

EFFECT OF THE NO CONCENTRATION ON THE RATIO $I_{557.7}/I_{427.8}$ IN AURORAS

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Abstract. We have examined the effect of the nitrogen oxide concentration on the ratio between $\lambda 557.7$ nm and $\lambda 427.8$ nm emission intensities in auroras caused by precipitating electron fluxes, using the numerical simulation method. The ratio $I_{557.7}/I_{427.8}$ has been shown to strongly depend on the NO concentration: the ratio decreases from 7 to 2 with increasing NO maximum concentration at the height profile from 10^7 to $3 \cdot 10^9$. This fact is in satisfactory agreement with experimental data. The effect of nitric oxide on the ratio has been demonstrated to occur through the excitation channel of

the emission $\lambda 557.7$ nm, namely, the dissociative recombination of the molecular oxygen ion $O_2^+ + e_{th}$ due to the ion deactivation by collision reaction with nitric oxide $O_2^+ + NO$.

Keywords: nitric oxide, 557.7 nm and 427.8 nm emissions, intensity ratio, aurora, modeling, electron precipitation.

INTRODUCTION

The results of previous studies indicate that the ratio $I_{557.7}/I_{427.8}$ varies in a fairly wide range from 2 to 10 [Maseide, 1967; Brekke, Henriksen, 1972; Gattinger, Vallance Jones, 1972; Henriksen, 1973; Mende, Eather, 1975; Shepherd, Gerdjikova, 1988; Steel, McEwen, 1990; Dashkevich et al., 2006]. Possible causes of the observed variability of the ratio were discussed in [Shepherd, Gerdjikova, 1988; Shepherd, Shepherd, 1995; Gattinger et al., 1996], in which the influence of two processes on the excitation of the 1S state of atomic oxygen in a neutral atmosphere was analyzed, namely variations in the parameters of the precipitating electron flux and variations in the atomic oxygen density. At the same time, the models describing excitation channels of the 1S state of atomic oxygen include only two main sources: a direct electron impact $O + e^* \rightarrow O(^1S) + e$ and a collision reaction $N_2(A^3\Sigma_u^+) + O \rightarrow O(^1S) + N_2(X^1\Sigma_g^+)$. As a result, in [Shepherd, Gerdjikova, 1988; Shepherd, Shepherd, 1995] it has been shown that the observed range of the $I_{557.7}/I_{427.8}$ variation cannot be caused by variations in the energy spectrum of the precipitating electron flux, but can be explained by variations in the atomic oxygen [O] density. In this case, the [O] density should vary within $(0.6 \div 2)MSIS[O]$. Gattinger et al. [1996] have drawn similar conclusions and have determined that the range of variation in [O] is $(0.5 \div 1)MSIS[O]$. Yet, such variations in oxygen concentration in the dark ionosphere are unlikely to occur during electron precipitation events.

In [Shepherd, Gerdjikova, 1988; Shepherd, Shepherd, 1995; Gattinger et al., 1996], the dissociative recombination reaction $O_2^+ + e_{th} \rightarrow O(^1S) + O(^1D)$ was not considered as one of the possible excitation channels

of the 1S state of atomic oxygen. This was due to the fact that, according to estimates obtained in [Gattinger et al., 1985, 1996], the dissociative recombination contribution to the excitation of the 1S state of atomic oxygen is less than 10 %. Note, however, that the contribution of the dissociative ion recombination O_2^+ largely depends on the nitric oxide concentration since NO is the main deactivator of the molecular oxygen ion in the reaction $O_2^+ + NO \rightarrow NO^+ + O_2$. In [Gattinger et al., 1985, 1996], the NO concentration was set as $4 \cdot 10^8$ cm $^{-3}$ and 10^9 cm $^{-3}$ in its height profile maximum, which led to assessing the contribution of the dissociative recombination reaction to the excitation of 1S atomic oxygen at less than 10 %. Direct estimates of the nitric oxide concentration in auroras demonstrate a fairly wide range of NO concentration variation $[NO]_{max}$ [Swider, Narcisi, 1977; Sharp, 1978; Siskind et al., 1989; Dashkevich, Ivanov, 2019]. Figure 1 shows the [NO] height profiles obtained from rocket and ground-based observations in auroras.

It is seen that $[NO]_{max}$ lies in a wide range from $3 \cdot 10^7$ to $3 \cdot 10^9$ cm $^{-3}$. Deans, Shepherd [1978] observed from mass spectroscopic measurements that $[NO]_{max}$ in the auroral region does not exceed 10^8 cm $^{-3}$. With a decrease in $[NO]_{max}$ less than 10^8 cm $^{-3}$, the effect of deactivation of molecular oxygen ion with nitric oxide will also decrease. It can therefore be expected that the contribution of the dissociative recombination reaction to the excitation of the atomic oxygen 1S state will increase and exceed the estimate of 10 %, which will directly affect $I_{557.7}/I_{427.8}$.

The purpose of this work is to study the degree of influence of $[NO]_{max}$ on $I_{557.7}/I_{427.8}$ observed in auroras. This paper focuses on studying the effect of $[NO]_{max}$ on the efficiency of the dissociative recombination reaction $O_2^+ + e_{th} \rightarrow O(^1S) + O(^1D)$, which is one of the significant excitation channels of the 1S state of atomic oxygen.

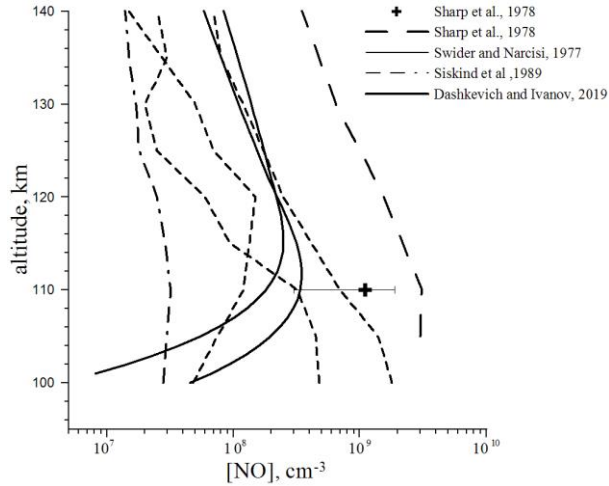
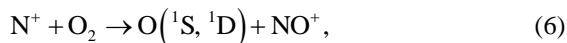
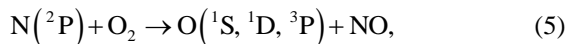
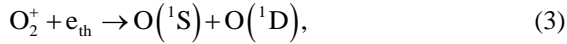
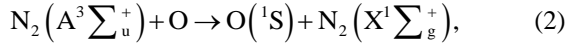


Figure 1. Estimated vertical profiles of NO concentration obtained from rocket and ground-based observations

1. THE EFFECT OF NITRIC OXIDE ON $\lambda 557.7$ nm EMISSION EXCITATION

The $\lambda 557.7$ nm emission arises from a transition from the 1S to the 1D level of atomic oxygen. In auroras, $O(^1S)$ atoms are excited both by the direct electron impact and by the collisional interactions between atmospheric components. Currently, six excitation channels of the 1S state of atomic oxygen are considered:



where e^* is a precipitating energetic electron; e_{th} is a thermal electron of ionospheric plasma.

Let us examine how $I_{557.7}$ can depend on $[NO]$. One of the excitation channels of the 1S state is reaction of dissociative recombination of molecular nitrogen ion (3). The effectiveness of this channel primarily depends on the quantity of molecular oxygen ions O_2^+ , generated in the region of electron precipitation, which depends on the effectiveness of reactions of O_2^+ deactivation with odd nitrogen $N(^4S)$, $N(^2D)$, and NO . The reaction rate constants of $O_2^+ + N(^4S)$, $O_2^+ + N(^2D)$, $O_2^+ + NO$ are comparable [Fensenfeld, 1977; Goldan et al., 1966], whereas $N(^4S)$ and $N(^2D)$ concentrations in auroras are by orders of magnitude lower than NO concentrations. The main process of ion deactivation O_2^+ can therefore be considered as $O_2^+ + NO$. A possible channel affecting $I_{557.7}$ is also the reaction of deactivation of the 1S state of atomic oxygen with nitric oxide $O(^1S)+NO$. The effect

of this reaction on $I_{557.7}$ is, nonetheless, insignificant due to the low rate of the reaction [Black et al., 1969].

The vertical profiles of the $\lambda 557.7$ volume emission rate are determined as follows:

$$\eta_{557.7}(h) = A_{1S \rightarrow 1D} [O(^1S), h],$$

where $\eta_{557.7}$ is the volume emission rate; $A_{1S \rightarrow 1D}$ is the Einstein coefficient for radiative transition $O(^1S \rightarrow ^1D)$ emitting $\lambda 557.7$ nm; $[O(^1S)]$ is the atomic oxygen concentration in the 1S state; h is the height.

Taking into account the mechanisms of excitation and deactivation of the 1S state of atomic oxygen [Dashkevich et al., 2017], the balance equation for calculating $[O(^1S), h]$ is as follows:

$$\begin{aligned} \frac{d}{dt} [O(^1S), h] = & Q_{1S}(h) + \sum_{ij} k_{ij} [N_i, h] [N_j, h] - \\ & - (A_{1S \rightarrow 1D}) [O(^1S), h] - \sum_i k_i [N_i, h] [O(^1S), h], \end{aligned}$$

where $Q_{1S}(h)$ is the production rate of the 1S state by an electron impact at a height h ; the second term describes the 1S state production by collisional interactions of i -type particles with j -type particles (1)–(6); the third term is applied to the deactivation of 1S state through the radiative transition $^1S \rightarrow ^1D$; the fourth term denotes the deactivation of the 1S state by collisional interactions; k_{ij} are the reaction rate constants; $A_{1S \rightarrow 1D}$ is the Einstein coefficient for the transition $^1S \rightarrow ^1D$.

Height profiles of the production rate of the 1S state due to electron impact (1) were calculated using the energy dissipation function and "energy costs" obtained by modeling the electron transfer process in atmospheric gases in accordance with the formulas

$$Q_{1S}(h) = P_O(h) \rho(h) \frac{1}{\varepsilon_{1S}} \Phi(F(E), h),$$

$$\Phi(F(E), h) = \int_E \frac{EF(E)}{R(E)} \lambda \left(E, \frac{z(h)}{R(E)} dE \right),$$

where $\Phi(F(E), h)$ is the total energy dissipated at a height h ; $P_O(h)$ is part of the energy used to excite atomic oxygen at a height h ; $\rho(h)$ is the neutral atmosphere density; ε_{1S} is the energy cost of excitation of 1S state of oxygen atom; $z(h)$ is the mass passed by an electron to a height h ; $R(E)$ is the integral path length; $F(E)$ is the energy spectrum of a precipitating electron flux; $\lambda \left(E, \frac{z(h)}{R(E)} \right)$ is the dimensionless energy dissipation function [Sergienko, Ivanov, 1993].

The $\lambda 557.7$ nm emission intensity

$$I_{557.7} = \int_{h_2}^{h_1} \eta_{557.7}(h) dh,$$

where h_1 and h_2 are the heights of the upper and lower boundaries of the aurora.

Numerical simulation of the excitation process of the 1S state of atomic oxygen caused by a precipitating electron flux has been carried out using the time-dependent model of polar ionosphere, described in [Dashkevich et al., 2017]. The model includes 56 physicochemical reactions describing the redistribution of dissipation energy of auroral electrons. MSIS-90 was used as a neutral-atmosphere model. Dashkevich, Ivanov [2022] have shown that $I_{557.7}/I_{427.8}$ weakly depends on the shape of the energy spectrum of auroral precipitation, but strongly depends on the average energy of the flux. In this paper, the energy spectrum of the precipitating electron flux is therefore given as Maxwell distribution

$$N(E) = N_0 E \exp(-E/E_0) / E_0^2,$$

where N_0 and E_0 are the initial particle flux and the characteristic energy respectively. The average energy of the flux E_{aver} , which has a Maxwellian distribution, corresponds to $2E_0$. The pitch angle distribution is taken as isotropic in the lower hemisphere.

Examine the effect of [NO] on the relative contributions of reactions (1)–(6) to the $\lambda 557.7$ nm emission excitation, assuming the total $I_{557.7}$ to be 1. In the calculations, E_{aver} varies in the range 1–20 keV, which is typical for auroral electrons [Vorobjev et al., 2013]. $[\text{NO}]_{\text{max}}$ varies in the range 10^7 – $3 \cdot 10^9$ cm^{-3} , which corresponds to the values observed in auroras. Figure 2 presents the results of modeling of relative contributions of reactions (1)–(6) on $[\text{NO}]_{\text{max}}$ for electron fluxes with an average energy of 1, 3, 7, and 15 keV.

The relative contributions of reactions (1), (2), (5), and (6) are seen to weakly depend on $[\text{NO}]_{\text{max}}$ for all average energies of the precipitating electron flux. Only the contributions of reactions (3) and (4) show a strong dependence: $\text{O}_2^+ + e_{\text{th}}$, $\text{O}_2^+ + \text{N}(^4S)$. Nonetheless, the absolute value of the relative contribution of $\text{O}_2^+ + \text{N}(^4S)$ is insignificant and amounts to less than 1 % over the entire range of average energies of the electron flux. We therefore examine in more detail the dependence of the relative contribution of $\text{O}_2^+ + e_{\text{th}}$ on $[\text{NO}]_{\text{max}}$. The calculated dependences of the $\text{O}_2^+ + e_{\text{th}}$

contribution to the excitation of the 1S state of atomic oxygen are shown in Figure 3 for average electron flux energies in the range from 1 to 20 keV.

Given that $[\text{NO}]_{\text{max}} > 2 \cdot 10^8$ cm^{-3} , the O_2^+ dissociative recombination contribution to the excitation of the $\lambda 557.7$ nm emission is seen to be less than 10 % and continues to decrease with an increase in the content of nitric oxide in the auroral region. This is consistent with the estimates obtained in [Gattinger et al., 1985, 1996]. However, the relative contribution of the dissociative recombination begins to increase when $[\text{NO}]_{\text{max}}$ decreases from $2 \cdot 10^8$ cm^{-3} . When $[\text{NO}]_{\text{max}}$ is 10^7 cm^{-3} , the relative contribution of $\text{O}_2^+ + e_{\text{th}}$ ranges from 20 to 41 % if E_{aver} is from 1 to 20 keV.

A similar behavior of this reaction as a source of excitation of the 1S state of atomic oxygen will inevitably lead to $I_{557.7}$ variations depending on [NO] during the aurora.

2. INTENSITY RATIO

$I_{557.7}/I_{427.8}$

Let us study the effect of [NO] on $I_{557.7}/I_{427.8}$. The $\lambda 427.8$ nm emission is one of the intense bands in ING N_2^+ resulting from the transition

$$\text{N}_2^+ \left(\text{B}^2 \sum_u^+, v'=0 \rightarrow \text{X}^2 \sum_g^+, v''=1 \right),$$

where v is a vibrational quantum number. The $\lambda 427.8$ nm volume emission rate at a height h is defined as

$$\eta_{427.8}(h) = A_{\text{B}^2, v'=0 \rightarrow \text{X}^2, v''=1} \left[\text{N}_2^+ \left(\text{B}^2 \sum_u^+, v'=0 \right) h \right],$$

where $\left[\text{N}_2^+ \left(\text{B}^2 \sum_u^+, v'=0 \right), h \right]$ is the concentration $\text{N}_2^+ \left(\text{B}^2 \sum_u^+, v'=0 \right)$; $A_{\text{B}^2, v'=0 \rightarrow \text{X}^2, v''=1}$ is the Einstein coefficient for the radiative transition $\text{N}_2^+ \left(\text{B}^2 \sum_u^+, v'=0 \rightarrow \text{X}^2 \sum_g^+, v''=1 \right)$, emitting $\lambda 427.8$ nm.

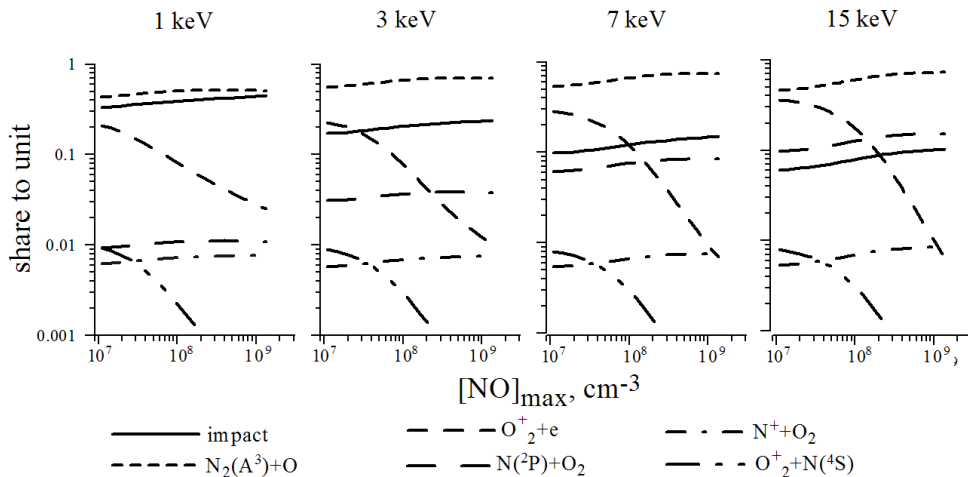


Figure 2. Dependence of relative contributions of six excitation channels of the 1S state of atomic oxygen on $[\text{NO}]_{\text{max}}$ for the average electron flux energies of 1, 3, 7, and 15 keV

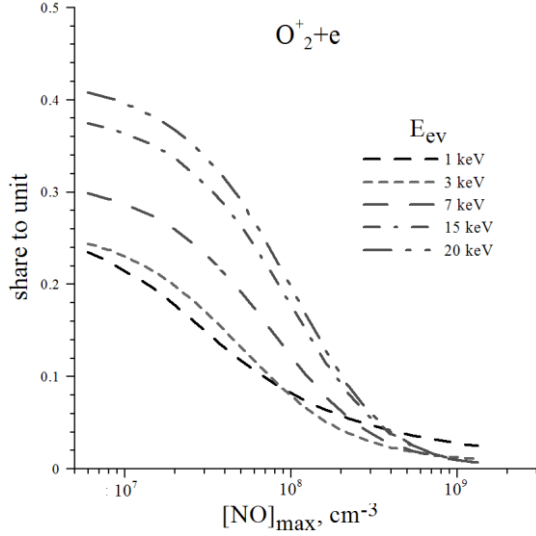


Figure 3. Dependence of the relative contribution of the O_2^+ dissociative recombination to excitation of the 1S state of atomic oxygen on $[NO]_{\max}$ for the average electron flux energies of 1, 3, 7, 15, and 20 keV

Given the short lifetime of the term $B^2 \sum_u^+$ ($\sim 10^{-7}$ s), the collisional deactivation of this state can be neglected, assuming that it is entirely excited only by an electron impact and is deactivated due to radiation transitions to the term $X^2 \sum_g^+$. In this case, the concentration of the molecular nitrogen ion N_2^+ in $B^2 \sum_u^+$, $v'=0$ under photochemical equilibrium conditions will be determined by a simple steady-state balance equation

$$0 = Q_{B^2, v'=0}(h) - \sum_{v''} A_{B^2, v'=0 \rightarrow X^2, v''} \left[N_2^+ \left(B^2 \sum_u^+, v'=0 \right), h \right],$$

where $Q_{B^2, v'=0}(h)$ is the production rate of the state $B^2 \sum_u^+$, $v'=0$ of N_2^+ by an electron impact at a height h , $A_{B^2, v'=0 \rightarrow X^2, v''}$ is the probability of radiative transition $N_2^+ \left(B^2 \sum_u^+, v'=0 \rightarrow X^2 \sum_g^+, v''=1 \right)$,

Then

$$\eta_{427.8}(h) = \frac{A_{B^2, v'=0 \rightarrow X^2, v''=0}}{\sum_{v''} A_{B^2, v'=0 \rightarrow X^2, v''}} Q_{v'=0}(h).$$

The height profiles of the production rate of the state $B^2 \sum_u^+$, $v'=0$, $Q_{B^2, v'=0}(h)$, were calculated in the same way as the height profiles of the atomic oxygen 1S state production rate, using the energy dissipation function and energy costs:

$$Q_{B^2, v'=0}(h) = P_{N_2}(h) \rho(h) \frac{q_{B^2, v'=0}}{\varepsilon_{B^2}} \Phi(F(E), h),$$

where $P_{N_2}(h)$ is the part of energy consumed to the

excitation of the nitrogen molecule at a height h ; $\rho(h)$ is the density of the neutral atmosphere at h ; $q_{B^2, v'=0}$ is the Franck—Condon factor defining the relative population $v'=0$ of vibrational level of $B^2 \sum_u^+$; ε_{B^2} is the energy cost of excitation of the state $B^2 \sum_u^+$ of N_2^+ ; $\Phi(F(E), h)$ is the total energy dissipated at a height h ; $F(E)$ is the energy spectrum of the precipitating electron flux.

The $\lambda 427.8$ nm emission intensity in the aurora

$$I_{427.8} = \int_{h_2}^{h_1} \eta_{427.8}(h) dh.$$

We calculated the intensity ratio $I_{557.7}/I_{427.8}$ for E_{aver} of the precipitating electron flux ranging from 1 to 20 keV. The value of $[NO]_{\max}$ varied from 10^7 to $4 \cdot 10^9$ cm^{-3} . The calculated dependences of $I_{557.7}/I_{427.8}$ on $[NO]_{\max}$ are shown in Figure 4.

The ratio $I_{557.7}/I_{427.8}$ is seen to strongly depend on $[NO]_{\max}$ in the entire range of average energies of the precipitating electron flux considered. The ratio $I_{557.7}/I_{427.8}$ decreases from ~ 7 to ~ 2 with an increase in $[NO]_{\max}$ from 10^7 to $3 \cdot 10^9$ cm^{-3} . The obtained $I_{557.7}/I_{427.8}$ values are in satisfactory agreement with the values observed in auroras. The effect of the precipitating electron average energy on $I_{557.7}/I_{427.8}$ is much weaker than the effect of $[NO]_{\max}$. In the range of average energies of precipitating electrons 1–20 keV, $I_{557.7}/I_{427.8}$ ranges from 6 to 7 when $[NO]_{\max}$ is 10^7 cm^{-3} and from 2 to 3 when $[NO]_{\max}$ is $3 \cdot 10^9$ cm^{-3} . This result is in agreement with the results obtained in [Shepherd, Gerdjikova, 1988; Shepherd, Shepherd, 1995].

Sharp et al. [1979] presented the results of simultaneous measurements of $I_{391.4}$, $I_{557.7}$ and $[NO]$ in the aurora region. The intensity $I_{391.4}$ was recalculated into $I_{427.8}$. The resulting ratio $I_{557.7}/I_{427.8}$ and measured $[NO]$ are shown in Figure 4. The results of the model calculations are seen to agree with experimental data.

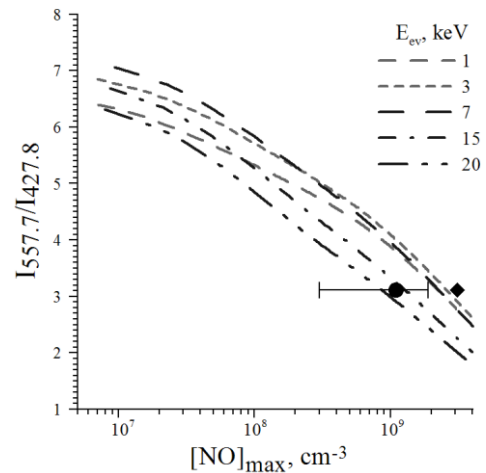


Figure 4. Dependence of the ratio $I_{557.7}/I_{427.8}$ on $[NO]_{\max}$ for average energies of 1, 3, 7, 15, and 20 keV. The solid circle and rhombus mark experimental data from [Sharp et al., 1979]

Thus, the $I_{557.7}/I_{427.8}$ variations observed in auroras may be caused not by variations in the concentration of atomic oxygen in the neutral atmosphere, as shown in [Shepherd, Gerdjikova, 1988; Shepherd, Shepherd, 1995; Gattinger et al., 1996], but by NO variations in the auroral region.

CONCLUSIONS

In this paper, we have examined the effect of the nitric oxide NO concentration on the intensity ratio $I_{557.7}/I_{427.8}$ in auroras produced by auroral electron fluxes. The ratio $I_{557.7}/I_{427.8}$ was demonstrated to strongly depend on $[\text{NO}]_{\text{max}}$ over the entire range of average energies typical for precipitating electron fluxes. The ratio decreases with increasing $[\text{NO}]_{\text{max}}$ from 10^7 to $3 \cdot 10^9 \text{ cm}^{-3}$. At the same time, $I_{557.7}/I_{427.8}$ ranges from 7 to 2, which is in satisfactory agreement with the range of ratio variations observed in auroras.

We have shown that the cause of the variability of the ratio $I_{557.7}/I_{427.8}$ is the deactivation of the molecular oxygen ion by nitric oxide, $\text{O}_2^+ + \text{NO}$, which leads to a change in the contribution of the dissociative recombination $\text{O}_2^+ + e_{\text{th}} \rightarrow \text{O}({}^1\text{S}) + \text{O}({}^1\text{D})$ to the production of the ${}^1\text{S}$ state of atomic oxygen.

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