084.7/6.58	2
$B'^2\Delta$	60,364.2/7.48	4
$E^2\Sigma^+$	60,628.8/7.52	2

Table 5.2 shows the band systems included together with the (0-0) band-origin wavelengths and wavenumbers of the systems and the approximate range of wavelengths over which each system radiates. All band systems are electric-dipole allowed.

EXCITATION/DEEXCITATION MECHANISMS

The processes included here for excitation and quenching of the excited electronic states are electron and heavy-particle collisions, spontaneous radiation and sunlight absorption. Table 5.3 shows the specific reactions incorporated in our model

Table 5.2. Band systems of NO included.

Band System	λ_{00} ($\text{\AA}$)	$\tilde{\nu}_{00}$ (cm^{-1})	Wavelength Region ($\text{\AA}$)
$A^2\Sigma^+-X^2\Pi$ (gamma)	2274.5	43,965.7	1600-2700
$B^2\Pi-X^2\Pi$ (beta)	2178.0	45,913.6	1800-4000
$C^2\Pi-X^2\Pi$ (delta)	1918.4	52,126	1650-2600
$C^2\Pi-A^2\Sigma^+$ (Heath)	12,254	8160.3	11,800-12,300
$D^2\Sigma^+-X^2\Pi$ (epsilon)	1883.8	53,084.7	1600-2300
$D^2\Sigma^+-A^2\Sigma^+$ (Feast 1)	10,966	9119.0	9200-11,500
$B'^2\Delta-X^2\Pi$ (beta prime)	1656.6	60,364.2	1500-2300
$E^2\Sigma^+-X^2\Pi$ (gamma prime)	1649.4	60,628.8	1500-2000
$E^2\Sigma^+-A^2\Sigma^+$ (Feast 2)	6001.3	16,663.1	5970-6002
$E^2\Sigma^+-C^2\Pi$	11,761	8502.8	11,700-12,200
$E^2\Sigma^+-D^2\Sigma^+$ (Feast-Heath)	13,255	7544.1	12,500-13,300

along with suggested values for the rate coefficients, Einstein A coefficients and ρB factors for sunlight. The deexcitation (forward) rate coefficients in Table 5.3 are expressed in the form

$$k = a e^{bT^{0.546}} \quad (\text{cm}^3 \text{sec}^{-1}) \quad (5.1)$$

and the excitation (reverse) rates are

$$k' = a' e^{-c'/T} k \quad (\text{cm}^3 \text{sec}^{-1}) \quad (5.2)$$

The quenching data available for our purposes leaves much to be desired. For quenching by heavy particles, only room-temperature data seem to be available and often the quenching products are not determined in the experiments. When these products are unknown, the reverse (excitation) reactions cannot be allowed for properly. Moreover, for certain states, especially $B'^2\Delta$ and, to a lesser degree, $E^2\Sigma^+$, the data are very fragmentary.

Table 5.3. Excitation/deexcitation mechanisms and assumed rates for states of NO.

	Reaction	a*	b*	a'	c'	Temperature (°K)	Reference
(5-1)	$e + NO(A^2\Sigma^+) \rightarrow e + NO(X^2\Pi)$	9.6 (-11)	9.66 (-4)	0.5	65119	300-30,000	see text
(5-2)	$e + NO(B^2\Pi) \rightarrow e + NO(X^2\Pi)$	9.5 (-13)	9.17 (-4)	1.0	71652	300-30,000	see text
(5-3)	$e + NO(C^2\Pi) \rightarrow e + NO(X^2\Pi)$	3.5 (-10)	8.93 (-4)	1.0	75349	300-30,000	see text
(5-4)	$e + NO(D^2\Sigma^+) \rightarrow e + NO(X^2\Pi)$	4.8 (-10)	8.56 (-4)	0.5	81291	300-30,000	see text
(5-5)	$e + NO(B'^2\Delta) \rightarrow e + NO(X^2\Pi)$	5.1 (-11)	8.00 (-4)	1.0	91938	300-30,000	see text
(5-6)	$e + NO(E^2\Sigma^+) \rightarrow e + NO(X^2\Pi)$	1.7 (-10)	7.97 (-4)	0.5	92658	300-30,000	see text
(5-7)	$NO(A^2\Sigma^+) + N_2 \rightarrow$ products + O_2 + NO	1.4 (-13) 1.5 (-10) 2.0 (-10)	0 0 0	- - -	- - -	~ 300 ~ 300 ~ 300	5.1 to 5.3 5.1 to 5.5, 5.32 5.2, 5.5 to 5.8
(5-8)	+ $CO_2 \rightarrow$ products	3.8 (-10)	0	-	-	~ 300	5.1, 5.2, 5.5
(5-9)	+ $H_2O \rightarrow$ products	7.7 (-10)	0	-	-	~ 300	5.1, 5.5, 5.32
(5-10)	$NO(X^2\Pi) + N_2(A^3\Sigma_u^+) \rightarrow NO(A^2\Sigma^+) + N_2(X^1\Sigma_g^+)$ $NO(X^2\Pi) + N_2(A^3\Sigma_u^+) \rightarrow NO(B^2\Pi) + N_2(X^1\Sigma_g^+)$ $NO(B^2\Pi) + N_2 \rightarrow$ products + O_2 + NO	6.9 (-11) 3.0 (-12) 7.2 (-12) 5.4 (-11) 2.0 (-10) 1.3 (-10)	0 0 0 0 0 0	- - - - - -	- - - - - -	~ 300 ~ 300 ~ 300 ~ 300 ~ 300 ~ 300	2.17 5.9 5.10, 5.32 5.10, 5.32 5.8, 5.10, 5.32 5.32, 5.33
(5-11)	+ $H_2O \rightarrow$ products	3.7 (-11)	0	0.33	3763	~ 300	2.17
(5-12)	$NO(C^2\Pi) + N_2(X^1\Sigma_g^+) \rightarrow NO(X^2\Pi) + N_2(A^3\Sigma)$ $NO(C^2\Pi) + N_2 \rightarrow NO(A^2\Sigma^+) + N_2$	6.0 (-10) 5.0 (-10)	0 0	- -	- -	~ 300 ~ 300	5.11 5.2, 5.7
(5-13)	+ $O_2 \rightarrow$ products	4.5 (-11)	0	-	-	~ 300	5.2, 5.12, 5.13
(5-14)	+ $NO \rightarrow$ products + CO_2	4.3 (-10) 5.0 (-10) 6.3 (-10)	0 0 0	- - -	- - -	~ 300 ~ 300 ~ 300	5.2 5.2, 5.7 5.2
(5-15)	+ $NO \rightarrow$ products + CO_2	1.4 (-11)	0	-	-	~ 300	5.14
(5-16)	$NO(B'^2\Delta) + N_2 \rightarrow$ $NO(E^2\Sigma^+) + N_2 \rightarrow$ products	5.0 (-11)	0	-	-	~ 300	5.15, 5.16

* Numbers in parentheses mean powers of 10.

** $k_{deex} = ae^{bT^{0.546}}$; $k_{e,z} = a'e^{-c'/T}k_{deex}$

Table 5.3. Excitation/deexcitation mechanisms and assumed rates for states of NO (Continued).

	Reaction	$A(\text{sec}^{-1})^*$	$\rho B(\text{sec}^{-1})^*$	Reference
(5-17)	$NO(A^2\Sigma^+) \rightarrow NO(X^2\Pi) + h\nu$	1.7 (6)	9.2 (-5)	See text
(5-18)	$NO(B^2\Pi) \rightarrow NO(X^2\Pi) + h\nu$	2.3 (4)	8.4 (-7)	See text
(5-19)	$NO(C^2\Pi) \rightarrow NO(X^2\Pi) + h\nu$	1.0 (7)	2.0 (-4)	See text
(5-20)	$NO(D^2\Sigma^+) \rightarrow NO(X^2\Pi) + h\nu$	1.8 (7)	6.6 (-5)	See text
(5-21)	$NO(B'^2\Delta) \rightarrow NO(X^2\Pi) + h\nu$	3.0 (6)	3.8 (-6)	See text
(5-22)	$NO(E^2\Sigma^+) \rightarrow NO(X^2\Pi) + h\nu$	1.0 (7)	5.5 (-6)	See text
(5-23)	$NO(C^2\Pi) \rightarrow NO(A^2\Sigma^+) + h\nu$	1.0 (7)	1.8 (1)	See text
(5-24)	$NO(D^2\Sigma^+) \rightarrow NO(A^2\Sigma^+) + h\nu$	1.3 (7)	8.0 (0)	See text
(5-25)	$NO(E^2\Sigma^+) \rightarrow NO(A^2\Sigma^+) + h\nu$	9.3 (5)	9.4 (-2)	See text
(5-26)	$NO(E^2\Sigma^+) \rightarrow NO(C^2\Pi) + h\nu$	2.9 (5)	1.2 (-1)	See text
(5-27)	$NO(E^2\Sigma^+) \rightarrow NO(D^2\Sigma^+) + h\nu$	1.6 (7)	1.7 (1)	See text
* Numbers in parentheses mean powers of 10.				

Electron-Impact Excitation/Deexcitation

For electron-impact excitation of the states, the only absolute cross-section data we have found in the literature pertain to certain bands of the gamma system (Ref. 5.17) and to the (4,0) band of the beta prime system (Ref. 5.18). To see if it is reasonable for us to use Equations 3.1 and 4.3, based on the Seaton cross sections (Ref. 3.1), to calculate the excitation rate coefficients, we compared the results obtained from the Seaton formula for the $\gamma(1,0)$ and $\gamma(1,5)$ bands with those calculated using Equation 2.3 and the cross sections in Reference 5.17. In both cases, the rate coefficients agree to within a factor of 2 for electron temperatures above about 3000 °K. For this reason, we have adopted Equations 3.1 and 4.3 for determination of the excitation rate coefficients 5.1 through 5.6 in Table 5.3.

When Equations 3.1 and 4.3 are combined, we can write the electron-excitation rate coefficients in the form

$$k_{ex} = 1.04 \times 10^{-6} \frac{\bar{f}}{\bar{E}^{3/2}} e^{2.478 \times 10^{-3} (T_e/\bar{E}_{ex})^{0.546}} e^{-11604.5 \bar{E}_{ex}/T_e} \quad (5.3)$$

where $\bar{f}$ is the average absorption oscillator strength connecting the ground state and electronically-excited state, $\bar{E}_{ex}$ is the average excitation energy (eV) and T_e is the electron temperature (°K). We define the average oscillator strength and excitation energy by the relations

$$\bar{f} = \sum_{v'=0}^{\infty} f_{0v'} q_{v'0} \quad (5.4)$$

$$\bar{E}_{ex} = \bar{\nu}/8065.48 \quad (5.5)$$

$$\bar{\nu} = \sum_{v'=0}^{\infty} \tilde{\nu}_{v'0} q_{v'0} \quad (5.6)$$

where $q_{v'0}$ is the Franck-Condon factor (Ref. 5.19) connecting the $v'' = 0$ vibrational state of the ground electronic state with the v' vibrational state of the excited electronic state and Equation 5.5 is the relation between the excitation energy, $\bar{E}_{ex}$, in eV units and $\bar{\nu}$ in cm^{-1} . To be more precise, the sums in Equations 5.4 and 5.6 should also be performed over v'' with appropriate weighting of the ground vibrational-state populations. However, measured oscillator strengths reported in the literature refer

mainly to $f_{0v'}$. Moreover, the values of $f_{0v'}$ we have found are usually restricted to $v' \leq 5$. Therefore, the actual Franck-Condon values used in Equations 5.4 and 5.6 are normalized ones that sum to unity over the range $v' = 0$ to v'_{max} rather than over the range $v' = 0$ to ∞ . The first six entries in Table 5.4 show the values for $\bar{f}$ and

Table 5.4. Average excitation energy and electronic-absorption oscillator strengths for NO transitions.

Transition	$\bar{E}_{ex}$ (eV)	$\bar{\nu}$ (cm ⁻¹)	$\bar{f}$	Reference
$A^2\Sigma^+ - X^2\Pi$	5.612	4.526 (4)	6.08 (-4)	5.20, 5.21
$B^2\Pi - X^2\Pi$	6.174	4.980 (4)	1.40 (-5)	5.22, 5.23
$C^2\Pi - X^2\Pi$	6.493	5.237 (4)	5.50 (-3)	5.24
$D^2\Sigma^+ - X^2\Pi$	7.005	5.650 (4)	4.30 (-3)	5.25
$B' ^2\Delta - X^2\Pi$	7.923	6.390 (4)	1.10 (-3)	5.18, 5.26
$E^2\Sigma^+ - X^2\Pi$	7.985	6.440 (4)	1.86 (-3)	5.15, 5.19
$C^2\Pi - A^2\Sigma^+$	-	8.160 (3)	4.55 (-1)	5.27 to 5.31
$D^2\Sigma^+ - A^2\Sigma^+$	-	9.119 (3)	2.40 (-1)	5.27, 5.31
$E^2\Sigma^+ - A^2\Sigma^+$	-	1.663 (4)	5.00 (-3)	5.31
$E^2\Sigma^+ - C^2\Pi$	-	8.503 (3)	3.00 (-3)	5.31
$E^2\Sigma^+ - D^2\Sigma^+$	-	7.544 (3)	4.10 (-1)	5.31

$\bar{E}_{ex}$ adopted for the various transitions and used in Equation 5.3 to compute the excitation rate coefficients. The remaining entries in Table 5.4, corresponding to "hot band" transitions, give values for $\bar{\nu} = \bar{\nu}_{00}$ from Table 5.2 and, for $\bar{f}$, values averaged over those reported in the indicated references.

Heavy-Particle-Impact Excitation/Deexcitation

Reactions 5-7 through 5-16 pertain to collisions with heavy particles. With the exception of Reactions 5-8, 5-9 and the reverse of 5-11, they all refer to quenching of the excited states. As indicated above, most measurements have been made at or near room temperature and the products of the reactions are usually not known. Therefore, application of the principle of detailed balance to the quenching rate coefficients to obtain the excitation rate coefficients, under the assumption that the states are quenched to the ground, is hazardous. Consequently, we have omitted the reverse

(excitation) processes except in the case of Reaction 5-11. These omissions, together with the adoption of temperature-independent rate coefficients for heavy-particle collisions, may be significant, particularly at high temperatures. However, the effect of these approximations is somewhat mitigated by the fact that the electron excitation/deexcitation collisions, described above, tend to dominate the heavy-particle collisions at high temperatures.

The measured rate coefficients are often sensitive to the particular vibrational state considered. In Table 5.3, the assigned values represent averages over those reported in the references shown in the last column.

Radiation Parameters

Entries 5-17 through 5-27 in Table 5.3 show the assumed Einstein A coefficients and the associated ρB factors for sunlight absorption. The A coefficients were calculated from Equation 3.3 using the $\bar{\nu}$ and $\bar{f}$ values in Table 5.4 and the ρB values were calculated from Equation 2.5.

DELTA-FACTOR EQUATIONS FOR NO

Table 5.5 shows the delta-factor notation used for the states of NO.

Table 5.5. Delta-factor notation for states of NO.

State	Delta	State	Delta
$X^2\Pi$	d_0^{NO}	$D^2\Sigma^+$	d_4^{NO}
$A^2\Sigma^+$	d_1^{NO}	$B'^2\Delta$	d_5^{NO}
$B^2\Pi$	d_2^{NO}	$E^2\Sigma^+$	d_6^{NO}
$C^2\Pi$	d_3^{NO}		

From Table 5.3 it is clear that, in our scheme, states A, C, D and E are coupled to each other and to the ground, whereas states B and B' are uncoupled except to the ground. In the following discussion we treat first the uncoupled states and then the coupled states.

States $B^2\Pi$ and $B'^2\Delta$

Determination of the delta factors for the $B^2\Pi$ and $B'^2\Delta$ states follows a procedure similar to that described in Section 2 for $d_4^{N_2}$. We solve the steady-state rate equations for the excited-state populations in terms of the ground-state population. The procedure is straightforward; only the results are presented here. They are as follows.

$$d_2^{NO} = \frac{[(k'_2 N_e + \rho B_{18})e^{71652/T} + 3 k_9 [N_2] d_1^{N_2} / Q_e^{N_2}] d_0^{NO}}{k_2 N_e + k_{10} [M] + A_{18}} \quad (5.7)$$

$$d_5^{NO} = \frac{(k'_5 N_e + \rho B_{21})e^{91938/T} d_0^{NO}}{k_5 N_e + k_{15} [N_2] + A_{21}}, \quad (5.8)$$

where $d_1^{N_2}$ is given by Equation 2.22, $Q_e^{N_2}$ by Equation 2.29 and

$$k_{10} [M] = k_{10} (N_2) [N_2] + k_{10} (O_2) [O_2] + k_{10} (NO) [NO] + k_{10} (H_2O) [H_2O] \quad (5.9)$$

The parameter numbering in Equations 5.7 through 5.9 follows that in Table 5.3.

For d_0^{NO} , the ground-state delta factor, we invoke an approximation analogous to 2.28 and write

$$d_0^{NO} \approx Q_e^{NO}(T) / g_{NO}(X^2\Pi) \quad (5.10)$$

Given the partition-function definition 2.10, the average state energies (cm^{-1}) in Table 5.4 and statistical weights in Table 5.1, Equation 5.10 becomes

$$d_0^{NO} \approx 1 + 0.5 e^{-65119/T} + e^{-71652/T} + e^{-75349/T} + 0.5 e^{-81291/T} \quad (5.11)$$

where the summation in Equation 2.10 is taken over the first 5 states. From Equation 5.11, we find that d_0^{NO} begins to depart significantly from unity only for $T > 15,000^\circ\text{K}$. Thus, for most applications of interest, $d_0^{NO} \approx 1$ is an excellent approximation.

States $A^2\Sigma^+$, $C^2\Pi$, $D^2\Sigma^+$ and $E^2\Sigma^+$

As mentioned above, these four states are coupled to each other as well as to the ground and values for their delta factors require simultaneous solution of four linear steady-state equations that are easily derived from the reaction set in Table 5.3. In particular, we find that the delta factors d_1^{NO} , d_3^{NO} , d_4^{NO} and d_6^{NO} are related to d_0^{NO} and to each other by the set of equations

$$b_1 d_1^{NO} - b_2 d_3^{NO} - b_3 d_4^{NO} - b_4 d_6^{NO} = b_5 d_0^{NO} \quad (5.12)$$

$$b_6 d_1^{NO} - b_7 d_3^{NO} + 0. d_4^{NO} + b_8 d_6^{NO} = -b_9 d_0^{NO} \quad (5.13)$$

$$b_{10} d_1^{NO} + 0. d_3^{NO} - b_{11} d_4^{NO} + b_{12} d_6^{NO} = -b_{13} d_0^{NO} \quad (5.14)$$

$$b_{14} d_1^{NO} + b_{15} d_3^{NO} + b_{16} d_4^{NO} - b_{17} d_6^{NO} = -b_{18} d_0^{NO} \quad (5.15)$$

where the coefficients are defined as follows:

$$b_1 = k_1 N_e + k_7 [M] + A_{17} + \rho B_{23} + \rho B_{24} + \rho B_{25}$$

$$b_2 = 2(k_{12} [N_2] + A_{23}) e^{-10230/T}$$

$$b_3 = A_{24} e^{-16172/T}$$

$$b_4 = A_{25} e^{-27538/T}$$

$$b_5 = 2[(k_1' N_e + \rho B_{17}) e^{65119/T} + 3k_8 [N_2] d_1^{N_2} e^{-6467/T} / Q_e^{N_2}]$$

$$b_6 = \rho B_{23}$$

$$b_7 = 2(k_3 N_e + k_{11} [N_2] d_0^{N_2} / Q_e^{N_2} + k_{12} [N_2] + k_{13} [M] + A_{19} + A_{23} + \rho B_{26}) e^{-10230/T}$$

$$b_8 = A_{26} e^{-27538/T}$$

$$b_9 = 2[(k_3' N_e + \rho B_{19}) e^{65119/T} + 3k_{11}' [N_2] d_1^{N_2} e^{-6467/T} / Q_e^{N_2}]$$

$$b_{10} = \rho B_{24}$$

$$b_{11} = (k_4 N_e + k_{14} [M] + A_{20} + A_{24} + \rho B_{27}) e^{-16172/T}$$

$$b_{12} = A_{27} e^{-27538/T}$$

$$b_{13} = 2(k'_e N_e + \rho B_{20}) e^{65119/T}$$

$$b_{14} = \rho B_{25}$$

$$b_{15} = 2\rho B_{26} e^{-10230/T}$$

$$b_{16} = \rho B_{27} e^{-16172/T}$$

$$b_{17} = (k_6 N_e + k_{16}[N_2] + A_{22} + A_{26} + A_{27}) e^{-27538/T}$$

$$b_{18} = 2(k'_6 N_e + \rho B_{22}) e^{65119/T}$$

By reference to Table 5.3, the quantities $k_7[M]$, $k_{13}[M]$ and $k_{14}[M]$ appearing above are defined as:

$$k_7[M] = k_7(N_2)[N_2] + k_7(O_2)[O_2] + k_7(NO)[NO] + k_7(CO_2)[CO_2] + k_7(H_2O)[H_2O]$$

$$k_{13}[M] = k_{13}([N_2] + [NO])$$

$$k_{14}[M] = k_{14}(N_2)[N_2] + k_{14}(O_2)[O_2] + k_{14}(NO)[NO] + k_{14}(CO_2)[CO_2]$$

The delta-factor solutions to Equations 5.12 through 5.15 are:

$$\begin{aligned} d_1^{NO} = & \{b_2[b_9(b_{11}b_{17} - b_{12}b_{16}) + b_8(b_{13}b_{16} + b_{11}b_{18})] + b_{15}[b_3(b_9b_{12} - b_8b_{13}) \\ & + b_{11}(b_4b_9 - b_5b_8)] + b_7[b_5(b_{11}b_{17} - b_{12}b_{16}) + b_{13}(b_4b_{16} + b_3b_{17}) \\ & + b_{18}(b_3b_{12} + b_4b_{11})]\} d_0^{NO} / D \end{aligned} \quad (5.16)$$

$$\begin{aligned} d_3^{NO} = & \{b_6[b_5(b_{11}b_{17} - b_{12}b_{16}) + b_{13}(b_3b_{17} + b_4b_{16}) + b_{18}(b_3b_{12} + b_4b_{11})] + b_9[b_1(b_{11}b_{17} \\ & - b_{12}b_{16}) - b_{10}(b_3b_{17} + b_4b_{16}) - b_{14}(b_3b_{12} + b_4b_{11})] + b_8[b_1(b_{13}b_{16} + b_{11}b_{18}) \\ & + b_{10}(b_5b_{16} - b_3b_{18}) + b_{14}(b_5b_{11} + b_3b_{13})]\} d_0^{NO} / D \end{aligned} \quad (5.17)$$

$$\begin{aligned} d_4^{NO} = & \{b_{10}[b_2(b_9b_{17} + b_8b_{18}) + b_7(b_5b_{17} + b_4b_{18}) + b_{15}(b_4b_9 - b_5b_8)] \\ & - b_{13}[b_1(b_8b_{15} - b_7b_{17}) + b_6(b_2b_{17} + b_4b_{15}) + b_{14}(b_2b_8 + b_4b_7)] \\ & + b_{12}[b_1(b_7b_{18} + b_9b_{15}) - b_6(b_2b_{18} - b_5b_{15}) + b_{14}(b_2b_9 + b_5b_7)]\} d_0^{NO} / D \end{aligned} \quad (5.18)$$

$$\begin{aligned} d_6^{NO} = & \{b_6[b_{15}(b_3b_{13} + b_5b_{11}) - b_2(b_{11}b_{18} + b_{13}b_{16})] + b_7[b_1(b_{11}b_{18} + b_{13}b_{16}) \\ & - b_{10}(b_3b_{18} - b_5b_{16}) + b_{14}(b_3b_{13} + b_5b_{11})] + b_9[b_2(b_{10}b_{16} + b_{11}b_{14}) \\ & - b_{15}(b_3b_{10} - b_1b_{11})]\} d_0^{NO} / D \end{aligned} \quad (5.19)$$

where

$$\begin{aligned} D = & b_{10}[b_3(b_8b_{15} - b_7b_{17}) - b_{16}(b_4b_7 + b_2b_8)] - b_{11}[b_1(b_8b_{15} - b_7b_{17}) \\ & + b_2(b_8b_{14} + b_6b_{17}) + b_4(b_8b_{15} + b_7b_{14})] - b_{12}[b_7(b_1b_{16} + b_3b_{14}) \\ & + b_6(b_3b_{15} - b_2b_{16})] \quad . \end{aligned} \quad (5.20)$$

SECTION 6

DELTA MODEL FOR NO⁺

STATES AND BAND SYSTEMS INCLUDED

The major band system of NO⁺, and the only one considered here, originates from the A¹Π-X¹Σ⁺ transition that gives rise to the Baer-Miescher (B.M.) bands in the vacuum UV. Because, as for O₂, only one electronically-excited state of NO⁺ is involved, we increase our delta-factor determinations to include vibrational states $v' = 0$ to 10 of the A¹Π state.

Table 6.1 shows some parameter values for the 0-0 band of the B.M. system. Energies for vibrational states of A¹Π up to $v' = 10$, and wavenumbers for associated band systems, are given by equations shown later in this section.

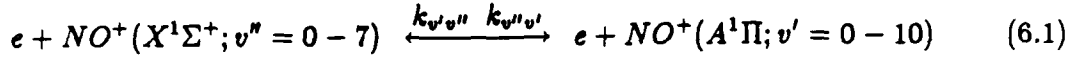
Table 6.1. States and band-system parameters for NO⁺.

State ($v=0$)	Energy (cm ⁻¹ /eV)	Statistical Weight g	Band System	λ_{00} (Å)	$\tilde{\nu}_{00}$ (cm ⁻¹)	Wavelength Region (Å)
X ¹ Σ ⁺	0.0/0.0	1	A ¹ Π - X ¹ Σ ⁺ (B.M.)	1368.3	73083.5	1200-1700
A ¹ Π	73083.5/9.06	2				

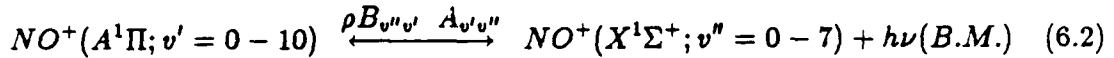
EXCITATION/DEEXCITATION MECHANISMS

The mechanisms included here for excitation and deexcitation of the A¹Π state are electron collisions, spontaneous radiation and sunlight absorption. We have found no data in the literature on quenching by heavy particles and, consequently, ignore the process here. The fact that thermal emission from NO⁺ will be significant only in regions of high NO⁺ concentration and, hence, of high electron density, together with the fact that electron excitation/deexcitation by electrons is relatively more efficient than that by heavy particles, should be ample justification for omission of the latter process.

The electron excitation and quenching reactions included in this delta model are



and the radiative processes included are



where, again, $k_{vv''}$ and $k_{v''v'}$ denote the rate coefficients for electron-impact excitation and deexcitation, respectively, and $A_{v'v''}$ and $\rho B_{v''v'}$ are the Einstein A coefficients and ρB factors, respectively. Note that Reactions 6.1 and 6.2 connect 8 vibrational states of the ground state, $X^1\Sigma^+$, with 11 vibrational states of $A^1\Pi$. As addressed again below, this limitation in the number of vibrational states v' and v'' considered corresponds to the size limitation of the Franck-Condon-factor array we have found in the literature for the Baer-Miescher system.

Electron Excitation/Deexcitation Rate Coefficients

In the absence of experimental data on cross sections or rate coefficients for Reactions 6.1, we again resort to use of the Seaton cross sections embodied in Equation 3.6 for the deexcitation rate coefficients. If, in this equation, we replace the excitation energy, $E_{ez}(eV)$, by its equivalent

$$E_{ez} \equiv \tilde{\nu}_{v',v''}/8065.479 \quad (6.3)$$

and recognize that, in our case,

$$A_{nm} = A_{n,v';m,v''} \equiv A_{v'v''} \quad , \quad (6.4)$$

we arrive at the result

$$k_{v'v''} = \frac{20.44 A_{v'v''}}{\tilde{\nu}_{v',v''}^3 T_e^{1/2}} \left(0.2 + 0.356 e^{-4.14 \tilde{\nu}_{v',v''}/T_e} \right) \quad (6.5)$$

where T_e , the electron temperature, is in °K. From detailed balance, the excitation rate coefficient is given by

$$k_{v''v'} = 2k_{v'v''} e^{-hc\tilde{\nu}_{v'v''}/k_b T_e} \quad (6.6)$$

where the factor 2 is the statistical-weight ratio, $g_{A^1\Pi}/g_{X^1\Sigma^+}$, and k_b is Boltzmann's constant.

The band wavenumbers, $\tilde{\nu}_{v'v''}$, are determined from the relation (Ref. 2.2)

$$\tilde{\nu}_{v'v''} = \tilde{\nu}(A^1\Pi; v') - \tilde{\nu}(X^1\Sigma^+; v'') \quad (6.7)$$

where the energies (cm^{-1}) of the upper and lower states are given, respectively, by

$$\tilde{\nu}(A^1\Pi; v') \approx \tilde{\nu}_e + \omega'_e(v' + 1/2) - \omega'_e x'_e(v' + 1/2)^2 + \omega'_e y'_e(v' + 1/2)^3 \quad (6.8)$$

and

$$\tilde{\nu}(X^1\Sigma^+; v'') \approx \omega''_e(v'' + 1/2) - \omega''_e x''_e(v'' + 1/2)^2 + \omega''_e y''_e(v'' + 1/2)^3 \quad (6.9)$$

Values (cm^{-1}) adopted for the parameters in Equations 6.8 and 6.9 are (Ref. 2.23):

$$\tilde{\nu}_e = 73083.5; \omega'_e = 1601.93; \omega'_e x'_e = 20.207; \omega'_e y'_e = -0.2683$$

$$\omega''_e = 2376.42; \omega''_e x''_e = 16.262; \omega''_e y''_e = -0.01562 \quad .$$

Einstein A Coefficients and ρB Factors

The Einstein A coefficient connecting an upper state n, v' with a lower state m, v'' can be written in terms of the Frank-Condon factor, $q_{v'v''}$, as (Ref. 2.2)

$$A_{n,v';m,v''} = \frac{64\pi^4}{3h} \tilde{\nu}_{n,v';m,v''}^3 \frac{|P_{nm}^e|^2}{g_n} q_{v'v''} \quad , \quad (6.10)$$

where P_e^{nm} is the matrix element of the electric-dipole moment connecting the upper and lower electronic states. Thus, for a given band system, Equation 6.10 can be recast in the form

$$A_{n,v';m,v''} = K \tilde{\nu}_{n,v';m,v''}^3 q_{v'v''} \quad (6.11)$$

where K is independent of the vibrational quantum numbers. To determine the constant K for the B.M. band system, we utilize the result of Hesser (Ref. 6.1) in Equation 6.11:

$$\sum_{v''} A_{0v''} = 1.8 \times 10^7 \text{ (sec}^{-1}\text{)} \quad , \quad (6.12)$$

together with the wavenumbers from Equation 6.7 and Franck-Condon factors of Nicholls (Ref. 6.2), to establish the result

$$A_{v'v''} = 6.43 \times 10^{-8} \tilde{\nu}_{v'v''}^3 q_{v'v''} \quad . \quad (6.13)$$

The ρB factors for sunlight are again based on Equation 2.5 which, in the present case, becomes

$$\rho B_{v'v''} = 1.08 \times 10^{-5} A_{v'v''} (e^{2.391 \times 10^{-4} \tilde{\nu}_{v'v''}} - 1)^{-1} \quad . \quad (6.14)$$

DELTA-FACTOR EQUATIONS FOR NO⁺

Formulation of the equations to determine delta factors for the states NO⁺ ($A^1\Pi; v' = 0 - 10$) follows a procedure similar to that described in Section 4 for the states of O₂. In particular, the steady-state concentration of state ($A^1\Pi; v'$), in terms of that for state ($X^1\Sigma^+; v''$), is

$$[NO^+(A; v')]_{ss} = \frac{\sum_{v''=0}^{\infty} (N_e k_{v''v'} + \rho B_{v''v'}) [NO^+(X; v'')]_{ss}}{\sum_{v''=0}^{\infty} (N_e k_{v'v''} + A_{v'v''})} \quad , \quad (6.15)$$

while the equilibrium populations are related in the usual way by

$$[NO^+(A; v')]_{eq} = (g_{A^1\Pi}/g_{X^1\Sigma^+})[NO^+(X; v'')]_{eq} e^{hc\tilde{\nu}_{v',v''}/k_bT} \quad (6.16)$$

Since the delta factors are defined by the relation

$$\delta_{NO^+(A;v')} \equiv \frac{[NO^+(A; v')]_{ss}}{[NO^+(A; v')]_{eq}} \quad (6.17)$$

Equations 6.15 through 6.17 lead to the result

$$\delta_{NO^+(A;v')} = \frac{\frac{1}{2} \sum_{v''=0}^{\infty} (N_e k_{v',v''} + \rho B_{v'',v'}) \frac{[NO^+(X; v'')]_{ss}}{[NO^+(X; v'')]_{eq}} e^{hc\tilde{\nu}_{v',v''}/k_bT}}{\sum_{v''=0}^{\infty} (N_e k_{v',v''} + A_{v',v''})} \quad (6.18)$$

By analogy with Equation 4.16 for the case of O_2 , the ground-state population ratio in Equation 6.18 can be expressed as

$$\delta_{NO^+(X;v'')} \equiv \frac{[NO^+(X; v'')]_{ss}}{[NO^+(X; v'')]_{eq}} = \frac{[NO^+(X)]_{ss}}{[NO^+(X)]_{eq}} \cdot \frac{P_{ss}(v'')}{P_{eq}(v'')} = \delta_e(X) \delta_v(v'') \quad (6.19)$$

where $\delta(X)$ is the delta factor for the ground electronic state of NO^+ and $\delta_v(v'')$ is the delta factor for vibrational state v'' of the ground electronic state.

Since NO^+ is infrared active, it is generally incorrect to assume a Boltzmann-population distribution for the vibrational states v'' as we did in the case of O_2 . However, for temperatures above about 2000 °K or so, there is a simple approximation that can be adopted. In particular, it can be shown (Ref. 6.3) that the vibrational delta factors for states $v'' > 1$ can be represented by the geometric relation

$$\delta_v(v'') \approx \delta_1 \left(\frac{\delta_1}{\delta_0} \right)^{v''-1} \quad (6.20)$$

Here, δ_0 and δ_1 , the vibrational delta factors for the $v'' = 0$ and 1 states, respectively, of the ground electronic state, can be determined from the infrared Delta model (Refs. 1.1, 6.3, 6.4).

For $\delta_e(X)$, we adopt the usual approximation (2.28) which, in the present case, yields

$$\delta_e(X) \approx Q_e^{NO^+}(T) \quad (6.21)$$

Values for $Q_e^{NO^+}$, the electronic partition function for NO^+ , can be obtained from its definition (2.10). In the present case, by use of the lowest four excited states (Ref. 2.23), we can recast this definition in the form

$$Q_e^{NO^+}(T) \approx 1 + 3e^{-75090/T} + 6e^{-85234/T} + 6e^{-89032/T} + 3e^{-97435/T} \quad (6.22)$$

After combining Equations 6.18 through 6.21, we can write the final expression for the $NO^+(A^1\Pi; v' = 0 - 10)$ delta factors as

$$\begin{aligned} \delta_{NO^+(A;v')} = & \left[\delta_1 \sum_{v''=1}^{\infty} \left(N_e k_{v'v''} e^{1.4388\tilde{\nu}_{v',v''}(\frac{1}{T} - \frac{1}{T_e})} + \frac{\rho B_{v''v'}}{2} e^{1.4388\tilde{\nu}_{v',v''}/T} \right) \left(\frac{\delta_1}{\delta_0} \right)^{v''-1} \right. \\ & \left. + \left(N_e k_{v'0} e^{1.4388\tilde{\nu}_{v',0}(\frac{1}{T} - \frac{1}{T_e})} + \frac{\rho B_{0v'}}{2} e^{1.4388\tilde{\nu}_{v',0}/T} \right) \delta_0 \right] Q_e^{NO^+}(T) / \sum_{v''=0}^{\infty} (N_e k_{v'v''} + A_{v'v''}) \quad (6.23) \end{aligned}$$

In practice, because of limitations in size of the Franck-Condon array in Reference 6.2, the sums in Equation 6.23 are taken only over values of v'' up to 7.

SECTION 7

SOME NUMERICAL EXAMPLES

As mentioned earlier, the Delta models described in Sections 2 through 6 have been computerized with a main driver program DELTAVU and separate subroutines for each of the molecules included. In this section we present three numerical examples of delta factors calculated by code DELTAVU based on NORSE-code output of species concentrations and temperatures. In each example, results are given for both day and night conditions.

Table 7.1 shows delta factors at 1 sec in a cell at 200-km altitude, displaced 140 km horizontally from a MT-class burst at 200-km altitude. The species concentrations and temperatures input to DELTAVU are shown at the top of the table. NE denotes electron density (cm^{-3}) and T and TE are, respectively, the neutral and electron temperatures. The delta-factor notation for N_2 , N_2^+ and NO corresponds to that shown in Tables 2.4, 3.4 and 5.5, respectively. Notice that, in this case, the electron and neutral temperatures are equal.

Two observations are apparent from the results shown in Table 7.1. First, with the exception of d_1 , the delta factor for $N_2(A^3\Sigma_u^+)$, the delta factors are all very small compared to unity. This is because the radiation is truly collision limited. At the high altitude involved, collisional processes, even at 7292 °K, cannot populate the states fast enough to compete with their rapid depopulation by radiation. This results in state populations that are orders-of-magnitude less than their Boltzmann values. The exception occurs for $N_2(A^3\Sigma_u^+)$ that is metastable, with a lifetime of about 2 sec, for which its population/depopulation rates are controlled more by collisional processes than by radiative ones.

The second observation is simply that the delta factors for daylight conditions are larger than those for nighttime. This, of course, is due to the effectiveness of sunlight absorption in populating the states. The effect is particularly dramatic for the high-lying Rydberg states $c_3\ ^1\Pi_u$ and $c_4\ ^1\Sigma_u^+$ of N_2 (delta factors d_7 and d_8 , respectively) that have large transition probabilities to the ground and whose daytime populations are enhanced about four orders-of-magnitude over those at night.

Table 7.2 shows the results at 1 sec in a cell at 140-km altitude, directly above a MT-class burst at 90 km. Due to the lower altitude involved, the species concentrations are typically one-to-two orders of magnitude larger than those for the

case corresponding to Table 7.1 although the electron density is considerably lower. A more significant difference, however, is that the electron temperature is about six times larger than the neutral temperature. This difference manifests itself in an enormous increase in the magnitude of the delta factors. For example, from Table 7.2 we see that for the $c'_5 \ ^1\Sigma_u^+$ state of N_2 , the delta factor d_{10} has the value 2.81×10^{45} at night and 8.52×10^{51} in the day. The reasons for these very large numbers have to do with our definition of the deltas themselves and with the fact that, in the present case, most of the excitation is produced by electron impact. The steady-state population of the state, which forms the numerator of the delta-factor ratio (compare Equation 2.8 for the case of $N_2(b^1\Pi_u)$), is determined mainly by electrons at a temperature of 6438 °K, whereas the equilibrium (Boltzmann) population, which forms the denominator of the delta-factor ratio, is (by definition) determined by the neutral temperature of 1046 °K. For the $c'_5 \ ^1\Sigma_u^+$ state of N_2 , at an energy of 14.37 eV (see Table 2.1), the equilibrium population in the present case is 8.9×10^{-59} molecules cm^{-3} . As for the numerator of the delta-factor ratio, if there were no collision limiting, that is, if collisions denominated the excitation/deexcitation processes, then the steady-state population of $N_2(c'_5 \ ^1\Sigma_u^+)$ would equal its Boltzmann population at 6438 °K which, in the present case, has a value 8.44×10^{-1} molecules cm^{-3} . Thus, the ratio (delta factor) in this case would be 9.5×10^{57} . However, due to the large Einstein A coefficient for depopulation of the state by radiation to the ground state (Table 2.3, Reaction 2.26), collision limiting is very significant. The steady-state population is less than the Boltzmann population and the delta factors for day and night conditions are reduced, accordingly, by factors of 9×10^{-7} and 3×10^{-13} , respectively, from the value of 9.5×10^{57} to the values indicated above and in Table 7.2.

This example, illustrated by Table 7.2, serves to point out the importance of proper application of the delta factors in converting LTE emission values to NLTE emission values, especially when the electron and neutral temperatures differ. To obtain the proper conversion, it is necessary that the LTE emission be calculated using the neutral gas temperature, not the electron temperature.

Table 7.3 is an example showing delta factors calculated from NORSE-code output at 1 sec following a MT-class burst at 600 km. The air cell involved here is at 140-km altitude, displaced horizontally by 50 km from the burst point. In this case, although the burst and cell altitudes are quite different from those in Table 7.1, the delta factors are not greatly different in the two cases. The electron and neutral temperatures in Table 7.3 differ by less than 0.1 percent and so the situation with very large deltas that we saw in Table 7.2 does not arise here. For those states whose excitation rates are dominated by neutral collisions, the associated delta factors in Table 7.3 (d_1 , d_2 , d_3 for N_2 , N_2^+ and NO) are larger than they are in Table 7.1 where

the cell altitude is higher. Other differences arise due to the different temperatures and electron densities. However, the results presented in Table 7.3 are a further example of the effect of collision limiting in reducing the LTE emission from permitted electronic transitions in the visible and UV by typically 4 to 8 orders-of-magnitude at altitudes above about 100 km.

Table 7.1. Delta factors at 1 sec in a cell at 200-km altitude, horizontally displaced 140 km from a MT-class burst at 200-km altitude.

$N_2=2.50E+09$ $O_2=1.80E+08$ $NO=8.00E+06$ $CO_2=1.50E+06$ $H_2O=5.00E+04$ $N=1.00E+09$ $O=5.00E+09$ $NE=1.00E+09$ $T=7.292E+03$ $TE=7.292E+03$

DELTA FACTORS FOR ELECTRONIC STATES OF N_2 (DAY)

d0	d1	d2	d3	d4	d5	d6	d7	d8	d9	d10
1.00E+00	8.75E-01	8.78E-06	8.61E-08	8.50E-08	8.20E-08	6.89E-08	6.88E-08	6.34E-08	4.32E-08	4.35E-08

DELTA FACTORS FOR ELECTRONIC STATES OF N_2^+ (DAY)

d0	d1	d2	d3
1.34E+00	1.46E-04	6.71E-06	9.39E-07

DELTA FACTORS FOR $O_2(B \text{ triplet } \Sigma^+; v=0 \text{ to } 19)$ (DAY)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
2.05E-06	2.03E-06	1.93E-06	1.73E-06	1.53E-06	1.40E-06	1.36E-06	1.32E-06	1.25E-06	1.19E-06	1.17E-06

v=11	v=12	v=13	v=14	v=15	v=16	v=17	v=18	v=19	v=20
1.13E-06	1.09E-06	1.06E-06	1.07E-06	1.03E-06	1.02E-06	1.01E-06	1.00E-06	9.89E-07	9.82E-07

DELTA FACTORS FOR ELECTRONIC STATES OF NO (DAY)

d0	d1	d2	d3	d4	d5	d6
1.00E+00	2.55E-06	1.58E-06	4.07E-07	3.29E-07	3.90E-07	1.45E-07

DELTA FACTORS FOR $NO^+(A \text{ singlet } \Pi; v=0 \text{ to } 10)$ (DAY)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
3.16E-08	1.05E-07	2.34E-07	3.00E-07	3.56E-07	3.26E-07	3.04E-07	2.60E-07	1.62E-07	1.56E-07	1.24E-07

DELTA FACTORS FOR ELECTRONIC STATES OF N_2 (NIGHT)

d0	d1	d2	d3	d4	d5	d6	d7	d8	d9	d10
1.00E+00	7.28E-01	5.28E-06	8.61E-08	4.38E-09	1.08E-08	5.11E-12	2.40E-12	4.38E-10	7.97E-12	2.37E-11

DELTA FACTORS FOR ELECTRONIC STATES OF N_2^+ (NIGHT)

d0	d1	d2	d3
1.34E+00	1.40E-04	4.18E-06	4.60E-07

DELTA FACTORS FOR $O_2(B \text{ triplet } \Sigma^+; v=0 \text{ to } 19)$ (NIGHT)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
3.15E-07	3.38E-07	3.24E-07	2.61E-07	1.92E-07	1.87E-07	1.54E-07	1.48E-07	1.31E-07	1.20E-07	1.17E-07

v=11	v=12	v=13	v=14	v=15	v=16	v=17	v=18	v=19	v=20
1.09E-07	1.00E-07	9.58E-08	9.74E-08	9.26E-08	9.06E-08	8.86E-08	8.71E-08	8.49E-08	8.37E-08

DELTA FACTORS FOR ELECTRONIC STATES OF NO (NIGHT)

d0	d1	d2	d3	d4	d5	d6
1.00E+00	3.42E-07	7.59E-07	2.79E-08	1.81E-08	1.88E-08	7.16E-09

DELTA FACTORS FOR $NO^+(A \text{ singlet } \Pi; v=0 \text{ to } 10)$ (NIGHT)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
1.03E-08	3.41E-08	7.63E-08	9.79E-08	1.17E-07	1.07E-07	1.00E-07	8.63E-08	5.42E-08	5.22E-08	4.18E-08

Table 7.2. Delta factors at 1 sec in a cell at 140-km altitude, directly above a MT-class burst at 90-km altitude.

N2=1.49E+11 O2=2.20E+10 NO=4.63E+08 CO2=1.09E+07 H2O=6.79E+02 N=5.24E+09 O=4.41E+10 NE=5.66E+07 T=1.046E+03 TE=6.438E+03

DELTA FACTORS FOR ELECTRONIC STATES OF N2 (DAY)

d0	d1	d2	d3	d4	d5	d6	d7	d8	d9	d10
1.00E+00	1.56E+23	1.63E+23	1.45E+36	3.11E+44	7.93E+45	1.33E+46	1.65E+46	7.75E+46	6.37E+51	8.52E+51

DELTA FACTORS FOR ELECTRONIC STATES OF N2+ (DAY)

d0	d1	d2	d3
1.00E+00	3.03E-01	2.38E+07	3.80E+26

DELTA FACTORS FOR O2(B triplet SIGMA u-; v=0 to 19) (DAY)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
1.44E+13	2.08E+14	1.88E+15	1.27E+16	6.67E+16	2.74E+17	1.01E+18	3.22E+18	9.33E+18	2.43E+19	5.67E+19

v=11	v=12	v=13	v=14	v=15	v=16	v=17	v=18	v=19	v=20
1.23E+20	2.45E+20	4.50E+20	8.00E+20	1.21E+21	1.79E+21	2.51E+21	3.29E+21	4.09E+21	4.81E+21

DELTA FACTORS FOR ELECTRONIC STATES OF NO (DAY)

d0	d1	d2	d3	d4	d5	d6
1.00E+00	7.11E+17	2.96E+19	8.18E+20	2.53E+22	1.88E+26	1.24E+26

DELTA FACTORS FOR NO+(A singlet PI; v=0 to 10) (DAY)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
3.35E+29	7.01E+30	9.37E+31	6.80E+32	4.34E+33	2.02E+34	9.00E+34	3.46E+35	9.16E+35	3.49E+36	1.03E+37

DELTA FACTORS FOR ELECTRONIC STATES OF N2 (NIGHT)

d0	d1	d2	d3	d4	d5	d6	d7	d8	d9	d10
1.00E+00	1.40E+23	1.15E+23	1.45E+36	6.10E+40	3.79E+42	8.44E+38	4.72E+38	1.82E+42	8.16E+44	2.81E+45

DELTA FACTORS FOR ELECTRONIC STATES OF N2+ (NIGHT)

d0	d1	d2	d3
1.00E+00	1.31E-01	1.07E+06	2.10E+24

DELTA FACTORS FOR O2(B triplet SIGMA u-; v=0 to 19) (NIGHT)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
2.33E+10	3.04E+11	2.52E+12	1.58E+13	7.77E+13	3.02E+14	1.06E+15	3.20E+15	8.91E+15	2.24E+16	5.04E+16

v=11	v=12	v=13	v=14	v=15	v=16	v=17	v=18	v=19	v=20
1.06E+17	2.06E+17	3.69E+17	6.40E+17	9.54E+17	1.39E+18	1.92E+18	2.49E+18	3.08E+18	3.59E+18

DELTA FACTORS FOR ELECTRONIC STATES OF NO (NIGHT)

d0	d1	d2	d3	d4	d5	d6
1.00E+00	1.13E+16	8.17E+18	8.91E+17	1.87E+19	9.89E+22	6.69E+22

DELTA FACTORS FOR NO+(A singlet PI; v=0 to 10) (NIGHT)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
1.44E+27	2.90E+28	3.74E+29	2.62E+30	1.62E+31	7.29E+31	3.17E+32	1.19E+33	3.06E+33	1.14E+34	3.30E+34

Table 7.3. Delta factors at 1 sec in a cell at 140-km altitude, horizontally displaced 50 km from a MT-class burst at 600-km altitude.

N2=5.43E+10 O2=3.05E+09 NO=3.72E+09 CO2=1.41E+04 H2O=5.01E+01 N=2.77E+10 O=3.47E+10 NE=3.80E+08 T=8.927E+03 TE=8.398E+03

DELTA FACTORS FOR ELECTRONIC STATES OF N2 (DAY)

d0	d1	d2	d3	d4	d5	d6	d7	d8	d9	d10
1.00E+00	1.64E+00	2.62E-05	1.08E-07	4.41E-09	7.80E-09	1.62E-09	1.60E-09	1.59E-09	6.85E-10	7.44E-10

DELTA FACTORS FOR ELECTRONIC STATES OF N2+ (DAY)

d0	d1	d2	d3
1.48E+00	1.17E-03	9.36E-06	4.87E-06

DELTA FACTORS FOR O2(B triplet SIGMA u-; v=0 to 19) (DAY)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
7.43E-07	7.44E-07	6.94E-07	5.85E-07	4.76E-07	4.55E-07	3.95E-07	3.79E-07	3.44E-07	3.19E-07	3.09E-07
v=11	v=12	v=13	v=14	v=15	v=16	v=17	v=18	v=19	v=20	
2.92E-07	2.74E-07	2.63E-07	2.66E-07	2.53E-07	2.48E-07	2.43E-07	2.40E-07	2.35E-07	2.32E-07	

DELTA FACTORS FOR ELECTRONIC STATES OF NO (DAY)

d0	d1	d2	d3	d4	d5	d6
1.00E+00	1.17E-05	3.50E-05	2.40E-07	4.80E-08	4.55E-08	1.63E-08

DELTA FACTORS FOR NO+(A singlet PI; v=0 to 10) (DAY)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
5.40E-09	1.77E-08	3.90E-08	4.93E-08	5.81E-08	5.28E-08	4.89E-08	4.16E-08	2.59E-08	2.47E-08	1.96E-08

DELTA FACTORS FOR ELECTRONIC STATES OF N2 (NIGHT)

d0	d1	d2	d3	d4	d5	d6	d7	d8	d9	d10
1.00E+00	1.48E+00	2.15E-05	1.08E-07	2.29E-09	6.12E-09	1.67E-11	8.26E-12	2.12E-10	2.31E-11	8.28E-11

DELTA FACTORS FOR ELECTRONIC STATES OF N2+ (NIGHT)

d0	d1	d2	d3
1.48E+00	1.17E-03	8.25E-06	4.82E-06

DELTA FACTORS FOR O2(B triplet SIGMA u-; v=0 to 19) (NIGHT)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
1.34E-07	1.44E-07	1.38E-07	1.11E-07	8.24E-08	8.00E-08	6.59E-08	6.37E-08	5.64E-08	5.15E-08	5.01E-08
v=11	v=12	v=13	v=14	v=15	v=16	v=17	v=18	v=19	v=20	
4.69E-08	4.33E-08	4.13E-08	4.20E-08	3.99E-08	3.91E-08	3.82E-08	3.76E-08	3.67E-08	3.61E-08	

DELTA FACTORS FOR ELECTRONIC STATES OF NO (NIGHT)

d0	d1	d2	d3	d4	d5	d6
1.00E+00	1.01E-05	3.14E-05	1.68E-07	7.59E-09	7.87E-09	2.99E-09

DELTA FACTORS FOR NO+(A singlet PI; v=0 to 10) (NIGHT)

v=0	v=1	v=2	v=3	v=4	v=5	v=6	v=7	v=8	v=9	v=10
3.85E-09	1.28E-08	2.88E-08	3.70E-08	4.42E-08	4.06E-08	3.82E-08	3.28E-08	2.06E-08	1.99E-08	1.59E-08

SECTION 8

COMMENTS AND RECOMMENDATIONS

By way of comment, we would like to re-emphasize certain points inferred from the foregoing sections. First, as in most models, assumptions and approximations have been made that limit the accuracy of the results in one way or another. Specifically, with respect to the wavelength dependence of the NLTE emission from a given band system of N_2 , N_2^+ and NO , the largest error probably stems from our assumption that all bands of the system have the same delta factor. That is, we have treated these three molecules as if they were vibrationless. To do otherwise, would involve a substantial expansion in the scope of the present model because of the large number of vibrational states of each electronic state for which delta factors would need to be provided. It seems to us that an expansion in scope such as this is not presently justified. This is mainly because the NORSE code is not designed to take advantage of this level of detail in converting LTE emission to NLTE emission. NORSE cannot distinguish contributions from each band of a given band system to the LTE emission in a specified wavenumber interval. Moreover, the required excitation/deexcitation rate coefficients connecting the upper and lower states of most bands of each system are not yet known.

How much error is introduced by this single delta-factor assumption for electronic states of N_2 , N_2^+ and NO ? It is hard to generalize, although some idea can perhaps be obtained by referring to the results in Tables 7.1 through 7.3 for the cases of O_2 and NO^+ . For O_2 , our model provides delta factors for 21 vibrational states of $B^3\Sigma_u^-$ and, for NO^+ , 11 vibrational states of $A^1\Pi$. In Tables 7.1 and 7.3, where the electron and neutral temperatures are nearly equal, the variation in the deltas over the vibrational states of O_2 is at most a factor of 4 while, for NO^+ , it is at most a factor of 10. For the case represented by Table 7.2, however, where the electron temperature is much greater than the neutral temperature, the variation in the deltas for O_2 and for NO^+ is several orders of magnitude. Therefore, depending on circumstances, it appears that the error resulting from the assumption that the deltas for all bands of a given band system are the same can range from small to very large. Large errors are likely to occur only when the electron and neutral temperatures differ significantly from one another.

Other sources of error include assumptions made on quenching rate coefficients for which no laboratory data are available. For electron-impact excitation of

the states, we have made liberal use of the Seaton formulas — an approximation that is accurate to within a factor of about 2 when compared with the limited laboratory data that do exist. As for quenching by heavy particles, reliable rate-coefficient data are harder to come by. Where no data were found, we omitted the process entirely rather than including it with a guess on its rate coefficient. Assessment of the impact of such omissions on the results would require a sensitivity study that we have not had time to perform.

A second comment that needs to be emphasized here relates to the delta-factor definition used in our models, and to the proper application of the deltas in converting the computed LTE emission to NLTE emission. The delta factor for each radiating state considered is defined as the ratio between the actual steady-state population of the state to its Boltzmann population — where the latter is evaluated at the neutral gas temperature. In view of this definition, it is very important that the LTE emission that we wish to convert to NLTE emission be computed using the neutral gas temperature. For cases where the neutral and electron temperatures are nearly equal, it clearly doesn't matter which is used. However, when the electron temperature greatly exceeds the neutral temperature, as in Table 7.2, then the calculated NLTE emission may be orders-of-magnitude too large if the electron temperature, rather than the neutral temperature, is used for determination of the LTE emission.

Finally, by way of recommendations for improvement and expansion of the present model, we suggest the following items.

(1) Addition of other species whose visible/UV radiation in a nuclear environment may be significant. Such species should include the atoms O and N and their corresponding ions O^+ and N^+ . Emission from the metastable states of these species has recently been added to NORSE, but thermal emission from their permitted states may also be important in high-temperature regions. Other species that should be considered for addition are CO , CO_2 , NO_2 and H_2O . As for O_3 , because of its low binding energy (1.05 eV), and hence propensity to dissociate at even moderate temperatures, it is unlikely to be an important thermal emitter in the visible/UV region except, possibly, under conditions similar to those corresponding to Table 7.2 where the neutral temperature is low and the electron temperature is high.

(2) Upgrading the rate coefficients is an obvious area where improvements can and should be done periodically. In this context, three items may be worth mentioning. First, the ρB factors for sunlight absorption in the present models are input as constants, independent of altitude. It is not difficult to allow for attenuation of sunlight by the intervening ambient atmosphere by introducing altitude-dependent values of ρB for each of the bands considered. Second, as new data on rate coefficients

for quenching reactions included in the present model become available, it is a simple matter to make the data changes in the appropriate subroutines, and this should be done. Beyond that, when data become available on processes not included in the current models, such as certain quenching reactions involving heavy particles, the appropriate models should be modified by adding the processes to the production- and destruction-rate terms for the states in question following the procedure outlined in the foregoing sections. Third, where laboratory data are lacking, it is probably worthwhile to perform sensitivity studies, using the codes developed here, to assess the importance of each reaction on the resulting delta factors. Such studies can be useful in helping to order the priorities of laboratory research programs.

(3) If future developments permit the NORSE code to distinguish the contributions to the LTE emission, in a given wavenumber interval, from the separate bands of each band system, then the way is open for expanding the present model to include delta factors for a whole array of vibrational states of each electronic state. This would provide for a much improved wavelength dependence of the NLTE visible/UV emission. As mentioned earlier, however, such a model would be rather unwieldy and, moreover, we would still be faced with the need to provide excitation/deexcitation rate coefficients for a large number of states for which laboratory data might largely be lacking. Nevertheless, for altitudes above about 100 km, where electron processes are likely to dominate, this need could perhaps be satisfied sufficiently by use of the Seaton approximation for rate coefficients that we employed to advantage in the present model. Thus, expansion of the model to include many more vibrational states is probably feasible if the need appears to warrant it.

SECTION 9

REFERENCES

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APPENDIX

FORTRAN LISTING OF PROGRAM DELTAVU AND ASSOCIATED SUBROUTINES

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PROGRAM DELTAVU
C THIS PROGRAM COMPUTES DELTA FACTORS FOR SELECTED ELECTRONIC STATES OF
C AIR MOLECULES AND IONS. ONLY ELECTRIC- DIPOLE ALLOWED TRANSITIONS ARE
C INCLUDED. THE STATES AND TRANSITIONS INCLUDED CORRESPOND, GENERALLY,
C TO THOSE IN THE AFAL CODE. THE MOLECULAR SPECIES INCLUDED ARE: N2,N2+,
C O2,NO AND NO+. WITH THE EXCEPTION OF O2 AND NO+, A SINGLE DELTA FACTOR IS
C COMPUTED FOR EACH ELECTRONIC STATE CONSIDERED--AND SO THE SAME DELTA
C FACTOR IS ASSUMED TO APPLY TO ALL VIBRATIONAL STATES OF A GIVEN ELECTR-
C ONIC STATE. THUS, IN CONVERTING LTE VISIBLE/UV EMISSION TO NLTE EMISSION,
C THE SAME DELTA FACTOR IS APPLIED TO ALL BANDS OF A GIVEN BAND SYSTEM.
C THE EXCEPTIONS ARE O2 AND NO+. FOR O2, SEPARATE DELTAS ARE COMPUTED
C FOR EACH OF THE VIBRATIONAL STATES 0,1,2,---,20 OF ELECTRONIC STATE
C O2(B tripletSigma u-) THAT GIVES RISE TO THE SCHUMANN-RUNGE BAND SYSTEM.
C FOR NO+, SEPARATE DELTAS ARE COMPUTED FOR EACH OF THE VIBRATIONAL STATES
C 0,1,2,---,10 OF ELECTRONIC STATE NO+(A singlet Pi) THAT GIVES RISE TO
C THE BAER-MIESCHER BAND SYSTEM.
      DIMENSION DN2(11),DN2P(4),DO2(21),DNO(7),DNOPI(11)
C SPECIES CONCENTRATIONS FOR N2,O2,NO,CO2,H2O,N,O,ELECTRONS.
      DATA XN2,O2,XNO,CO2,H2O,XN,O,XNE/1.49E11,2.20E10,4.63E8,1.09E7,
      1 6.79E2,5.24E9,4.41E10,5.66E7/
C NEUTRAL AND ELECTRON TEMPERATURES
C CAUTION !!!!! FOR MACHINES THAT ACCEPT NUMBERS ONLY SMALLER THAN ABOUT
C 10**38, OVERFLOWS IN SUBROUTINE DELN2 MAY OCCUR FOR TEMPERATURES < 1600
C (DEG. K) UNLESS DOUBLE PRECISION IS USED.
      DATA T,TE/1046.,6438./
C DO AND D1 ARE DELTA FACTORS FOR VIBRATIONAL STATES 0 AND 1 OF THE GROUND
C ELECTRONIC STATE OF NO+ AS DETERMINED BY THE INFRARED DELTA MODEL.
      DATA D0,D1/2.7,4.36E-3/
C DAY(K=1)/NIGHT(K=0) INDEX.
      K=0
      IF(K.EQ.1)WRITE(1,20) XN2,O2,XNO,CO2,H2O,XN,O,XNE,T,TE
      IF(K.EQ.1)WRITE(1,25)
      IF(K.EQ.0)WRITE(1,26)
      WRITE(1,30)
      CALL DELN2(XN2,O2,XNO,XN,O,XNE,T,TE,K,DN2)
      WRITE(1,40) (DN2(I),I=1,11)
      CALL DELN2P(XN2,O2,XN,O,XNE,T,TE,K,DN2P)
      IF(K.EQ.1)WRITE(1,45)
      IF(K.EQ.0)WRITE(1,46)
      WRITE(1,50)
      WRITE(1,55) (DN2P(I),I=1,4)
      CALL DELO2(XNE,T,TE,K,DO2)
      IF(K.EQ.1)WRITE(1,60)
      IF(K.EQ.0)WRITE(1,61)
      WRITE(1,65)
      WRITE(1,70) (DO2(I),I=1,11)

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```

WRITE(1,75)
WRITE(1,72) (D02(I),I=12,21)
IF(K.EQ.1)WRITE(1,80)
IF(K.EQ.0)WRITE(1,81)
WRITE(1,85)
CALL DELNO(XN2,O2,XNO,CO2,H2O,XNE,T,TE,DN2,K,DNO)
WRITE(1,90) (DNO(I),I=1,7)
IF(K.EQ.1)WRITE(1,95)
IF(K.EQ.0)WRITE(1,96)
WRITE(1,100)
CALL DELNOP(XNE,T,TE,K,DO,D1,DNOP)
WRITE(1,70)(DNOP(I),I=1,11)
20 FORMAT(5X,'N2='1PE8.2,' O2='1PE8.2,' NO='1PE8.2,' CO2='1PE8.2,' H2
10='1PE8.2,' N='1PE8.2,' O='1PE8.2,' NE='1PE8.2,' T='1PE9.3,' TE='1
2PE9.3/)
25 FORMAT(11X,'DELTA FACTORS FOR ELECTRONIC STATES OF N2 (DAY)')
26 FORMAT(11X,'DELTA FACTORS FOR ELECTRONIC STATES OF N2 (NIGHT)')
30 FORMAT(8X,'      d0      d1      d2      d3      d4
1 d5      d6      d7      d8      d9      d10')
40 FORMAT(9X,11(1PE10.2)/)
45 FORMAT(11X,'DELTA FACTORS FOR ELECTRONIC STATES OF N2+ (DAY)')
46 FORMAT(11X,'DELTA FACTORS FOR ELECTRONIC STATES OF N2+ (NIGHT)')
50 FORMAT(8X,'      d0      d1      d2      d3')
55 FORMAT(9X,4(1PE10.2)/)
60 FORMAT(11X,'DELTA FACTORS FOR O2(B triplet SIGMA u- ;v=0 to 19) (D
1AY)')
61 FORMAT(11X,'DELTA FACTORS FOR O2(B triplet SIGMA u- ;v=0 to 19) (N
1IGHT)')
65 FORMAT(8X,'      v=0      v=1      v=2      v=3      v=4
1v=5      v=6      v=7      v=8      v=9      v=10')
70 FORMAT(9X,11(1PE10.2)/)
72 FORMAT(9X,10(1PE10.2)/)
75 FORMAT(8X,'      v=11      v=12      v=13      v=14      v=15
1v=16      v=17      v=18      v=19      v=20')
80 FORMAT(11X,'DELTA FACTORS FOR ELECTRONIC STATES OF NO (DAY)')
81 FORMAT(11X,'DELTA FACTORS FOR ELECTRONIC STATES OF NO (NIGHT)')
85 FORMAT(8X,'      d0      d1      d2      d3      d4
1 d5      d6')
90 FORMAT(9X,7(1PE10.2)/)
95 FORMAT(11X,'DELTA FACTORS FOR NO+(A singlet PI;v=0 to 10) (DAY)')
96 FORMAT(11X,'DELTA FACTORS FOR NO+(A singlet PI;v=0 to 10) (NIGHT)')
100 FORMAT(8X,'      v=0      v=1      v=2      v=3      v=4
1v=5      v=6      v=7      v=8      v=9      v=10')
END

```

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SUBROUTINE DELN2(XN2,Q2,XNO,XN,O,XNE,T,TT,K,DN2)
C THIS SUBROUTINE COMPUTES DELTA FACTORS FOR 11 ELECTRONIC STATES OF N2.
  DIMENSION R(29),RP(29),DN2(11),A(19),B(19),C(19),D(19),F(19),
  1 AA(10),RB(10)
C ELECTRONIC PARTITION FUNCTION FOR N2.
  QEN2(X)=1.+3.*EXP(-71587.2/X)+6.*(EXP(-85330.6/X)+EXP(-85435.9/X))
  1 +3.*EXP(-94748.4/X)+EXP(-97463.3/X)+2.*(EXP(-99207.0/X)+EXP(-1031
  2 59.8/X))+5.*EXP(-112082.5/X)+6.*(EXP(-125319.5/X)+EXP(-128021.3/X
  3 ))+10.*EXP(-134096.2/X)+3.*EXP(-137800.4/X)+6.*EXP(-140432.0/X)+
  4 EXP(-142211.4/X)+2.*EXP(-145056.2/X)
C TWO-BODY RATE COEFFICIENTS FOR COLLISIONAL DEEXCITATION (Ith REACTION)
C ARE IN THE FORM: R(I)=A(I)*T**B(I)*EXP(-C(I)/T). THE RATE COEFFICIENTS
C FOR THE REVERSE (EXCITATION) REACTIONS ARE IN THE FORM: RP(I)=D(I)*
C EXP(-F(I)/T)*R(I). HERE, T MAY BE EITHER THE NEUTRAL OR THE ELECTRON
C TEMPERATURE.
  DATA A/2.18E-13,6.12E-11,1.59E3,5.85E4,1.78E-15,5.5E2,2.6E4,6.68E-
  1 9,1.2E-10,1.5E-13,1.E-11,2.8E-10,2.7E-11,1.1E-10,2.4E-10,4.6E-12,
  2 6.9E-11,2.1E-11,4.6E-7/
  DATA B/.861,.427,-2.469,-2.681,1.068,-2.469,-2.681,-.102,.2245,
  1 .8539,8*0.,-1.5/
  DATA C/385.1,6759.8,97547.3,101251.,-4454.7,92502.4,101251.6,
  1 3599.9,2297.1,-2225.5,9*0./
  DATA D/2.,1.,2.,1.,2.,2.,1.,6.,6.,3.,5*6.,4*3./
  DATA F/145054.9,149160.2,149832.7,150099.,152094.7,166375.4,
  1 166720.9,128020.1,85329.9,71586.5,2*128020.1,3*85329.9,4*71586.5/
C AA(I) ARE THE EINSTEIN "A" COEFFICIENTS (SEC-1) AND RB(I) ARE THE
C CORRESPONDING RHO*B FACTORS (SEC-1) FOR SUNLIGHT CONDITIONS.
  DATA AA/2*1.E8,1.4E8,1.E9,1.E8,6.2E7,4.5E7,2.E7,1.4E5,0.5/
  DATA RB/3.7E-8,9.3E-9,2.3E-8,7.9E-8,1.1E-8,6.6E-10,2.3E-10,9.E-2,
  1 .17,5.5E-11/
  DO 10 I=1,10
    R(I)=A(I)*TT**B(I)*EXP(-C(I)/TT)
    RP(I)=D(I)*EXP(-F(I)/TT)*R(I)
  10 CONTINUE
  DO 15 I=11,19
    R(I)=A(I)*T**B(I)*EXP(-C(I)/T)
    RP(I)=D(I)*EXP(-F(I)/T)*R(I)
  15 CONTINUE
  DO 20 I=20,29
    J=I-19
    R(I)=AA(J)
    RP(I)=FLOAT(K)*RB(J)
  20 CONTINUE
C DN2(1) IS THE DELTA FACTOR FOR THE GROUND ELECTRONIC STATE (X singlet
C SIGMA g+) OF N2. IT IS APPROXIMATELY EQUAL TO THE ELECTRONIC PARTITION
C FUNCTION.
  DN2(1)=QEN2(T)
  A1=(EXP(71586.5*(1./T-1./TT))*R(10)*XNE+R(16)*O2+R(17)*XNO+R(18)*O
  1 +R(19)*XN)*DN2(1)

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A2=R(10)*XNE+R(16)*O2+R(17)*XNO+R(18)*O+R(19)*XN+R(29)
A3=2.*R(28)*EXP(-13743.4/T)
B1=R(9)*XNE*EXP(85329.9*(1./T-1./TT))+R(13)*XN2+R(14)*O2+R(15)
1 *XNO)*DN2(1)
B2=RP(28)*EXP(13743.4/T)/2.
B3=R(9)*XNE+R(13)*XN2+R(14)*O2+R(15)*XNO+R(28)
B4=R(27)*EXP(-42690.2/T)
C1=R(8)*XNE*EXP(128020.1*(1./T-1./TT))+R(11)*XN2+R(12)*O2
1 *DN2(1)
C3=RP(27)*EXP(42690.2/T)
C4=R(8)*XNE+R(11)*XN2+R(12)*O2+R(27)
G=A2*(B3*C4-R(27)*RP(27))-A3*B2*C4
C THE DELTA FACTORS DN2(I) (I=2 TO 11) REFER, RESPECTIVELY, TO DELTAS FOR
C THE 5 VALENCE STATES: A triplet SIGMA ut, B triplet PI g, C triplet PI u,
C b singlet PI u, b' singlet SIGMA ut, AND THE 5 RYDBERG STATES: c3 singlet
C PI u, c4' singlet SIGMA ut, o3 singlet PI u, c4 singlet PI u, c5' singlet
C SIGMA ut.
DN2(2)=(A1*(B3*C4-R(27)*RP(27))+A3*(B1*C4+B4*C1))/G
DN2(3)=(A1*B2*C4+A2*(B1*C4+B4*C1))/G
DN2(4)=(A1*B2*C3+A2*(B3*C1+B1*C3)-R(28)*RP(28)*C1)/G
E=0.
C CAUTION!!!! FOR MACHINES THAT ACCEPT NUMBERS ONLY SMALLER THAN ABOUT
C 10**38, THE FOLLOWING LINES MAY PRODUCE OVERFLOW FOR TEMPERATURES < 1600
C (DEG. K) UNLESS DOUBLE PRECISION IS USED.
IF(K.EQ.1)E=EXP(145054.9/T+ALOG(.5*RB(1)))
DN2(5)=(R(1)*XNE*EXP(145054.9*(1./T-1./TT))+E)/(R(1)*XNE+R(20))
1 *DN2(1)
E=0.
IF(K.EQ.1)E=EXP(149160.2/T+ALOG(RB(2)))
DN2(6)=(R(2)*XNE*EXP(149160.2*(1./T-1./TT))+E)/(R(2)*XNE+R(21))
1 *DN2(1)
E=0.
IF(K.EQ.1)E=EXP(149832.7/T+ALOG(.5*RB(3)))
DN2(7)=(R(3)*XNE*EXP(149832.7*(1./T-1./TT))+E)/(R(3)*XNE+R(22))
1 *DN2(1)
E=0.
IF(K.EQ.1)E=EXP(150099./T+ALOG(RB(4)))
DN2(8)=(R(4)*XNE*EXP(150099.0*(1./T-1./TT))+E)/(R(4)*XNE+R(23))
1 *DN2(1)
E=0.
IF(K.EQ.1)E=EXP(152094.7/T+ALOG(.5*RB(5)))
DN2(9)=(R(5)*XNE*EXP(152094.7*(1./T-1./TT))+E)/(R(5)*XNE+R(24))
1 *DN2(1)
E=0.
IF(K.EQ.1)E=EXP(166375.4/T+ALOG(.5*RB(6)))
DN2(10)=(R(6)*XNE*EXP(166375.4*(1./T-1./TT))+E)/(R(6)*XNE+R(25))
1 *DN2(1)
E=0.
IF(K.EQ.1)E=EXP(166720.9/T+ALOG(RB(7)))

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DN2(11)=(R(7)*XNE*EXP(166720.9*(1./T-1./TT))+E)/(R(7)*XNE+R(26))
1 *DN2(1)
RETURN
END

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SUBROUTINE DELN2P(XN2,02,XN,0,XNE,T,TT,K,DN2P)
C THIS SUBROUTINE COMPUTES DELTA FACTORS FOR 4 ELECTRONIC STATES OF N2+.
  DIMENSION R(14),RP(14),DN2P(4),A(11),B(11),C(11),D(11),G(11),
1 D1(11),F(11),AA(3),RB(3)
C ELECTRONIC PARTITION FUNCTION FOR N2+.
  QEN2P(X)=2.*(1.+2.*EXP(-12972.68/X)+EXP(-36784.02/X)+2.*EXP(-75057
1 .9/X)+EXP(-92862.18/X))
C TWO-BODY RATE COEFFICIENTS FOR COLLISIONAL DEEXCITATION (Ith REACTION)
C ARE IN THE FORM:
C      R(I)=A(I)*T**B(I)*(D(I)+G(I)*EXP(-C(I)/T)).
C THE RATE COEFFICIENTS FOR THE REVERSE (EXCITATION) REACTIONS ARE IN THE
C FORM:
C      RP(I)=D1(I)*EXP(-F(I)/T)*R(I).
C HERE, T MAY BE EITHER THE NEUTRAL OR THE ELECTRON TEMPERATURE.
  DATA A/1.68E-6,1.72E-5,1.52E-6,7.5E-10,6.2E-10,5.E-11,1.E-9,1.E-9,
1 1.E-10,1.E-9,1.E-10/
  DATA B/3*-.5,8*0./
  DATA C/37405.5,105870.9,267182.1,8*0./
  DATA D/3*0.2,8*0./
  DATA G/3*0.356,8*1./
  DATA D1/2.,1.,1.,3*2.,5*1./
  DATA F/12997.0,36786.3,92836.0,3*12997.0,3*36786.3,2*92836.0/
C AA(I) ARE EINSTEIN 'A' COEFFICIENTS (SEC-1) AND RB(I) ARE THE
C CORRESPONDING RHO*B FACTORS (SEC-1) FOR SUNLIGHT CONDITIONS.
  DATA AA/6.E4,1.4E7,2.E7/
  DATA RB/8.5E-2,.17,2.1E-5/
  DO 10 I=1,3
    R(I)=A(I)*TT**B(I)*(D(I)+G(I)*EXP(-C(I)/TT))
    RP(I)=D1(I)*EXP(-F(I)/TT)*R(I)
10 CONTINUE
  DO 20 I=4,11
    R(I)=A(I)*T**B(I)*(D(I)+G(I)*EXP(-C(I)/T))
    RP(I)=D1(I)*EXP(-F(I)/T)*R(I)
20 CONTINUE
  DO 30 J=1,3
    I=J+11
    R(I)=AA(J)
    RP(I)=FLOAT(K)*RB(J)
30 CONTINUE
C DN2P(1) IS THE DELTA FACTOR FOR THE GROUND ELECTRONIC STATE (X doublet

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C SIGMA γ) OF N2+. IT IS APPROXIMATELY EQUAL TO ONE-HALF THE ELECTRONIC
 C PARTITION FUNCTION.
 DN2P(1)=QEN2P(T)/2.
 C THE DELTA FACTORS DN2P(I) (I=2 TO 4) REFER, RESPECTIVELY, TO DELTAS FOR
 C THE 3 STATES: A doublet PI u, B doublet SIGMA u+, AND C doublet SIGMA u+.
 E=0.
 IF(K.EQ.1)E=EXP(12997.0/T+ALOG(.5*RB(1)))
 FAC=EXP(12997.0*(1./T-1./TT))
 DN2P(2)=(R(1)*XNE*FAC+R(4)*XN2+R(5)*O2+R(6)*(XN+O)+E)/
 1 (R(1)*XNE+R(4)*XN2+R(5)*O2+R(6)*(XN+O)+R(12))*DN2P(1)
 E=0.
 IF(K.EQ.1)E=EXP(36784.0/T+ALOG(RB(2)))
 FAC=EXP(36784.0*(1./T-1./TT))
 DN2P(3)=(R(2)*XNE*FAC+R(7)*XN2+R(8)*O2+R(9)*(XN+O)+E)/
 1 (R(2)*XNE+R(7)*XN2+R(8)*O2+R(9)*(XN+O)+R(13))*DN2P(1)
 E=0.
 IF(K.EQ.1)E=EXP(92862.2/T+ALOG(RB(3)))
 FAC=EXP(92862.2*(1./T-1./TT))
 DN2P(4)=(R(3)*XNE*FAC+R(10)*(XN2+O2)+R(11)*(XN+O)+E)/
 1 (R(3)*XNE+R(10)*(XN2+O2)+R(11)*(XN+O)+R(14))*DN2P(1)
 RETURN
 END

SUBROUTINE DELO2(XNE,T,TT,K,D02)
 C THIS SUBROUTINE COMPUTES DELTA FACTORS FOR THE VIBRATIONAL STATES $V'=0$
 C TO 20 OF ELECTRONIC STATE O2(B TRIPLET SIGMA U MINUS) .THESE DELTA
 C FACTORS CAN BE USED TO CONVERT LTE EMISSION RATES FOR THE SCHUMANN-
 C RUNGE BANDS(B; $V' \rightarrow X;V''$) TO NLTE RATES.
 DIMENSION QP(24,21),A(21,24),F(21,24),Q(21,24),XNU(21,24),E(24),
 1 RB(21,24),D02(21),XK(21,24)
 DATA QP/3.55E-9,1.02E-7,1.43E-6,1.28E-5,8.26E-5,4.09E-4,1.61E-3,
 1 5.15E-3,1.36E-2,3.04E-2,5.77E-2,9.28E-2,1.28E-1,.15,.152,.132,
 2 9.97E-2,6.6E-2,3.82E-2,1.93E-2,8.48E-3,3.24E-3,1.13E-3,3.81E-4,
 3 3.49E-8,9.09E-7,1.14E-5,9.07E-5,5.11E-4,2.17E-3,7.16E-3,1.88E-2,
 4 3.91E-2,6.54E-2,8.64E-2,8.59E-2,5.85E-2,1.98E-2,1.97E-5,1.95E-2,
 5 6.82E-2,.114,.131,.115,8.11E-2,4.73E-2,2.38E-2,1.09E-2,2.14E-7,
 6 5.06E-6,5.7E-5,4.E-4,1.96E-3,7.11E-3,1.95E-2,4.09E-2,6.46E-2,
 7 7.48E-2,5.77E-2,2.17E-2,9.87E-5,1.82E-2,5.76E-2,7.12E-2,4.13E-2,
 8 4.67E-3,8.84E-3,5.54E-2,.104,.119,.102,7.29E-2,9.14E-7,1.96E-5,
 9 1.98E-4,1.23E-3,5.24E-3,1.61E-2,3.62E-2,5.9E-2,6.62E-2,4.49E-2,
 1 1.08E-2,1.7E-3,2.95E-2,5.38E-2,3.59E-2,3.27E-3,1.16E-2,5.29E-2,
 2 6.42E-2,2.84E-2,1.86E-4,2.27E-2,7.71E-2,.125,2.91E-6,5.68E-5,
 3 5.16E-4,2.84E-3,1.05E-2,2.71E-2,4.9E-2,5.94E-2,4.17E-2,9.66E-3,
 4 2.09E-3,2.86E-2,4.4E-2,1.96E-2,9.66E-5,2.55E-2,5.E-2,2.56E-2,
 5 1.65E-6,2.71E-2,6.18E-2,4.46E-2,5.58E-3,1.26E-2,7.66E-6,1.36E-4,

6 1.11E-3,5.42E-3,1.73E-2,3.71E-2,5.26E-2,4.37E-2,1.39E-2,4.5E-4,
 7 2.22E-2,3.95E-2,1.65E-2,4.18E-4,2.57E-2,3.91E-2,1.04E-2,4.61E-3,
 8 3.96E-2,4.05E-2,5.22E-3,1.08E-2,5.02E-2,5.06E-2,1.73E-5,2.81E-4,
 9 2.07E-3,8.92E-3,2.45E-2,4.32E-2,4.6E-2,2.26E-2,5.67E-4,1.26E-2,
 1 3.39E-2,1.99E-2,1.1E-5,1.33E-2,3.31E-2,7.8E-3,5.86E-3,3.55E-2,
 2 2.47E-2,2.E-6,2.61E-2,4.44E-2,1.29E-2,4.86E-3,3.5E-5,5.2E-4,
 3 3.46E-3,1.32E-2,3.09E-2,4.42E-2,3.33E-2,6.55E-3,3.41E-3,2.6E-2,
 4 2.55E-2,2.22E-3,1.02E-2,2.95E-2,1.08E-2,2.83E-3,2.88E-2,2.05E-2,
 5 9.68E-5,2.6E-2,3.26E-2,2.57E-3,1.49E-2,4.15E-2,6.3E-5,8.59E-4,
 6 5.17E-3,1.74E-2,3.49E-2,3.94E-2,1.88E-2,1.4E-4,1.36E-2,2.74E-2,
 7 9.54E-3,2.03E-3,2.29E-2,1.68E-2,5.78E-5,2.01E-2,2.18E-2,1.95E-4,
 8 1.91E-2,2.7E-2,1.27E-3,1.69E-2,3.36E-2,5.26E-3,1.01E-4,1.27E-3,
 9 6.94E-3,2.07E-2,3.53E-2,3.07E-2,7.57E-3,2.09E-3,2.09E-2,1.91E-2,
 1 6.35E-4,1.15E-2,2.13E-2,2.66E-3,8.8E-3,2.28E-2,3.44E-3,9.29E-3,
 2 2.48E-2,3.39E-3,1.11E-2,2.88E-2,5.04E-3,1.E-2,1.48E-4,1.72E-3,
 3 8.61E-3,2.29E-2,3.31E-2,2.15E-2,1.59E-3,7.53E-3,2.2E-2,8.8E-3,
 4 1.39E-3,1.79E-2,1.13E-2,6.04E-4,1.76E-2,1.12E-2,1.16E-3,2.E-2,
 5 9.57E-3,3.07E-3,2.39E-2,8.44E-3,4.57E-3,2.54E-2,1.96E-4,2.14E-3,
 6 9.79E-3,2.33E-2,2.85E-2,1.31E-2,1.06E-7,1.22E-2,1.78E-2,2.1E-3,
 7 6.44E-3,1.69E-2,2.77E-3,6.12E-3,1.65E-2,1.61E-3,9.07E-3,1.61E-2,
 8 1.84E-4,1.43E-2,1.43E-2,2.64E-4,1.9E-2,1.17E-2,2.4E-4,2.45E-3,
 9 1.04E-2,2.23E-2,2.31E-2,7.13E-3,9.34E-4,1.42E-2,1.19E-2,2.05E-5,
 1 1.05E-2,1.16E-2,1.36E-5,1.09E-2,9.79E-3,3.26E-4,1.38E-2,6.59E-3,
 2 2.86E-3,1.64E-2,2.55E-3,8.23E-3,1.72E-2,3.83E-4,2.7E-4,2.6E-3,
 3 1.03E-2,2.E-2,1.77E-2,3.36E-3,2.57E-3,1.36E-2,6.77E-3,6.81E-4,
 4 1.15E-2,6.19E-3,1.06E-3,1.16E-2,3.78E-3,3.27E-3,1.22E-2,9.51E-4,
 5 8.04E-3,1.04E-2,1.83E-4,1.37E-2,6.92E-3,2.69E-3,2.81E-4,2.58E-3,
 6 9.58E-3,1.17E-2,1.3E-2,1.34E-3,3.81E-3,1.16E-2,3.33E-3,2.05E-3,
 7 1.03E-2,2.57E-3,2.95E-3,9.55E-3,7.7E-4,5.83E-3,7.99E-3,8.04E-5,
 8 9.81E-3,4.18E-3,3.02E-3,1.2E-2,8.9E-4,7.74E-3,2.72E-4,2.4E-3,
 9 8.47E-3,1.4E-2,9.29E-3,4.29E-4,4.33E-3,9.06E-3,1.43E-3,3.01E-3,
 1 8.08E-3,7.94E-4,4.11E-3,6.74E-3,7.23E-6,6.55E-3,4.25E-3,1.16E-3,
 2 8.51E-3,9.59E-4,5.45E-3,7.48E-3,1.15E-4,9.11E-3,2.48E-4,2.12E-3,
 3 7.15E-3,1.12E-2,6.52E-3,9.27E-5,4.21E-3,6.75E-3,5.29E-4,3.32E-3,
 4 5.9E-3,1.42E-4,4.32E-3,4.34E-3,1.81E-4,5.92E-3,1.94E-3,2.19E-3,
 5 6.18E-3,4.04E-5,5.98E-3,3.76E-3,1.23E-3,7.61E-3,2.13E-4,1.77E-3,
 6 5.76E-3,8.52E-3,4.51E-3,5.82E-6,3.69E-3,4.84E-3,1.61E-4,3.11E-3,
 7 4.1E-3,1.67E-6,3.87E-3,2.65E-3,4.93E-4,4.72E-3,7.72E-4,2.56E-3,
 8 4.06E-3,8.12E-5,5.22E-3,1.62E-3,2.13E-3,5.32E-3,1.74E-4,1.41E-3,
 9 4.5E-3,6.4E-3,3.1E-3,3.49E-6,3.03E-3,3.41E-3,3.63E-5,2.64E-3,
 1 2.79E-3,2.4E-5,3.17E-3,1.59E-3,6.64E-4,3.52E-3,2.74E-4,2.41E-3,
 2 2.55E-3,2.94E-4,4.06E-3,6.21E-4,2.73E-3,3.43E-3,1.35E-4,1.08E-3,
 3 3.37E-3,4.66E-3,2.11E-3,1.69E-5,2.34E-3,2.34E-3,3.88E-6,2.09E-3,
 4 1.87E-3,6.36E-5,2.42E-3,9.46E-4,6.74E-4,2.5E-3,8.45E-5,2.01E-3,
 5 1.57E-3,4.14E-4,2.94E-3,2.13E-4,2.14E-3,2.11E-3,8.81E-5,6.99E-4,
 6 2.15E-3,2.91E-3,1.25E-3,2.13E-5,1.52E-3,1.4E-3,3.43E-8,1.37E-3,
 7 1.09E-3,7.E-5,1.56E-3,5.03E-4,5.11E-4,1.52E-3,2.05E-5,1.35E-3,

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      8 3.48E-4,3.64E-4,1.8E-3,6.05E-5,1.51E-3,1.14E-3/
C VIBRATIONAL PARAMETERS FOR O2(X)
      DATA W,WX,WY,WZ/1580.193,11.981,.04747,-.001273/
      DO 20 I=1,21
      VP=FLOAT(I-1)
      DO 10 J=1,24
      VPP=FLOAT(J-1)
C WAVENUMBERS FOR THE SCHUMANN-RUNGE BANDS (V'--;V'') :
      XNU(I,J)=49793.28+709.31*(VP+.5)-10.65*(VP+.5)**2-.139*(VP+.5)**3
      1 -(W*(VPP+.5)-WX*(VPP+.5)**2+WY*(VPP+.5)**3+WZ*(VPP+.5)**4)
C FRANCK-CONDON FACTORS FOR THE SCHUMANN- RUNGE BANDS:
      Q(I,J)=QP(J,I)
C ABSORPTION OSCILLATOR STRENGTHS,F(I,J),DEFINED IN TERMS OF THE FRANCK-
C CONDON FACTORS:
      F(I,J)=2.36E-6*Q(I,J)*XNU(I,J)
C EINSTEIN A COEFFICIENTS (SEC-1) DEFINED:
      A(I,J)=0.667*XNU(I,J)**2*F(I,J)
C RHO*B FACTORS (SEC-1) FOR SUNLIGHT EXCITATION OF O2(B;V') DEFINED:
      RB(I,J)=5.4E-6*A(I,J)/(EXP(2.391E-4*XNU(I,J))-1.)*FLOAT(K)
C RATE COEFFICIENT FOR ELECTRON EXCITATION OF THE STATE O2(B;V') FROM
C THE STATE O2(X;V'') :
      XK(I,J)=.754*F(I,J)/XNU(I,J)**1.5*EXP(.3366*(TT/XNU(I,J))**.546-
      1 1.4388*XNU(I,J)/TT)
      10 CONTINUE
      20 CONTINUE
C DO IS THE GROUND-STATE DELTA FACTOR
      DO=1.+1.336E-2*T**.445*EXP(-10309.1/T)
      DO 40 I=1,21
      S1=0.
      S2=0.
      S3=0.
      DO 30 J=1,24
      S1=S1+XK(I,J)*EXP(1.4388*XNU(I,J)/TT)
      S2=S2+A(I,J)
      S3=S3+(RB(I,J)+XNE*XK(I,J))*EXP(1.4388*XNU(I,J)/T)
      30 CONTINUE
      FN=S3*DO
      FD=S2+XNE*S1
C DELTA FACTORS FOR THE STATES O2(B;V'=0 TO 20) DEFINED:
      DO2(I)=FN/FD
      40 CONTINUE
      RETURN
      END

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SUBROUTINE DELNO(XN2,O2,XNO,CO2,H2O,XNE,T,TT,DN2,K,DNO)
C THIS SUBROUTINE COMPUTES DELTA FACTORS FOR 7 ELECTRONIC STATES OF NO.
  DIMENSION R(27),RP(27),AA(11),RB(11),DNO(7),A(6),B(6),C(6),D(6),
  1 XK(10),DN2(11)
C ELECTRONIC PARTITION FUNCTION FOR N2.
  QEN2(X)=1.+3.*EXP(-71587.2/X)+6.*(EXP(-85330.6/X)+EXP(-85435.9/X))
  1 +3.*EXP(-94748.4/X)+EXP(-97463.3/X)+2.*(EXP(-99207.0/X)+EXP(-1031
  2 59.8/X))+5.*EXP(-112082.5/X)+6.*(EXP(-125319.5/X)+EXP(-128021.3/X
  3 ))+10.*EXP(-134096.2/X)+3.*EXP(-137800.4/X)+6.*EXP(-140432.0/X)+
  4 EXP(-142211.4/X)+2.*EXP(-145056.2/X)
C ELECTRONIC PARTITION FUNCTION FOR NO.
  QENO(X)=4.*(1.+5*EXP(-65119.5/X)+EXP(-71651.6/X)+EXP(-75349.3/X)+
  1 .5*EXP(-81291.5/X)+EXP(-91938.5/X)+.5*EXP(-92657.9/X))
C TWO-BODY RATE COEFFICIENTS FOR ELECTRON-IMPACT DEEXCITATION ARE IN
C THE FORM: R(I)=A(I)*EXP(B(I)*TT**.546). THE CORRESPONDING ELECTRON-
C IMPACT EXCITATION RATE COEFFICIENTS ARE IN THE FORM: RP(I)=C(I)*EXP(
C -D(I)/TT)*R(I) WHERE TT IS THE ELECTRON TEMPERATURE( DEGREES KELVIN).
  DATA A/9.6E-11,9.5E-13,3.5E-10,4.8E-10,5.1E-11,1.7E-10/
  DATA B/9.66E-4,9.17E-4,8.93E-4,8.56E-4,8.E-4,7.97E-4/
  DATA C/.5,1.,1.,.5,1.,.5/
  DATA D/65119.,71652.,75349.,81291.,91938.,92658./
C AA(I) ARE THE EINSTEIN "A" COEFFICIENTS (SEC-1) AND RB(I) ARE THE
C CORRESPONDING RHO*B FACTORS (SEC-1) FOR SUNLIGHT CONDITIONS.
  DATA AA/1.7E6,2.3E4,1.E7,1.8E7,3.E6,1.E7,1.E7,1.3E7,9.3E5,2.9E5,
  1 1.6E7/
  DATA RB/9.2E-5,8.4E-7,2.E-4,6.6E-5,3.8E-6,5.5E-6,18.,8.9,9.4E-2,
  1 .12,17./
C XK ARE RATE COEFFICIENTS FOR COLLISIONAL QUENCHING BY HEAVY PARTICLES
  DATA XK/1.4E-13,6.9E-11,3.E-12,7.2E-12,3.7E-11,6.E-10,5.E-10,
  1 4.5E-11,1.4E-11,5.E-11/
  DO 10 I=1,6
    R(I)=A(I)*EXP(B(I)*TT**.546)
    RP(I)=C(I)*EXP(-D(I)/TT)*R(I)
  10 CONTINUE
  DO 15 I=7,16
    J=I-6
    R(I)=XK(J)
  15 CONTINUE
  RP(11)=.3*EXP(-3763./T)*R(11)
C OTHER COLLISIONAL QUENCHING RATE COEFFICIENTS.
  R7O2=1.5E-10
  R7NO=2.E-10
  R7CO2=3.8E-10
  R7H2O=7.7E-10
  R1O02=5.4E-11
  R1ONO=2.E-10
  R1OH2O=1.3E-10
  R14O2=4.3E-10

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R14N0=5.E-10
R14C02=6.3E-10
DO 20 I=17,27
J=I-16
R(I)=AA(J)
RP(I)=FLOAT(K)*RB(J)
20 CONTINUE
C DNO(1) IS THE DELTA FACTOR FOR THE GROUND ELECTRONIC STATE (X doublet
C P1) OF NO. IT IS APPROXIMATELY EQUAL TO ONE-QUARTER OF THE ELECTRONIC
C PARTITION FUNCTION.
DNO(1)=QENO(T)/4.
B1=R(1)*XNE+R(7)*XN2+R702*02+R7N0*XN0+R7C02*C02+R7H20*H20+R(17)+
1 RP(23)+RP(24)+RP(25)
B2=2.*(R(12)*XN2+R(23))*EXP(-10230./T)
B3=EXP(ALOG(R(24)))-16172./T)
B4=EXP(ALOG(R(25)))-27538./T)
E=0.
IF(K.EQ.1)E=EXP(65119./T+ALOG(RB(1)))
B5=2.*(5*EXP(65119./T-1./TT))*R(1)*XNE+E+3.*R(8)*XN2*DN2(2)*
1 EXP(-6467./T)/QEN2(T))
B6=RP(23)
B7=2.*(R(3)*XNE+R(11)*XN2*DN2(1)/QEN2(T)+R(12)*XN2+R(13)*(02+XN0)
1 +R(19)+R(23)+RP(26))*EXP(-11741./T)
B8=EXP(ALOG(R(26)))-27538./T)
E=0.
IF(K.EQ.1)E=EXP(65119./T+ALOG(RB(3)))
B9=2.*(EXP(65119./T-75349./TT))*R(3)*XNE+E+3.*RP(11)*XN2*DN2(2)*
1 EXP(-6467./T)/QEN2(T))
B10=RP(24)
B11=EXP(ALOG(R(4)*XNE+R(14)*XN2+R1402*02+R14N0*XN0+R14C02*C02+
1 R(20)+R(24)+RP(27)))-16172./T)
B12=EXP(ALOG(R(27)))-27538./T)
E=0.
IF(K.EQ.1)E=EXP(65119./T+ALOG(RB(4)))
B13=2.*(5*EXP(65119./T-81291./TT))*R(4)*XNE+E)
B14=RP(25)
B15=0.
IF(K.EQ.1)B15=EXP(ALOG(2.*RB(10)))-10230./T)
B16=0.
IF(K.EQ.1)B16=EXP(ALOG(RB(11)))-16172./T)
B17=EXP(ALOG(R(6)*XNE+R(16)*XN2+R(22)+R(26)+R(27)))-27538./T)
E=0.
IF(K.EQ.1)E=EXP(65119./T+ALOG(RB(6)))
B18=2.*(5*EXP(65119./T-92658./TT))*R(6)*XNE+E)
G=B10*(B3*(B8*B15-B7*B17)-B16*(B4*B7+B2*B8))-B11*(B1*(B8*B15-
1 B7*B17)+B2*(B8*B14+B6*B17)+B4*(B6*B15+B7*B14))-B12*(B7*(B1*B16+
2 B3*B14)+B6*(B3*B15-B2*B16))
A1=B5*DNO(1)

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A2=B9*DN0(1)
A3=B13*DN0(1)
A4=B13*DN0(1)
C THE DELTA FACTORS DN0(I) (I=2 TO 7) REFER, RESPECTIVELY, TO DELTAS FOR
C THE STATES: A doublet SIGMA +, B doublet PI, C doublet PI, D doublet
C SIGMA +, B' doublet DELTA, AND E doublet SIGMA +.
DN0(2)=(B2*(A2*(B11*B17-B12*B16)+B8*(A3*B16+A4*B11))+B15*(B3*(A2*
1 B12-A3*B8)+B11*(A2*B4-A1*B8))+B7*(A1*(B11*B17-B12*B16)+A3*(B4*B16
2 +B3*B17)+A4*(B3*B12+B4*B11)))/G
DN0(3)=((RP(2)*XNE+RP(18))*EXP(71652./T)+3.*R(9)*XN2*DN2(2)/QEN2(T
1 ))*DN0(1)/(R(2)*XNE+R(10)*XN2+R1002*02+R10N0*XN0+R10H20*H20+R(18)
2 )
DN0(4)=(B6*(A1*(B11*B17-B12*B16)+A3*(B3*B17+B4*B16)+A4*(B3*B12+B4*
1 B11))+A2*(B1*(B11*B17-B12*B16)-B10*(B3*B17+B4*B16)-B14*(B3*B12+B4
2 *B11))+B8*(B1*(A3*B16+A4*B11)+B10*(A1*B16-A4*B3)+B14*(A1*B11+A3*
3 B3)))/G
DN0(5)=(B10*(B2*(A2*B17+A4*B8)+B7*(A1*B17+A4*B4)+B15*(A2*B4-A1*B8)
1 )-A3*(B1*(B8*B15-B7*B17)+B6*(B2*B17+B4*B15)+B14*(B2*B8+B4*B7))+
2 B12*(B1*(A4*B7+A2*B15)-B6*(A4*B2-A1*B15)+B14*(A2*B2+A1*B7)))/G
DN0(6)=(RP(5)*XNE+RP(21))*EXP(91938./T)*DN0(1)/(R(5)*XNE+R(15)*XN2
1 +R(21))
DN0(7)=(B6*(B15*(A3*B3+A1*B11)-B2*(A4*B11+A3*B16))+B7*(B1*(A4*B11+
1 A3*B16)-B10*(A4*B3-A1*B16)+B14*(A3*B3+A1*B11))+A2*(B2*(B10*B16+
2 B11*B14)-B15*(B3*B10-B1*B11)))/G
RETURN
END

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SUBROUTINE DELNOP(XNE,T,TT,K,D0,D1,DNOP)
C THIS SUBROUTINE COMPUTES DELTAFACORS FOR THE VIBRATIONAL STATES v'=0
C TO 10 OF ELECTRONIC STATE NO+(A singlet PI). THESE DELTA FACTORS CAN
C BE USED TO CONVERT LTE EMISSION RATES FOR THE BAER-MIESCHER BANDS
C (A;v'-->X;v*) TO NLTE RATES.
DIMENSION Q(11,8),A(11,8),XNU(11,8),RB(11,8),XK(11,8),
1 DNOP(11)
C ELECTRONIC PARTITION FUNCTION FOR NO+
QENOP(X)=1.+3.*(EXP(-75090./X)+2.*EXP(-85234./X)+2.*EXP(-89032./X)
1 +EXP(-97435./X))
C TX AND TA ARE THE ABSOLUTE ENERGIES (CM-1) OF VIBRATIONAL STATES OF
C THE ELECTRONIC STATES (X singlet SIGMA+) AND (A singlet PI),RESPECTIVELY.
TX(X)=2376.42*(X+.5)-16.262*(X+.5)**2-.01562*(X+.5)**3
TA(X)=73083.5+1601.93*(X+.5)-20.207*(X+.5)**2-.2683*(X+.5)**3
DATA Q/.0217,.0643,.1068,.1321,.1363,.1246,.1047,.083,.063,.0465,
1 .0336,.0962,.1617,.1338,.0644,.0138,9.024E-5,.0121,.0323,.049,
2 .0581,.0596,.1958,.1329,.0158,.0101,.0555,.0744,.0569,.0274,
3 .0642,3.1E-7,4.598E-3,.2443,.0214,.0369,.0922,.0507,4.54E-3,

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4 6.733E-3,3.258E-2,4.857E-2,4.525E-2,3.037E-2,.21,.0181,.113,
5 .02764,7.03E-3,.0532,.0577,.0247,1.66E-3,4.31E-3,.0198,.133,
6 .1205,.05,.0187,.078,.0327,4.31E-5,.024,.0462,.0378,.0157,.0644,
7 .1835,1.47E-3,.0963,.0214,.0141,.0579,.0371,3.32E-3,5.96E-3,
8 .0266,.0246,.1549,.0788,.0509,.0209,.0712,.0142,9.919E-3,.0419,
9 .0392,.0123/
DO 20 I=1,11
VP=FLOAT(I-1)
DO 10 J=1,8
VPP=FLOAT(J-1)
C WAVENUMBERS FOR THE BAER-MIESCHER BANDS ( $\nu' \rightarrow \nu''$ ) :
XNU(I,J)=TA(VP)-TX(VPP)
C EINSTEIN A COEFFICIENTS (SEC-1) DEFINED :
A(I,J)=6.429E-8*XNU(I,J)**3*Q(I,J)
C RHO*B FACTORS (SEC-1) FOR SUNLIGHT EXCITATION OF NO+(A; $\nu'$ ) DEFINED :
RB(I,J)=1.08E-5*A(I,J)/(EXP(2.391E-4*XNU(I,J))-1.)*FLOAT(K)
C RATE COEFFICIENT FOR ELECTRON DEEXCITATION OF THE STATE NO+(A; $\nu'$ ) TO
C THE STATE NO+(X; $\nu''$ ) :
XK(I,J)=20.44*A(I,J)/(SQRT(TT)*XNU(I,J)**3)*(.2+.356*EXP(-4.14*
1 XNU(I,J)/TT))
10 CONTINUE
20 CONTINUE
DO 50 I=1,11
S1=0.
S2=0.
DO 30 J=2,8
E=0.
IF(K.EQ.1)E=EXP(ALOG(RB(I,J)/2.))+1.4388*XNU(I,J)/T)
S1=S1+(E+XNE*EXP(1.4388*XNU(I,J)*(1./T-1./TT))*XK(I,J))
1 *(D1/D0)**(J-2)
30 CONTINUE
DO 40 J=1,8
S2=S2+A(I,J)+XNE*XK(I,J)
40 CONTINUE
E=0.
IF(K.EQ.1)E=EXP(ALOG(RB(I,1)/2.))+1.4388*XNU(I,1)/T)
FN=(E+XNE*EXP(1.4388*XNU(I,1)*(1./T-1./TT))*XK(I,1))*D0+D1*S1
ONOP(I)=FN*QENOP(T)/S2
50 CONTINUE
RETURN
END

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