

Satellite Studies of N(²D) Emission and Ion Chemistry in Aurorae

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The incident particle flux ion and neutral composition data taken on the AE-D satellite have been used to investigate the quantal emission of N₂⁺ at 4278 Å, N(²D) at 5200 Å, and the ion chemistry in aurorae. The results of a time dependent auroral model have been compared to the data. The calculated 4278 Å emission of N₂⁺, the 5200 Å emission of N(²D), the densities of O₂⁺, NO⁺, N₂⁺, O⁺, and the electron density are generally in agreement with the measured values. These results are consistent with the branching ratios and quenching rates deduced from previous studies of the N(²D) densities in the day-time, mid-latitude ionosphere. It is found that in an auroral arc, the measured atomic oxygen density is lower than predicted by the MSIS model.

INTRODUCTION

The simultaneous and broad-based measurement capability of the Atmosphere Explorer (AE) satellites allows us to obtain unique data on auroral events as the satellite passes through an active region. Two previous studies [Torr *et al.*, 1975; Kasting and Hays, 1977] have taken advantage of the satellite's capability in order to investigate the ion chemistry and the energy degradation of electrons in aurorae. In this paper, the electron energy spectrum measured by the low-energy electron experiment (Lee) [R. Hoffman *et al.*, 1973] and the neutral atmosphere densities of N₂ and O measured by the open source mass spectrometer (OSS) [Nier *et al.*, 1973] are used as input to a time dependent model of the auroral ionosphere. The model has been previously applied to mid-latitude calculations of odd nitrogen and ion densities in the thermosphere, for comparison to satellite data [Rusch *et al.*, 1977; Cravens *et al.*, 1979], and to the calculation of auroral odd nitrogen and ionospheric densities, for comparison to rocket and satellite data [Gérard and Rusch, 1979].

The model is used here to calculate the ionization and dissociation rates in the atmosphere and the time dependent development of the auroral ionospheric and the odd nitrogen densities. We then compare the calculated airglow (4278 Å and 5200 Å) intensities and ionospheric densities to those measured on the satellite in an attempt to verify under auroral conditions the validity of mid-latitude odd nitrogen chemistry deduced by Rusch *et al.* [1975] and Frederick and Rusch [1977].

DATA

In this study we have concentrated on data from two AE-D orbits, 431 and 425, for which perigee is located in the auroral zone during a period of bright nighttime aurorae. On one of the orbits (425), we have performed individual calculations at two different times. The basic data are shown in Figures 1 and 2. The vertical intensities of the 4278 Å and 5200 Å emissions are taken from the visible airglow experiment (VAE) [Hays *et al.*, 1973], the electron density is from the cylindrical electrostatic probe (CEP) [Brace *et al.*, 1973], the ion densities of NO⁺ and O₂⁺ are from the magnetic ion-mass spectrometer

(Mims) [J. Hoffman *et al.*, 1973], and the electron energy flux from Lee is displayed versus universal time and satellite altitude. In both cases, AE-D was operating in a spinning mode, cart-wheeling along its orbit. In this mode, vertical intensities may be measured by both VAE channels, although not precisely at the same time.

The VAE data were averaged in the sector of the spin within 20° of the vertical. Dark count and galactic background emissions were removed by using data from the high-altitude segments of the orbits. The laboratory calibration was then applied to the data. The statistical error involved in this procedure is about 15% for the 15 R signal measured on orbit 425 and about 5% for the 29 R signal of orbit 431.

The low-energy electron experiment on AE-D scans the energy range from 0.2 Kev to 20 Kev in 1 second. The Lee spectra were averaged over the upward-looking hemisphere during one-half of a spin period, and each sum included seven or eight spectra. The individual spectra used in the averages did not show any significant pitch angle dependence, so we assume the distribution to be isotropic at all energies. The averaged Lee spectra for the three cases studied below are shown in Figure 3 and exhibit differences in the flux distribution and total energy. Note in particular the very rapid decrease in flux at high energies and the strong 'inverted V' event of orbit 431. The collected data used for comparison to the calculation are given in Table 1, where *H* is the satellite altitude.

The vertical distribution of the neutral atmosphere is needed as input for the calculations. To obtain this distribution we used the MSIS model [Hedin *et al.*, 1977] and normalized the N₂ density, by varying the *Ap* value in the model, to that measured by the OSS. We then normalized the atomic oxygen by multiplying the model O density by the ratio of the measured O density to the model O density at the value of *Ap* where the N₂ densities agreed. We found, in each case, that the model O densities had to be decreased by approximately a factor of two to match the measurement. The neutral temperature profile corresponding to the normalized MSIS model was adopted. A further difficulty arises in determining the appropriate molecular oxygen density profiles. For initial model calculations in each case we used the O₂ density profile attached to the MSIS model, realizing that no attempts were made to quantitatively describe the O₂ distribution in the

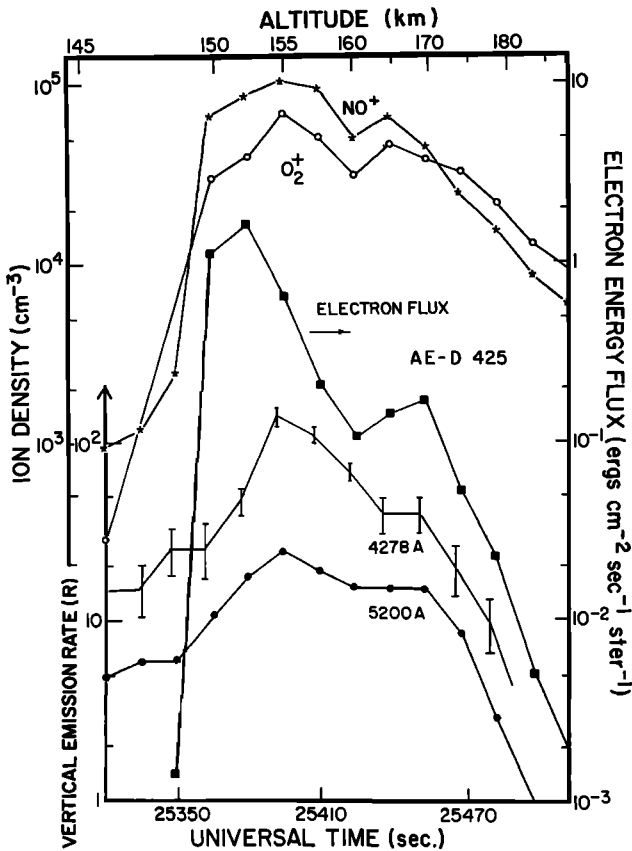


Fig. 1. The measured vertical intensities of 5200-Å and 4278-Å emission, ion densities, and electron flux for AE-D orbit 425 as a function of Universal Time in seconds and satellite altitude.

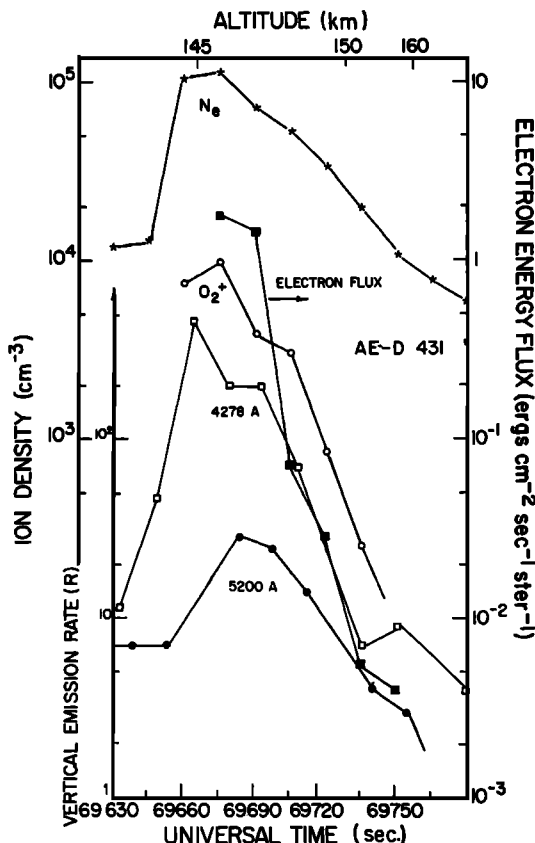


Fig. 2. Same as Figure 1 for orbit 431, except the electron density is included.

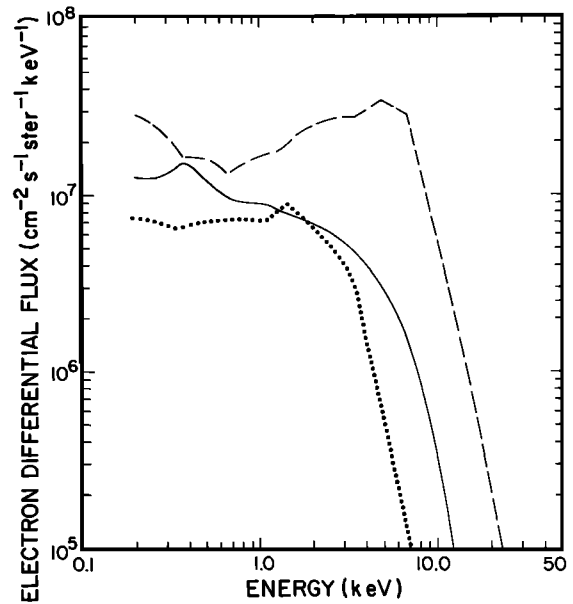


Fig. 3. The measured electron differential flux for orbit 425 at 25,425 seconds UT (···), 25,455 seconds UT (—), and for orbit 431 at 69,680 seconds UT (---).

model. In subsequent runs the O₂ density profile was adjusted, guided by the calculated ionospheric densities and airglow emissions. The final neutral atmosphere model adopted in each case resembled that used by Gérard and Rusch [1979] in their analysis of a coordinated satellite-rocket auroral experiment.

THE MODEL

The chemical model used in these calculations has been described in several papers [Rusch et al., 1977; Cravens et al., 1979; Gérard and Rusch, 1979]. The basic features of the model are given here.

The ionization rate profile is calculated by using a method developed in Lazarev [1967] for the case of monodirected-monoenergetic beam of electrons. This formula gives an analytical expression for the total ionization rate as a function of the penetration depth and depends on the energy of the primary electrons and the local mass density [Gérard, 1970]. The validity of this formulation was demonstrated in Gérard and Rusch [1979]. The ionization rate profile is calculated by assuming that the electron energy spectrum measured by the Lee detectors at the spacecraft altitude represents the spectrum of the primaries outside the atmosphere. This approximation would mostly affect the soft electron component (energies below ~ 500 eV) whose energy is degraded above the altitude of the spacecraft. Neglect of this component would influence the calculated 4278 and 5200 Å column intensities. The ionization rate is integrated over the energy spectrum, and an isotropic pitch angle distribution from 0° to 80° is assumed to be in agreement with the angular distribution measured by the detectors. The volume emission rate of the 4278-Å band of the N₂⁺ first-negative system, η(4278), is subsequently calculated from the total ionization rate *q* by using

$$\eta(4278) = q \frac{0.88[N_2]}{0.88[N_2] + 0.5[O] + [O_2]} \cdot \frac{1}{50}$$

The production rates of individual ions are obtained from the total ion production rate *q* by following the method described by Vallance-Jones [1975]. The relative production of

TABLE 1. Airglow and Ionosphere Data

Orbit	UT, s	Height, km	I 4278, R	I 5200, R	NO ⁺ , cm ⁻³	O ₂ ⁺ , cm ⁻³	O ⁺ , cm ⁻³	N ₂ ⁺ , cm ⁻³	N ⁺ , cm ⁻³	ΣN _i [†] , cm ⁻³	Ne [‡] , cm ⁻³
425	25425	160	60	15	5.0(4)*	3.1(4)	8.7(3)	1.5(3)	4.5(2)	9.2(4)	6.3(4)
425	25455	165	50	16	3.8(4)	4.7(4)	2.3(4)	3.1(2)	2.1(2)	1.1(5)	8.4(4)
431	69680	145	200	29	1.2(5)	9.7(3)	6.2(3)	—	—	1.2(5)	—

*Read 5.0(4) as 5.0 × 10⁴.

†ΣN_i is the sum of the densities of the ions measured by Mims.

‡Ne is the electron density from CEP.

O⁺ ions in the three lower levels ⁴S, ²D, and ²P is 0.48, 0.32, and 0.20, respectively, of the total O⁺ production [Torr and Torr, 1978]. The ion and odd nitrogen densities are then calculated with a time-dependent model which uses a general second-order differential equation solver developed at the National Center for Atmospheric Research by Hastings and Roble [1977]. The continuity equations are solved for N₂⁺, NO⁺, O₂⁺, N⁺, O(⁴S), O(²D), O(²P), N(²D), N(²P), N(⁴S) and NO with the chemical reactions listed in Table 2. The NO and N(⁴S) calculations include molecular and eddy diffusion and appropriate flux conditions at the lower (50 km) and upper (300 km) boundaries. Most of the reaction rates and their temperature dependence that are used in the calculations have been measured in the laboratory and their values confirmed by the analysis of the AE (satellite) measurements of the thermospheric ion composition [Torr and Torr, 1978]. However, a few branching ratios and quenching rates have not been measured, and a choice must be made on the basis of the odd nitrogen daytime chemistry. The reaction of N₂⁺ with O (reaction 7) is assumed to produce only N(²D) atoms, and the dissociation of N₂ by fast electron impact yields 60% N(²D), and 20% of N(⁴S) and 20% N(²P) in the model. In the model, effective quenching of N(²P) by atomic oxygen to the N(²D) state makes the overall efficiency of this reaction for N(²D) production near 80%. These values are in agreement with the [NI] 5200 Å airglow analysis by Frederick and Rusch [1977] and give satisfactory agreement with the nitric oxide densities observed in the mid-latitude lower thermosphere [Cravens et al., 1979].

ANALYSIS AND RESULTS

The measured airglow and ionospheric parameters are compared in detail to the results of the model calculations in Tables 3, 4, and 5. The 4278-Å and 5200-Å emission rates listed are obtained by integrating the calculated volume emission rates above the spacecraft altitude.

Two calculations are presented for each time selected, for it is instructive to show the results as specific parameters are varied. The comments refer to the parameter variations. In all the calculations, except case 2 of Table 5, the densities and emissions shown are for the fully developed ionosphere. The saturation time for the ionosphere at these altitudes is on the order of 500 seconds. The comparisons are difficult, of course, as we have no knowledge of the history of the event. It does appear, however, that for the two cases of orbit 425, the ionosphere was fully developed, and for the case of orbit 431 it was not. This is consistent with the known lifetimes (~10 seconds) of inverted-V events, such as the one which occurred on orbit 431.

In each case the [O] density was normalized to the MSIS model, as described earlier. The objective of each calculation was to reproduce the observed optical emissions, then to see if the calculated ion densities compared favorably with the measurements. We were guided in our choice of the O₂ profiles primarily by their effect on the calculated O₂⁺ and O⁺ densities. We found good agreement with the airglow, the NO⁺ and O₂⁺ densities could be achieved, but N₂⁺ and O⁺ were not in as good agreement. Note that it was necessary to triple the O₂ densities in the cases of Tables 3 and 4, but this resulted in a calculated to measured O⁺ ratio of 0.15 for case 2 of Table 4. This case for orbit 431 was one of hard precipitation, probably short lived, and the results of the calculation after 6.0 seconds are in good agreement with the measurement.

TABLE 2. Reactions and Reaction Rates

Reaction	Reaction Rate*	Source
1. $O + e \rightarrow O^+(^4S, ^2, ^2D, ^2P) + 2e$	see text: $f(^4S) = 0.484, f(^2D) = 0.323,$ $f(^2P) = 0.194$	f 's from Torr and Torr [1978]
2. $O_2 + e \rightarrow O_2^+ + 2e$	see text	
3. $O_2 + e \rightarrow O + O^+(^4S, ^2D, ^2P) + 2e$	see text ($f(^4S), f(^2D), f(^2P)$, same as R1)	
4. $N_2 + e \rightarrow N_2^+ + 2e$	see text	
5. $N_2 + e \rightarrow N(^4S) + N(^2D, ^2P) + e$	see text	
6. $N_2 + e \rightarrow N(^4S, ^2D, ^2P) + N^+ + 2e$	see text	
7. $N_2^+ + O \rightarrow NO^+ + N(^2D)$	$1.4 \times 10^{-10}(T/300)^{-0.44}$	McFarland et al. [1974]
8. $N_2^+ + O_2 \rightarrow O_2^+ + N_2$	$5 \times 10^{-11}(T/300)^{-0.8}$	Lindinger et al. [1974]
9. $N_2^+ + e \rightarrow N(^4S) + N(^2D)$	$1.8 \times 10^{-7}(T_e/300)^{-0.39}$	Mehr and Biondi [1969]
10. $O^+ + N_2 \rightarrow NO^+ + N(^4S)$	5×10^{-13}	Lindinger et al. [1974]
11. $O^+ + O_2 \rightarrow NO^+ + O$	$2 \times 10^{-11}(T_n/300)^{-0.4}$	McFarland et al. [1974]
12. $O_2^+ + NO \rightarrow NO^+ + O_2$	4.4×10^{-10}	Lindinger et al. [1974]
13. $O_2^+ + N(^2D) \rightarrow NO^+ + O$	1.8×10^{-10}	Goldan et al. [1966]
14. $O_2^+ + e \rightarrow O + O$	$1 \times 10^{-5}T_e^{-0.7}$	D. Torr et al. [1976]
15. $N^+ + O_2 \rightarrow NO^+ + O$	2.75×10^{-10}	McFarland et al. [1973]
16. $NO^+ + e \rightarrow N(^4S, ^2D) + O$	$4.2 \times 10^{-7}(T_e/300)^{-0.85}$	Walls and Dunn [1974]
17. $N(^4S) + O_2 \rightarrow NO + O$	$2.4 \times 10^{-11} \exp(-3975/T_n)$	Wilson [1967]
18. $N(^2D) + O_2 \rightarrow NO + O$	6×10^{-12}	Lin and Kaufman [1971]
19. $N(^2D) + e \rightarrow N(^4S) + e$	$6 \times 10^{-10}(T_e/300)^{0.5}$	Frederick and Rusch [1977]
20. $N(^2D) + O \rightarrow N(^4S) + O$	5×10^{-13}	Frederick and Rusch [1977]
21. $N(^4S) + NO \rightarrow N^2 + O$	2.1×10^{-11}	Phillips and Schiff [1962]
22. $N(^2D) \rightarrow N(^4S) + h\nu_{5200}$	$A_{2D} = 1.07 \times 10^{-5} s^{-1}$	Garstang [1956]
23. $O^+(^2D) + N_2 \rightarrow N_2^+ + O$	1×10^{-9}	Rutherford and Vroom [1971]
24. $N(^2P) + O \rightarrow N(^2D) + O$	1×10^{-11}	Young and Dunn [1975]
25. $N(^2P) + e \rightarrow N(^2D) + e$	$6 \times 10^{-10}(T_e/300)^{-5}$	Assumed
26. $N(^2P) \rightarrow N(^2D) + h\nu$	$A = 0.079 s^{-1}$	Garstang [1956]
27. $N(^2P) \rightarrow N(^4S) + h\nu$	$A = 0.0054 s^{-1}$	Garstang [1956]
28. $O^+(^2P) + O \rightarrow O^+(^2D) + O$	5.2×10^{-11}	Rusch et al. [1977]
29. $O^+(^2P) + e \rightarrow O^+(^2D) + e$	$1.89 \times 10^{-7}(T_e/300)^{-0.5}$	Henry et al. [1969]
30. $O^+(^2P) \rightarrow O^+(^2D) + h\nu$	$A = 0.17 s^{-1}$	Seaton and Osterbrock [1957]
31. $O^+(^2P) \rightarrow O^+(^4S) + h\nu$	$A = 0.048 s^{-1}$	Seaton and Osterbrock [1957]
32. $O^+(^2P) + N_2 \rightarrow N_2^+ + O$	4.8×10^{-10}	Rusch et al. [1977]
33. $N(^2D) + NO \rightarrow N_2 + O$	7×10^{-11}	Black et al. [1969]
34. $N(^2P) + O_2 \rightarrow NO + O$	2.6×10^{-12}	Husain et al. [1974]

*Rates are in units of cm^3s^{-1} unless otherwise noted.

TABLE 3. Data and Theory for Orbit 425 at 25,425 Seconds UT

	I 4278	I 5200	NO ⁺	O ₂ ⁺	N ₂ ⁺	O ⁺	N ⁺	ΣN _i	Ne	Comment
Data	60	15	5 (4)	3.1 (4)	1.5 (3)	8.7 (3)	4.5 (2)	9.1 (4)	6.3 (4)	
					Theory					
1.	28	20	6.2 (4)	1.2 (4)	6.4 (2)	6.4 (3)	2.4 (2)	8.1 (4)	8.1 (4)	0.6 × [O]
2.	28	13	6.4 (4)	1.7 (4)	5.8 (2)	3.6 (3)	8.2 (1)	8.5 (4)	8.5 (4)	0.6 × [O] 2.9 × [O ₂]

TABLE 4. Data and Theory for Orbit 425 at 25,455 Seconds UT

	I 4278	I 5200	NO ⁺	O ₂ ⁺	N ₂ ⁺	O ⁺	N ⁺	ΣN _i	Ne	Comment
Data	50	16	3.8 (4)	4.7 (4)	3.1 (2)	2.3 (4)	2.1 (2)	1.1 (5)	5.8 (4)	
					Theory					
1.	30	25	6.5 (4)	1.2 (4)	8.0 (2)	9.2 (3)	3.2 (2)	8.7 (4)	8.7 (4)	0.6 × [O]
2.	29	17	6.7 (4)	1.7 (4)	7.4 (2)	5.0 (3)	1.1 (2)	9.0 (4)	9.0 (4)	0.6 × [O] 3.0 × [O ₂]

TABLE 5. Data and Theory for Orbit 431 at 69,680 Seconds UT

	I 4278	I 5200	NO ⁺	O ₂ ⁺	N ₂ ⁺	O ⁺	N ⁺	ΣN _i	Comment
Data	200	29	1.2 (5)	9.7 (3)	—	6.2 (3)	—	1.2 (5)	
					Theory				
1.	198	62	1.6 (5)	2.5 (4)	3.7 (3)	1.6 (4)	8.4 (2)	2.0 (5)	0.5 × [O]
2.	198	26	8.9 (4)	2.7 (4)	1.5 (3)	6.5 (3)	3.6 (2)	1.2 (5)	0.5 × [O] $t = 6.0$ seconds

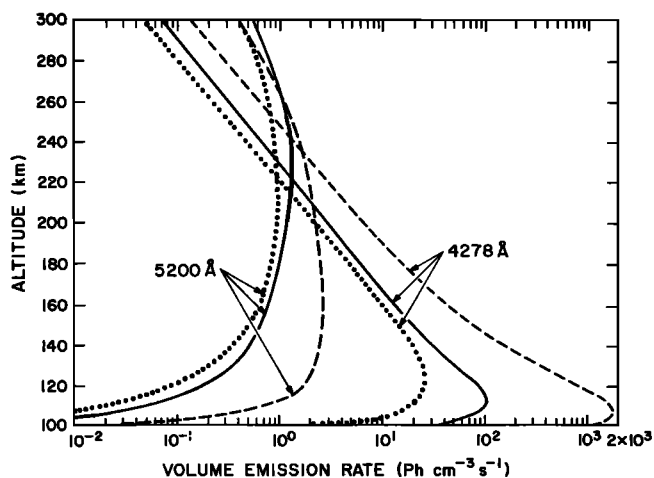


Fig. 4. The calculated altitude distribution of 4278-Å and 5200-Å emission for orbit 425 at 25,425 seconds UT for case 3 of Table 3 (---), for orbit 425 at 25,455 seconds UT for case 2 of Table 4 (—), for orbit 431 at 69,680 seconds UT for case 2 of Table 5 (---).

The agreement between the calculated and measured 4278-Å emission rates is within a factor of two for orbit 425. A similar discrepancy was encountered by *Kasting and Hays* [1977] upon comparing the 4278-Å intensities measured by VAE with those calculated from the particle flux.

In Figure 4 we show the volume emission rate profiles for case 2 of Tables 3, 4, and 5. The maximum volume emission rates for 4278-Å intensities are 26, 100, and 1.6×10^3 ph $\text{cm}^{-3}\text{s}^{-1}$, which correspond to 5200-Å maximum volume emission rates of 0.93, 1.3, and 2.1 ph $\text{cm}^{-3}\text{s}^{-1}$, respectively. This indicates that the shape of the incident energy flux and the neutral atmosphere play important roles in determining the 5200-Å intensity profile. Note that the peak intensity of 5200-Å for orbit 431 occurs at 140 km.

DISCUSSION AND CONCLUSIONS

Detailed comparison of the production and loss rates for N(²D) in the aurora and in the mid-latitude daytime ionosphere [*Frederick and Rusch*, 1977] show that the dominant sources of N(²D) are different in the aurorae. The production rates for N(²D) are displayed in Figure 5 for case 2 of orbit 425, at 25,425 seconds for the individual reactions. In the daytime, dissociative recombination of NO⁺ (reaction 16) and ionization interchange of N₂⁺ with O (reaction 7) dominate at altitudes above 150 km, and dissociative excitation of N₂ by energetic electrons (reaction 5) is a 10% source. In the aurora, at the altitudes studied, the three sources are very nearly equal if the efficiency for production of N(²D) by reaction 5 is effectively 80%. Also, the major quenching species in the standard model in the aurora is molecular oxygen due to the relatively low atomic oxygen density. At mid-latitudes, quenching by atomic oxygen dominates in the 200- to 240-km region, a fact which led *Frederick and Rusch* [1977] to infer the low quenching rate of N(²D) by O.

In the aurora, about four nitrogen atoms are produced for each N₂ ionization. Two nitrogen atoms are produced from each N₂⁺ ion, one from reaction 7 and one from the subsequent NO⁺ recombination, reaction 16. Further, the total cross section for the dissociation of N₂ by electrons [*Winters*, 1966] is nearly equal to the ionization cross section, so the rate of ionization of N₂ is nearly equal to the rate of N₂ dis-

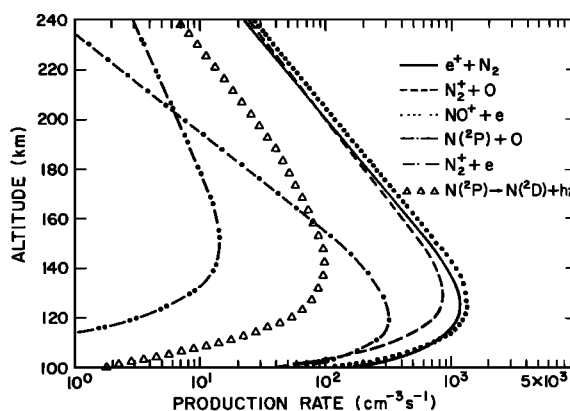


Fig. 5. The calculated production rates for N(²D) for case 2 orbit 425 at 25,425 seconds.

sociation. Thus four N atoms are produced for each N₂ ionization.

If we accept the efficiencies for the production of N(²D) by reactions 5, 6, 7, and 16 as 80%, 80%, 100%, and 80%, respectively, the total auroral efficiency for all sources for N(²D) production is 83%. This extremely high efficiency is required to satisfy the 5200-Å measurements. The efficiency for production of N(²D) by reaction 26 has been measured in the laboratory by *Kley et al.* [1977], and the 100% efficiency for reaction 6 is required by the dayglow measurements [*Frederick and Rusch*, 1977] and supported by the theoretical calculations of *Oran et al.* [1975]. However, there has been no firm indication of the combined efficiency of reactions 5 and 6. From this study we infer that this efficiency must be large, probably near 80%, in agreement with the value inferred from studies of the nitric oxide density in the lower thermosphere [*Cravens et al.*, 1979].

The calculations are subject to uncertainties, because the auroral histories are unknown, and time variations in the electron precipitation during the measurement period are difficult to discern.

We conclude that the chemistry adopted adequately explains the measured 5200-Å emission in the aurora. This chemistry is consistent with the requirements of the daytime mid-latitude ionosphere and measurements of the N(²D) density in the mid-latitude dayglow.

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