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Study of the Earth's Own Radiation of the Upper Atmosphere (Herzberg I Bands) as a Function of Solar Activity, Atmospheric Temperature, and Seasons of the Year

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Abstract—The processes of excitation and quenching of electronically excited molecular oxygen $O_2(A^3\Sigma_u^+)$ in the Earth's atmosphere at nightglow sky heights are considered. The Herzberg I bands in the range of 250–360 nm have a wide spectrum of luminescence in the nightglow of the Earth. The volume intensity profiles of the Herzberg I bands of molecular oxygen in the Earth's atmosphere are calculated at night using data from a semiempirical model of the temperature response of the middle atmosphere depending on altitude, season, and solar activity at the Earth's midlatitudes. The calculations of the luminescence intensities of the Herzberg I bands are compared with the experimental data obtained from the Space Shuttle Discovery (STS-53) and from standard SP-48, SP-49, and SP-50 spectrographs from the 1950s–1960s. It is shown that the calculation results are in good agreement with the experimental data obtained from both the space shuttle and ground-based observations.

Keywords: atomic oxygen concentrations, calculations of luminescence intensities

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1. INTRODUCTION

The upper atmosphere of the Earth (above 80 km) is a very rarefied gaseous medium, the main components of which are atoms and molecules of nitrogen and oxygen, as well as hydrogen and helium. The so-called minor components—nitric oxide, carbon monoxide, etc., as well as metastable atoms and molecules, are important for the photochemistry and radiation of the upper atmosphere. As a result of exposure to the ionizing ultraviolet radiation of the Sun, numerous photochemical processes occur in the upper atmosphere, the consequence of which is the atmosphere's own radiation [1]. In this altitude region, molecular oxygen is dissociated by solar UV radiation. The processes of recombination of atomic oxygen lead to the formation of electronically excited O_2 molecules, which cause many emissions and affect the radiative balance of this region [1]. It is known that one of the sources of the glow of the Earth's night atmosphere is the electronically excited molecular oxygen $O_2(A^3\Sigma_u^+)$, which is formed during triple collisions in the Earth's atmosphere with the participation of two O atoms and a third particle

$$O + O + M \rightarrow O_2(A^3\Sigma_u^+; v') + M, \qquad (1)$$

where ν' are the vibrational levels of the $A^3\Sigma_u^+$ state and M is the third particle in the collision. Oxygen atoms are formed in the Earth's atmosphere during the daytime during the photodissociation of O_2 molecules by solar UV radiation $O_2 + h\nu \rightarrow O + O$. Triple collisions (1) with the formation of $O_2(A^3\Sigma_u^+)$ are most effective in a layer of the Earth's atmosphere about 10 km in thickness with a center at an altitude of about 90 km [1, 2]. Subsequently, the electronically excited oxygen molecule passes from the $A^3\Sigma_u^+$ state to the ground state $X^3\Sigma_g^-$ while emitting Herzberg I bands. In this work, the processes of excitation and quenching of electronically excited molecular oxygen $O_2(A^3\Sigma_u^+)$ are considered. At the same time, it should be noted that the Herzberg I bands in the range of 250–360 nm have a wide emission spectrum in the own radiation of the Earth's upper atmosphere at night.

$$O_2(A^3\Sigma_u{}^+, v') \rightarrow O_2\ (X^3\Sigma_g{}^-, v'') + h\nu_{HI}. \qquad (2)$$

This paper uses experimental data on the characteristic of [O] concentrations in the aforementioned layer based on the luminescence characteristics of atomic oxygen O for different months of the year under low ($F_{10.7}$ = 75, 1976 and 1986) and high ($F_{10.7}$ = 203, 1980 and 1981) solar activity at midlati-

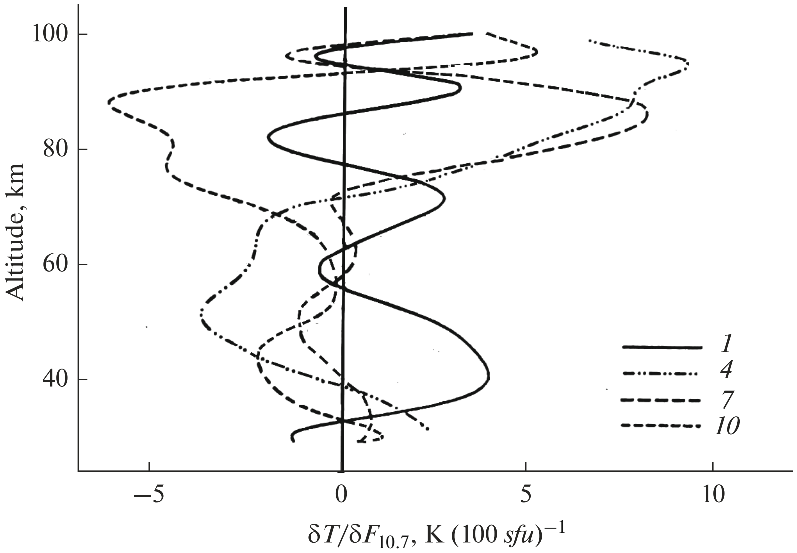

Fig. 1. Model altitude distributions of the temperature response to solar activity for 4 months of the year (*1* is January, *4* is April, *7* is July, and *10* is October) at altitudes of 30–100 km [1]. On the abscissa axis: $\delta T/\delta F_{10.7}$, K (100 sfu)$^{-1}$—the values of the atmospheric temperature response to solar activity at $F_{10.7}$ = 100 sfu; *y* axis: height values in kilometers.

tudes (55.7° N; 36.8° E), Zvenigorod Observatory at the Obukhov Institute of Atmospheric Physics, Russian Academy of Sciences (IAP RAS). Regular data on the luminescence of atomic oxygen were obtained from a semiempirical model integrating several types of different midlatitude measurements, regression relations, and theoretical calculations over several decades by the staff at the IAP RAS [1]. At middle latitudes, the 557.7 nm emission is excited mainly in the altitudinal region of 85–115 km with an intensity maximum at ~97 km. An increase in solar activity leads to an increase in the O concentration at the layer maximum and to a lowering of its lower boundary [4]. Results [1, 3] showed a significant scatter in the absolute concentration values of atomic oxygen at the maximum of the layer, the height of which was also not constant. The results of model calculations for the 557.7 nm emission revealed that there is a negative correlation between the height of the maximum concentrations of atomic oxygen and their values. Moreover, a negative correlation is clearly observed between the emission intensity of 557.7 nm and the height of the maximum of the emitting layer, both for seasonal variations and for the dependence on solar activity [5, 6]. As a result of changes in the concentration profiles of atomic oxygen, the rate profiles of the formation of electronically excited molecular oxygen O_2^* in the Earth's atmosphere inevitably change as a result of the process of triple collisions (1) and the emission intensity of various bands of molecular oxygen. Therefore, the glow intensity of the Herzberg I bands will depend both on the time of a year and on solar activity. In addition, paper [1] also presented the results of an analysis of the response of monthly average temperature values of the middle atmosphere on solar activity based on long-term data obtained using rockets and spectrophotometry of a number of emissions of its own radiation during several cycles of 11-year solar activity. The analysis was carried out in [7]. Based on these data, using the temperature differences for different heights of the profiles corresponding to the years of high and low solar activity, in a linear approximation it is possible to find the rate of temperature increase under the influence of solar activity:

$$\Delta T(Z) = \delta T_F(Z)(F_{10.7} - 130)/100, \text{ (K)}, \qquad (3)$$

where $\delta T_F(Z) = dt/df$ is the change in temperature at height Z at $\Delta F_{10.7}$ = 100 sfu. After determining the values of $\delta T_F(Z)$, seasonal temperature variations were plotted for individual altitude levels [1]. The altitude profiles of the rates of change in the temperatures of the middle atmosphere at different altitudes from solar activity indicate their pronounced altitude nonlinearity. Significant seasonal difference in the influence of solar activity in the mesopause region is obviously due to the difference in the altitude distributions of temperature depending on the time of a year [1]. Figure 1 presents the results of studies [1] based on an empirical model of temperature response to solar activity on height and season; the months are indicated by numbers: 1 is January, 4 is April, 7 is July, and 10 is October. On the abscissa: $\delta T/\delta F_{10.7}$, K (100 sfu)$^{-1}$ are values of the atmospheric temperature response to solar activity at $F_{10.7}$ = 100 sfu; along the *y* axis, altitude values are in km. Thus, the altitude distributions of the temperature response to solar activity at altitudes of 30–100 km indicate that significant seasonal temperature variations are observed at altitudes of ≈80–95 km

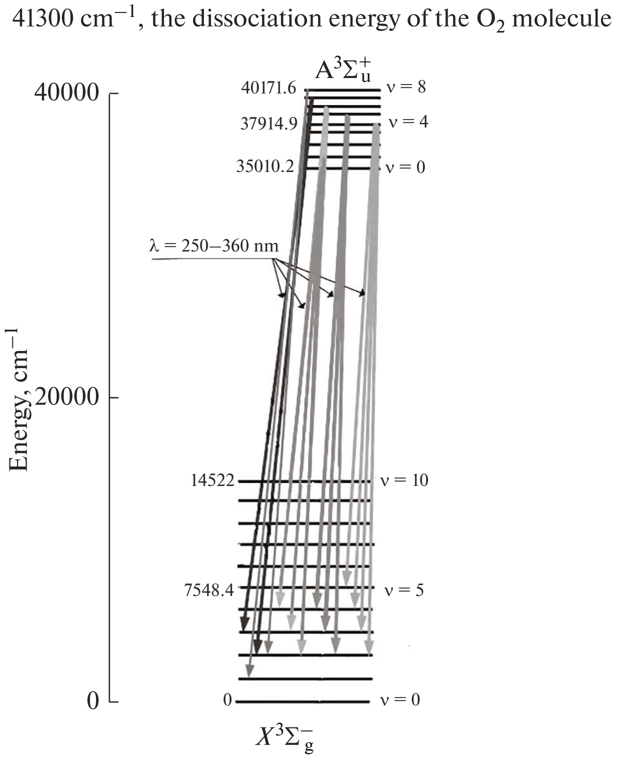

Fig. 2. Electronic transitions inside the O_2 molecule.

and minimal ones are at altitudes of ≈55–70 km. This is clearly seen from Fig. 1.

The purpose of this work is to compare the results of theoretical calculations of the luminescence intensities of the Herzberg I bands in the range of 250–360 nm with the experimental data on the intensity of the night-glow of molecular oxygen O_2^* in the own radiation of the Earth's upper atmosphere at night. Particular attention is paid to the peculiarities of the formation of different vibrational levels ν' of the electronically excited state $A^3\Sigma_u^+$ of the oxygen molecule as a result of triple collisions (1).

2. DESCRIPTION OF THE CALCULATION OF THE EXCITED OXYGEN $O_2(A^3\Sigma_u^+)$ CONCENTRATION

Figure 2 schematically shows several spontaneous radiative transitions from different vibrational levels of the electronically excited state $A^3\Sigma_u^+$ to different vibrational levels of the ground state $X^3\Sigma_g^-$ at which the Herzberg I bands are emitted. All of the above states are below the dissociation energy of the O_2 molecule ~41300 cm^{-1} (8065 cm^{-1} = 1 eV). Wavelength λ of the Herzberg I bands can be calculated using the formula

$$\lambda_{HI} = 1/(E_{A(v')} - E_{X(v'')}), \qquad (4)$$

where $E_{A(\nu')}$ (cm^{-1}) is the energy of the vibrational level ν' of the state $A^3\Sigma_u^+$; $E_{X(\nu'')}$ (cm^{-1}) is the energy of the vibrational level ν'' of the state $X^3\Sigma_g^-$. Since the transitions between the considered states are dipole-forbidden, then the characteristic radiative times of the states $A^3\Sigma_u^+$ are of the order of 1 and 0.1 s, respectively [8]. Therefore, when calculating the concentrations of electronically excited oxygen, it is necessary to take into account the quenching of the $O_2(A^3\Sigma_u^+)$ molecule not only during radiative transitions (2), but also during collisions with the main atmospheric components N_2 and O_2 in this altitude range [9]:

$$O_2(A^3\Sigma_u^+, v') + N_2 \rightarrow O_2 + N_2; \qquad (5a)$$

$$O_2(A^3\Sigma_u^+, v') + O_2 \rightarrow O_2 + O_2. \qquad (5b)$$

Since the concentrations of N_2 at altitudes of 90–100 km exceed 10^{13} cm^{-3} and the quenching constants of the $A^3\Sigma_u^+$ state are greater than ~10^{-12} cm^3 s^{-1} [9, 10], the collisional lifetimes of the considered vibrational levels of these states are either comparable or are much smaller than the radiative Herzberg I bands at night-glow heights. This means that the kinetics of Herzberg I states in the considered range of atmospheric altitudes is largely determined by collisional processes. Calculations of the concentration of excited oxygen $O_2(A^3\Sigma_u^+)$ at the heights of the Earth's upper atmosphere for vibrational levels ν' = 3–9 of this state for October 1976 and 1986 were carried out (low solar activity, $F_{10.7}$ = 75) [12]. The concentration of electronically excited oxygen $O_2(A^3\Sigma_u^+)$ was calculated according to the formula:

$$\begin{aligned}\left[O_2(A^3\Sigma_u^+, v')\right] &= q_{v'}^A \alpha_A k_1 [O]^2([N_2] \\ &+ [O_2])/(A_{v'}^A + k_{5a}[N_2] + k_{5b}[O_2]),\end{aligned} \qquad (6)$$

where α_A is the quantum yield of state $A^3\Sigma_u^+$ in triple collisions (1); $q_{v'}^A$ are the quantum yields of the vibrational levels ν' of this state; k_1 is the rate constant of the recombination reaction in triple collisions (1); k_{5a}, and k_{5b} are the rate constants of reactions (5a), (5b); and $A_{v'}^A$ is the sum of the Einstein coefficients for all spontaneous radiative transitions from the vibrational levels v' of the state $A^3\Sigma_u^+$. The recombination reaction rate constant k_1(cm^6 s^{-1}) was used as a calculated value depending on the temperature of the atmosphere in the considered height interval according to [1]; the quenching constants of electronically excited oxygen in collisions of molecular oxygen $O_2(A^3\Sigma_u^+)$ with atmospheric components N_2 and O_2, k_{5a}(cm^3 s^{-1}), k_{5b}(cm^3 s^{-1}), were taken into account according to [9, 10]; quantum yields $\alpha_{A'}$ and α_A were taken into account according to [13], and Einstein coefficients for all spontaneous transitions were taken into account according to [8]. An analytical formula for calculating quantum yields $q_{v'}^{A}$ was presented in [9]:

$$q_{v'} \sim \exp\left[-(E_{A',A(v')} - E_0)^2/\beta^2\right], \qquad (7)$$

where $E_0 = 40000$ cm^{-1}, $\beta = 1500$ cm^{-1} are the parameters determined by the least squares method by comparing the calculated vibrational populations of the $A^3\Sigma_u^+$ state with the results of ground-based observations. However, in [12], the quantum yields $q_{v'}^{A}$ were corrected based on a comparison of the calculated intensities of the Herzberg I bands measured from the Space Shuttle Discovery (STS-53). In this paper, we use $q_{v'}^{A}$ according to [11].

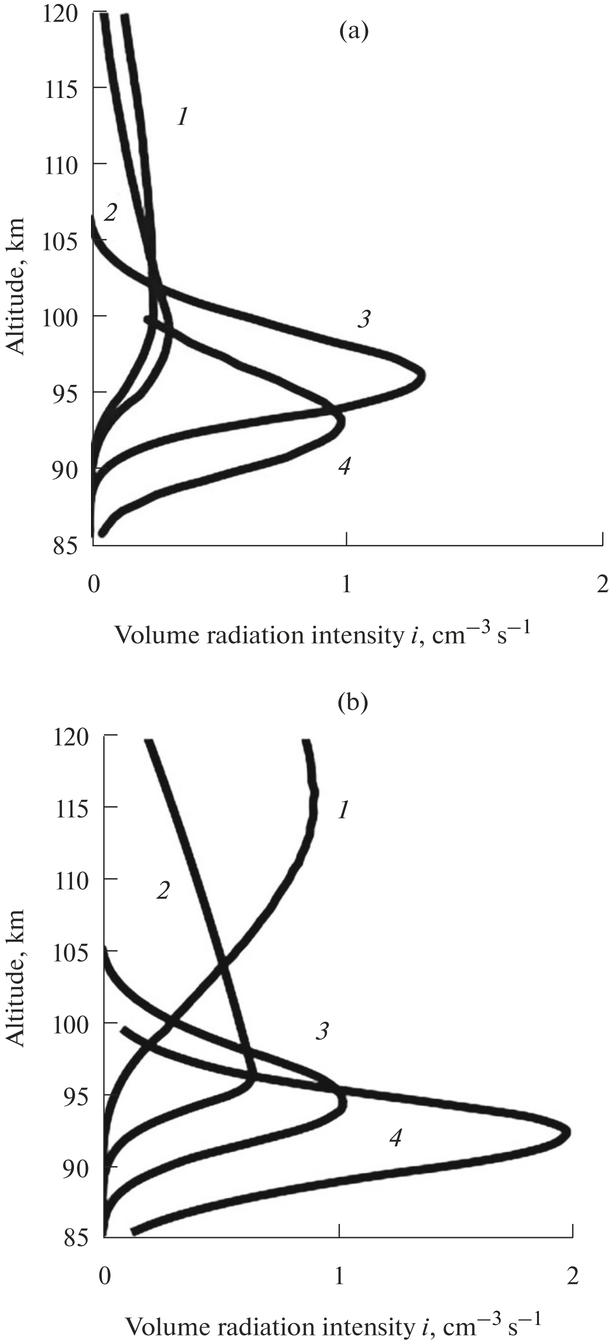

Fig. 3. Altitude distributions of the volume radiation intensity $i_{v'v''}$ (cm^{-3} s^{-1}) of Herzberg I (a) for high solar activity and (b) for low solar activity for different months of the year (1 is January, 2 is April, 3 is July, and 4 is October) at the middle latitudes of the Earth. The abscissa axes show the values of the volume radiation intensity i (cm^{-3} s^{-1}); the ordinate axes show heights in kilometers.

3. RESULTS OF CALCULATING THE EMISSION INTENSITY OF THE HERZBERG I BANDS

According to formula (6), the vertical distribution profiles of the concentrations of electronically excited molecular oxygen O_2^* were calculated for the $A^3\Sigma_u^+$ state in the Earth's upper atmosphere. When calculating the concentrations of electronically excited oxygen, we used altitude temperature profiles compiled on the basis of long-term (1960–2000) measurements of temperature profiles at altitudes of 30–110 km [7]. The method developed by these authors for calculating altitude profiles of temperature and total concentration of the atmosphere makes it possible to determine the temperature and density of the atmosphere at middle latitudes for given heliogeophysical conditions (altitude, solar activity level, and year number). The values of the volume intensities of the radiation bands corresponding to the transitions (2) were calculated by the formula

$$i_{v'v''}\left(\text{cm}^{-3}\text{s}^{-1}\right) = [O_2^*]\, A_{v'v''}, \qquad (8)$$

where $[O_2^*]$ (cm^{-3}) is the calculated concentration of electronically excited oxygen O_2^* depending on height h [12]; $A_{v'v''}$ (s^{-1}) is the Einstein coefficient corresponding to the spontaneous radiative transition from vibrational level v' of the upper state to the vibrational level v'' of the lower state in (2) [8]. Figure 3 shows the calculated height distributions of the volume emission intensities of the bands associated with the spontaneous transition $A^3\Sigma_u^+ (v' = 6) \rightarrow X^3\Sigma_g^- (v'' = 3)$ (3a, 3b) for low ($F_{10.7}$ = 75, 1976 and 1986) (3a) and high ($F_{10.7}$ = 203, 1980 and 1981) (3b) solar activity at the middle latitudes of the Earth. The numbers represent the months of the year: 1 is January, 2 is April, 3 is July, and 4 is October. The calculations used data on atomic oxygen concentrations and temperatures for the average months of each season. The abscissa axes show the values of the volume radiation intensity i (cm^{-3} s^{-1}); the ordinate axes show heights in kilometers. Figure 4a shows a fragment of the average night sky glow spectrum in the range of 250–360 nm, respectively, measured by the spectrograph from the

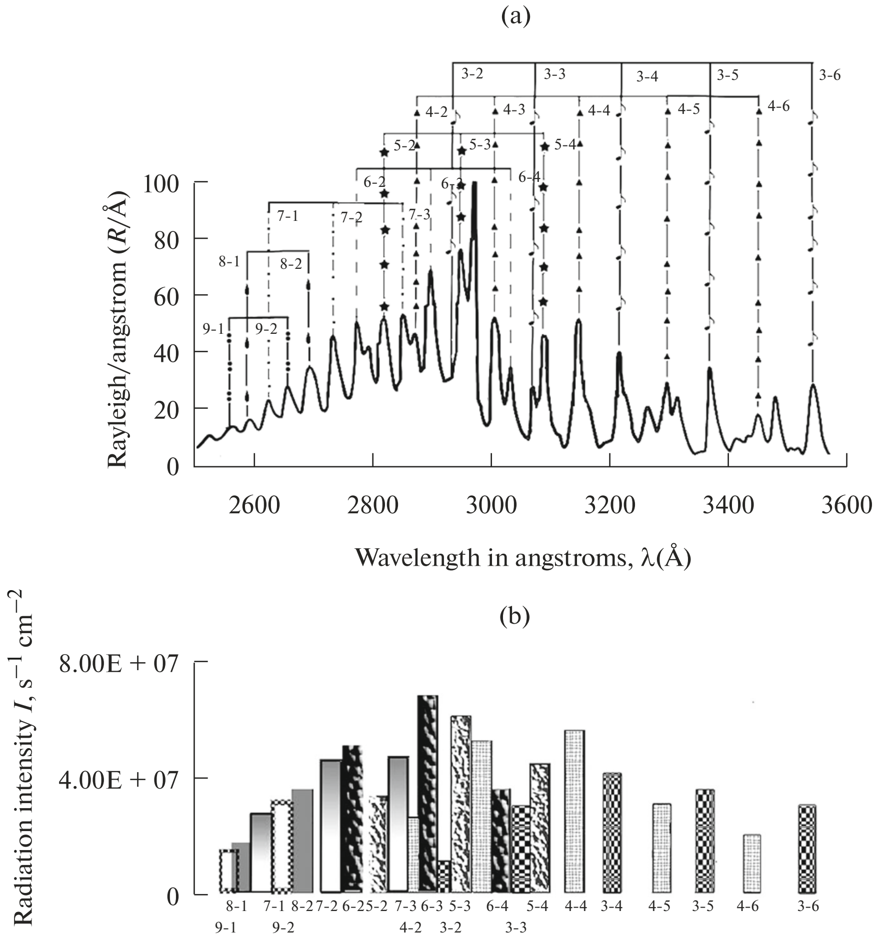

Fig. 4. (a) Fragment of the average night sky glow spectrum in the range of 250–360 nm measured by a spectrograph from the space shuttle [2]: the Rayleigh/angstrom values (R/Å) are along the ordinate axis; the wavelengths λ (Å) are along the abscissa axis; and the numbers above the peaks are (v'–v'') for radiative transitions (2). (b) Emission intensities for various Herzberg I bands.

Space Shuttle Discovery (STS-53) in the range from 115 to 900 nm during its 12-day mission in January 1995 (low solar activity conditions) [2]. The ordinate axes show the intensities in Rayleighs/angstroms (R/Å) (1 R = 10^6 photon/cm^2 s); the abscissa axes show the wavelengths in angstroms (λ(Å)). Both numbers above the luminescence peaks denote vibrational levels (v'–v'') during radiative transitions (2). The calculated values of the radiation intensity I (cm^{-2} s^{-1}) (histograms) for various Herzberg I bands due to radiative transitions (2) were obtained for October 1976 and 1986 (conditions of low solar activity $F_{10.7}$ = 75) in the same wavelength range. The results of the calculations are shown in Fig. 4b. While recalculating the volumetric radiation intensity $i_{v'v''}$ into the radiation intensity $I_{v'v''}$, the approximation of an optically thin layer is used; i.e., the absorption of photons inside the layer is neglected. In this case, in contrast to the results of [12], the radiative transitions from the ninth vibrational level v' = 9 of the $A^3\Sigma_u^+$ state are taken into account and the intensities of the Herzberg I bands (9-1) and (9-2) located in the range of 255–270 nm are given. As can be seen from Fig. 4, there is a good agreement between the calculated intensities of the excited oxygen emission bands O_2^* ($A^3\Sigma_u^+$, v' = 3–9) and the spectrum obtained from the shuttle [2]—the experimental data of the night sky glow in the range of 250–360 nm. Figure 5a shows the results obtained by ground-based long-term measurements of the emission spectrum of the nighttime upper atmosphere in the UV wavelength range of 305–395 nm, i.e., the Herzberg I band [14]. The observations were carried out during the period of high solar activity using standard Soviet SP-48, SP-49, and SP-50 spectrographs of the 1950s–1960s [1]. The theoretically calculated intensities of the Herzberg I bands for the period of high solar activity are shown in Fig. 5b. As can be seen from the comparison of Fig. 5a and Fig. 5b, the calculated intensities of the Herzberg I bands are in good agreement with the experimental data. A comparison of the theoretically calculated intensities of the Herzberg I bands with the experimental data [14] makes it possible to identify the max-

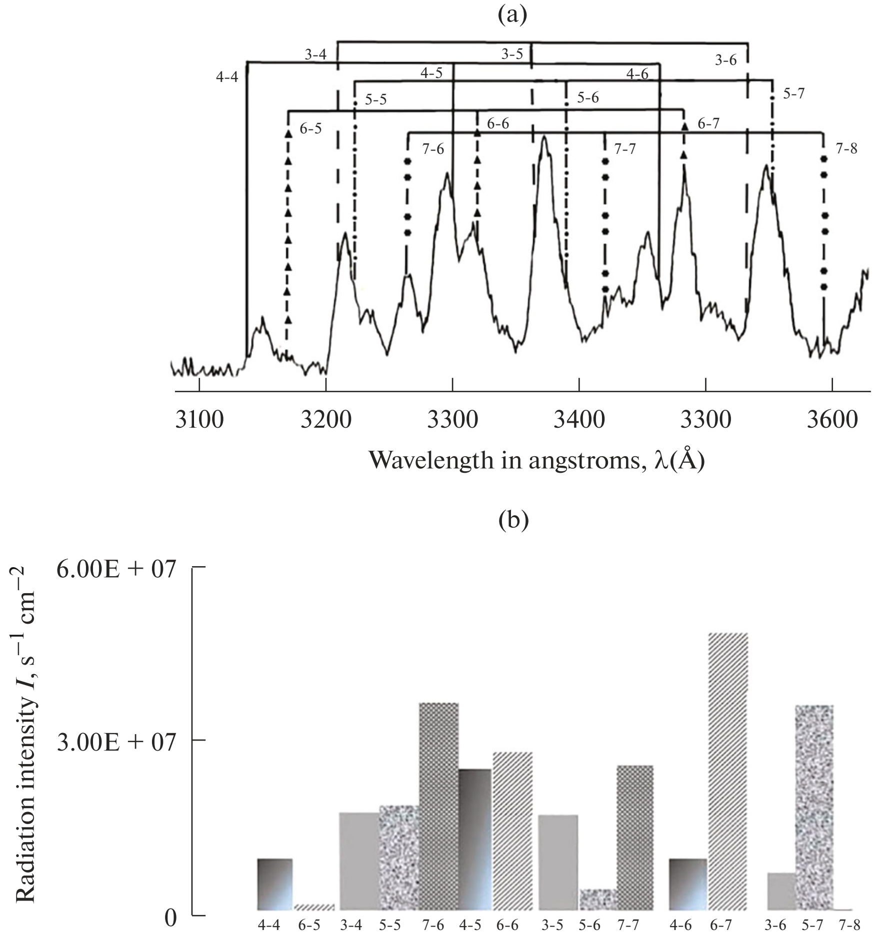

Fig. 5. (a) Radiation spectrum of the nighttime upper atmosphere in the UV wavelength range of 305—395 nm, Herzberg I bands, obtained by ground-based observations [14]. (b) Values of the emission intensity of the Herzberg I bands.

ima in the obtained spectra: the maximum at 315 nm is due to the band (4-4); 321—323 nm, bands (3-4) and (5-5); 327—332 nm, bands (7-6), (4-5), and (6-6); 337 nm, bands (3-5) and (5-6); 342—348 nm, bands (7-7), (4-6), and (6-7); 355 nm, bands (3-6) and (5-7).

4. CONCLUSIONS

Several spontaneous radiative transitions are schematically presented (Fig. 2) from different vibrational levels of the electronically excited state $A^3\Sigma_u^+$ to different vibrational levels of the ground state $X^3\Sigma_g^-$ at which Herzberg I bands are emitted. Calculations of the concentration of excited oxygen $O_2(A^3\Sigma_u^+)$ at the altitudes of the Earth's upper atmosphere for vibrational levels $v' = 3 - 9$ of this state have been carried out. When calculating the concentrations of electronically excited oxygen, the quenching of the $O_2(A^3\Sigma_u^+)$ molecule is taken into account not only during radiative transitions (2), but also during collisions with the main atmospheric components N_2 and O_2 in a given altitude range: 85—100 km [9]. The values of the emission intensity of the Herzberg I bands due to radiative transitions from the vibrational levels $v' = 3$—9 of electronically excited oxygen $O_2(A^3\Sigma_u^+)$ for low ($F_{10.7} = 75$, 1976 and 1986) and high ($F_{10.7} = 203$, 1958 and 1959) solar activity for middle latitudes are obtained. The emission intensity of the Herzberg I bands under conditions of low solar activity is compared with the experimental data obtained in the wavelength range of 250—360 nm by a spectrograph from the space shuttle during its 12-day STS 53 mission in September 1995 (years of low solar activity) [2]. The result of a comparison of the calculated values with the experimental data is a good agreement between the calculated intensities of the excited oxygen emission bands O_2^* ($A^3\Sigma_u^+$, $v' = 3$—9) and the spectrum obtained from the shuttle [2] the experimental data of the night sky glow in the range of 250—360 nm, which can be seen from Fig. 4. The calculated values of the emission intensity of the Herzberg I bands under conditions of high solar activity were also compared with experimental data obtained in the wavelength range of 305—395 nm by standard ground-based Soviet spectrographs of the 50s–60s [14]. The results obtained by these long-term measurements of the emission spectrum of the night-time upper atmosphere are in good agreement with the calculated values of the emission intensity of the Herzberg I bands. A comparison of the theoretically calculated intensities of the Herzberg I bands with experimental data [14] allows us to identify the maxima in the obtained spectra: the maximum at 315 nm is due to the band (4-4); that at 321–323 nm is due to bands (3-4) and (5-5); at 327–332 nm to bands (7-6), (4-5), and (6-6); at 337 nm to bands (3-5) and (5-6); at 342–348 nm to bands (7-7), (4-6), and (6-7); and at 355 nm to the bands (3-6) and (5-7).

CONFLICT OF INTERESTS

The authors declare that they have no conflicts of interest.

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