BRIGHTNESS OF THE O₂ ATMOSPHERIC BANDS IN THE DAYTIME THERMOSPHERE

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Abstract — The Fabry-Perot interferometer on *Dynamics Explorer* 2 was used as a low sensitivity photometer to study the O_2 Atmospheric A band during the daytime. A study of the brightness of the emission showed that the assumed source of $O_2(b^1\Sigma_g^+)$ in the thermosphere, $O(^1D)$, can account for the observed intensity up to about 250 km but with a significantly different scale height. This combined with an enhanced brightness above this altitude suggests an additional source for this emission.

INTRODUCTION

An extensive set of observational data exists for the emission of the O_2 atmospheric bands $(b^1\Sigma_a^+ - X^3\Sigma_a^-)$ under nighttime and auroral conditions. Reported studies of daytime observations, however, are limited to that of Wallace and Hunten (1968). They observed the (0-0) and (0-1) bands with rocket-borne photometers from approx. 40 to 130 km, and concluded that above 100 km quenching of $O(^{1}D)$ by O_{2} is the predominant mechanism for the excitation of the $O_2(b^1\Sigma_a^+)$ state. Since their observations did not extend above 130 km this hypothesis could not be checked for the upper thermosphere. The Fabry-Perot interferometer on Dynamics Explorer 2 (DE-FPI) had a filter which transmitted the A band of the O2 atmospheric band system. The instrument allowed the daytime emission to be observed from the lowest observation tangent point ($\simeq 60 \text{ km}$) to 300 km. In this paper these data will be used to infer the brightness of the O₂ bands on various occasions during the life of DE-2 (August 1981) to February 1983) and to confirm that O(1D) can account for the magnitude of the observed brightness of $O_2(b^1\Sigma_q^+)$ in the thermosphere up to about 250 km, although the scale heights are considerably different. Above this altitude the observed brightness exceeds the calculated one. This paper will address these issues and consider the possibility of additional sources of $O_2(b^1\Sigma_a^+)$ in the thermosphere.

MEASURED SURFACE BRIGHTNESS

The Fabry-Perot interferometer on *DE-2* has been discussed in some detail elsewhere (Hays *et al.*, 1981; Killeen *et al.*, 1982, 1983; Rees *et al.*, 1982; Skinner, 1984) and only the most salient points are mentioned here and summarized in Table 1. The interferometer

was a single etalon with solid spacers and had a 12-channel concentric ring detector which was used to scan in wavelength. A mirror system provided a limb scan consisting of 16 spectra. Depending on the satellite altitude and orientation the tangent point altitude ranged from roughly the satellite altitude to as low as 60 km. *DE*-2 was in a polar orbit and data were taken at all latitudes and solar zenith angles. This analysis is limited to conditions with low magnetic latitudes and low solar zenith angle.

The O₂ emission was studied by using the interferometer as a photometer. In order to relate the signal to the brightness it is necessary to consider the

Table 1. Characteristics of DE-FPI at 7650 Å

Parameter	Value
Etalon gap	1.2615 cm
Free spectral range (FSR)	0.39536 cm ⁻¹ 0.2316 Å
Number of channels per FSR	12.36
Fraction of FSR on detector	97.1%
Spacing/channel	0.032 cm ⁻¹
	0.019 Å
Reflectivity	62% @ 7650 Å
Filter	ZnS-Cryolite layers, single cavity, dielectric blocking to 5000 Å
Peak position	7668.3 Å
Peak transmission	63.5%
Halfwidth	30.2 Å
Detector	
anode structure	12 concentric rings equal area anodes
photocathode	S 20
Interferometer field of view	0.44 degrees
Sensitivity to O2 bands	360 Rayleighs per count

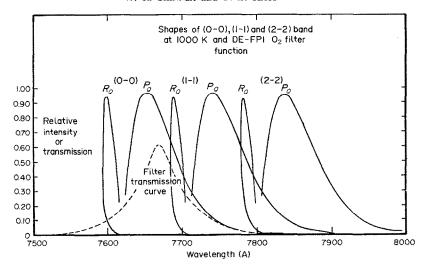


Fig. 1. Transmission function of *DE*-FPI O₂ filter (dashed line) and the envelope of the rotational intensity distribution of the (0-0), (1-1), and (2-2) atmospheric bands (solid lines). Only the envelopes for the ^RQ and ^PQ branches are shown but the P and R branches are very similar. The bands are shown with equal strength and with a temperature of 1000 K.

vibrational transitions transmitted by the filter. Besides the (0-0) band for which the filter was designed, it can also transmit the (1-1) and (2-2) bands. Figure 1 shows the filter transmission curve and the line strength envelopes of the main branches of the (0-0), (1-1), (2-2) bands. For purposes of illustration the bands are shown with the same intensity and reveals that the (1-1) band in particular can be significantly transmitted. The filter passes about 25% of the (0-0) band, 20% of the (1-1), and 2% of the (2-2), with these values nearly independent of temperature. If the bands are in thermodynamic equilibrium then in a hot thermosphere $(T \simeq 1500^{\circ})$ the (1-1) band can contribute up to 30% of the total signal while the (2-2) band will be insignificant. The atmospheric bands are so strong that it is unlikely that contaminant emission could compete in intensity. Because of the excess emission seen at high altitudes, however, the possibility of contaminant emission will be considered in the discussion section. The following data analysis assumes only the (0-0) and (1-1) bands are contributing to the signal.

The brightness of the O_2 emission band can be estimated by using the *DE*-FPI as a photometer instead of an interferometer. A Fabry-Perot interferometer behaves as a photometer if the signal is summed over a free spectral range. The situation is slightly complicated in this case due to the large number of lines transmitted. The brightness from a series of lines, such as the O_2 band, is just the summation of the brightness from each line (Skinner, 1984). The resulting signal from a given

detector channel k will be (Hays et al., 1981):

$$\begin{split} N_k &= C\Delta t \left(\frac{1-R}{1+R}\right) B \sum_{n=1}^{16} S_J T_F(v_J) \\ & \cdot \left[a_{0k} + \sum_{n=1}^{16} R^n \, \mathrm{e}^{-(\pi n G)^2} \right. \\ & \cdot \left[a_{nk} \cos \left(\frac{2\pi n (v_J - v_k)}{\Delta v_{\mathrm{FSR}}}\right) + b_{nk} \sin \left(\frac{2\pi n (v_J - v_k)}{\Delta v_{\mathrm{FSR}}}\right) \right] \end{split}$$

$$(1)$$

where k ranges from 1 to 12, C is the sensitivity, Δt is the integration time, B is the band brightness, S_J is the normalized line strength of line J, v_J is the position of line J, $T_F(v_J)$ is the filter transmission at v_J , a_{nk} and b_{nk} are the Fourier coefficients representing the instrument function, $\Delta v_{\rm FSR}$ is the free spectral range, R is the reflectivity of the etalon plates, v_k is the peak for detector channel k, and $G = \Delta v_e/\Delta v_{\rm FSR}$. All emission lines that have a significant intensity must be included in the sum. The molecular parameters needed to calculate the O_2 atmospheric band line strengths and positions were obtained from Babcock and Herzberg (1948) and the Hönl-London factors were from Schlapp (1937).

The 12 detector channels comprise almost exactly one free spectral range and since the value of each Fourier component does not vary much from channel to channel, then if the signal from each channel is summed [equation (1)] all the Fourier terms vanish

except for the zero order and the sum (N_{sum}) reduces to:

$$N_{\text{sum}} \simeq C\Delta t \left(\frac{1-R}{1+R}\right) B \sum_{J} S_{J} T_{F}(v_{J}) \sum_{k} a_{0k}$$

$$= C'B \tag{2}$$

 C^{\prime} a constant. Simulations indicate that the wavelength dependent term

$$\sum_I S_J T_F(v_J)$$

equals 0.25 for the (0-0) band and 0.20 for the (1-1) band, independent of temperature. This combined with the fact that the Franck–Condon factors for the (0-0) and (1-1) bands are only 15% apart (Nicholls, 1965) means that it is not necessary to be concerned about the origin of the emission as long as it is from the (0-0) or the (1-1) band. All other calibration constants are known leading to a value for C' of about 0.003 counts per Rayleigh.

This estimated photometric sensitivity of the DE-FPI was used to provide the brightness of the O_2 emission feature for approx. 10 orbits throughout the life of DE-2. Averaged data for individual orbits are plotted in Fig. 2 and show the horizontal line of sight

brightness for high sun conditions (solar zenith angle less than 65°) and low magnetic latitude (magnetic latitude is less than 55°). The data show this emission to be extremely bright in the daytime theremosphere, with a line of sight brightness exceeding 10 kR at 250 km.

THEORETICAL CALCULATION

The brightness of the $O_2(b^1\Sigma_g^+ - X^3\Sigma_g^-)$ emission as observed from the satellite was calculated assuming production from O(1D) and resonance scattering. Quenching of the $O_2(b^1\Sigma_a^+)$ state by N_2 and O_2 was included in the calculation but is negligible except at the lowest altitudes (Wallace and Hunten, 1968). At low altitudes the density of O(1D) was calculated from the photolysis of O₂. The density of O(¹D) at higher altitudes was estimated using volume emission rates obtained from the Visible Airglow Experiment (VAE) on the Atmosphere Explorer (AE) satellites (Havs et al., 1973). Two profiles were obtained, one from near solar minimum (Hays et al., 1978 and Torr et al., 1981) and another from AE-E near solar maximum in 1981 (V. J. Abreu, private communication, 1983). This latter profile was obtained using an inversion technique

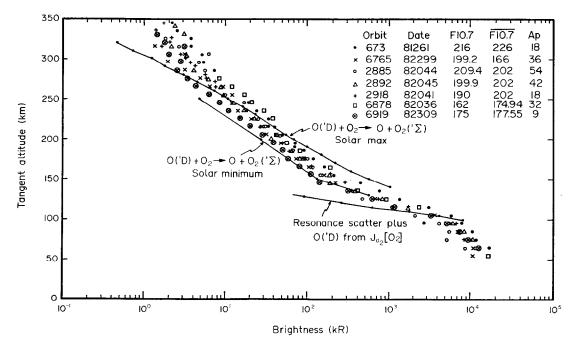


FIG. 2. SURFACE BRIGHTNESS OF THE O_2 ATMOSPHERIC BANDS AS OBSERVED BY DE-2. Data were taken for low magnetic latitude and low solar zenith angle conditions. Theoretically calculated brightnesses are also shown. The high altitude profiles were calculated from the quenching of $O(^1D)$. The $O(^1D)$ profiles were obtained from AE data. The low altitude profile included resonance scattering and quenching of $O(^1D)$. Here $O(^1D)$ was calculated from photolysis of O_2 .

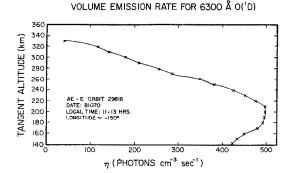


Fig. 3. O(1 D) red line volume emission rate for AE-E orbit 29818.

This corresponds to near solar maximum.

described by Fesen and Hays (1982) and is shown in Fig. 3. The shape of this profile was confirmed by comparing with measurements of 6300 Å emission taken by DE-FPI at the same time as the O_2 emissions. The volume emission rates were converted to densities by using the Einstein coefficient value of 0.00515 s⁻¹ given by Kernahan and Pang (1975).

The volume emission rate of $O_2(b^1\Sigma_g^+)$ in the thermosphere, where quenching is insignificant, is given by $k_O[O_2][O(^1D)]$. The O_2 densities were obtained from the MSIS-83 neutral atmosphere model (Hedin, 1983). Assuming the emission to be exponential in character the surface brightness will be (in Rayleighs):

$$B = 10^{-6}k_0[O_2][O(^1D)]\sqrt{2\pi(R_e + Z_T)H}$$
 (3)

with $k_0 = 2.5 \times 10^{-11}$ cm³ s⁻¹ (Link *et al.*, 1981), *H* the emission scale height, Z_T the tangent point altitude and R_s the radius of the Earth.

The results of the calculation are shown in Fig. 2 and the results at first appear encouraging. The calculated brightness at 200 km is 70 kR which is in reasonable agreement with the observed average of $\simeq 50$ kR. However, there are two distinct areas of disagreement. First, the scale heights of the profiles are considerably different. The calculated scale height of $O_2(b^1\Sigma_a^+)$ is a combination of the O(1D) and O2 scale heights. The scale height of the topside of the O(1D) profile is found from the DE-FPI data to be 56 km above 240 km. The MSIS-83 model gives an O_2 scale height of $\simeq 36$ km in the same region. This suggests that the emission profile should have roughly a scale height of 22 km. The average scale height of the $O_2(b^1\Sigma_q^+)$ emission is much larger and close to the predicted O₂ scale height, 37 km. It would take a major change in the scale heights to obtain agreement. The O2 scale height in this region would need to be over 100 km, while the O(1D) density

would need to be nearly constant with height. Slightly lower, near the peak of the $O(^1D)$ density, the O_2 emission scale height should be very close to the O_2 scale height. In this instance the $O(^1D)$ peak is near 200 km and the MSIS-83 O_2 scale height is $\simeq 28$ km. The actual emission scale height is still of the order of 35 km, a difference of 25%. The second problem concerns an excess of emission at high altitudes. The emission at 300 km is of the order of 3 kR which is about a factor of 3 more than is accounted for by the simple model. This discrepancy becomes increasingly worse at higher altitudes. This at first may appear to be a result of the smaller scale height of the calculated emission but a closer examination reveals the possibility that the emission scale height is increasing above 300 km.

DISCUSSION

Although the above arguments present strong evidence for another source of $O_2(b^1\Sigma_g^+)$ there are other alternatives that should be considered before a conclusion is reached. There is the possibility that the model atmosphere is not supplying reliable O_2 densities. Since O_2 is difficult to measure at these altitudes this alternative cannot be eliminated. As noted above the scale height of O_2 would have to be increased an unrealistic amount to obtain agreement.

One should also consider the possibility that emissions due to sources other than O2 may be responsible for the additional signal. Since the filter was about 60 Å wide there are several candidates. One possible source of contamination is the background continuum usually thought to be due to the chemiluminescence reaction $NO + O \rightarrow NO_2 + hv$. At night this process forms a layer near the height of the O2 atmospheric bands and has a value of roughly 1 R Å⁻¹ (Gadsden and Marovich, 1973). It would take an unrealistic enhancement during the day for this emission to be important to this measurement. For example, at 200 km the line of sight brightness of O₂ is about 60 kR. To be equal in intensity a continuum would have to be $\approx 1 \text{ kR Å}^{-1}$. At 100 km the band brightness rises to about 5000 kR and the background would need to be $\approx 85 \text{ kR Å}^{-1}$. These are clearly unrealistic and the background continuum can safely be ignored during the day.

The OH Meinel (9-4) band at 7748 Å can also be transmitted by the filter. OH emissions are usually considered mesospheric sources and should be unimportant at higher altitudes. The N_2 first positive bands are also a possibility. The (2-0) band at $\simeq 7754$ Å and the (3-1) band at $\simeq 7627$ Å (Vallance Jones and Gattinger, 1972) can both be transmitted to some extent. The total first positive band has an estimated

daytime vertical brightness of 6.6–28 kR (Feldman, 1972; Green and Barth, 1967) and the fraction in the (2-0) and (3-1) bands is probably much smaller than this. The $\rm O_2A$ band brightness during the day has an integrated vertical brightness of several hundred kR which means that unless the $\rm N_2$ first positive band is emitted from high altitudes, it cannot compete with the $\rm O_2$ emission.

One explanation for the additional emission might be direct excitation by photoelectrons $O_2 + e \rightarrow O_2(b^1\Sigma_g^+) + e$. This source can be estimated by the ratio of the production of $O(^1D)$ and $O_2(b^1\Sigma_g^+)$ by electrons:

$$\frac{P(O_{2}(b^{1}\Sigma_{g}^{+}))}{P(O(^{1}D))} = \frac{k_{O_{2}}n_{e}[O_{2}]}{k_{O}n_{e}[O]}$$

$$= \frac{k_{O_{2}}[O_{2}]}{k_{O}[O]} \tag{4}$$

where n_e is the density of electrons, $k_{\rm O_2}$ and $k_{\rm O}$ are unimolecular rate constants (Hays *et al.*, 1978). By referring to the cross sections for O and O₂ in Oran and Strickland (1976) a rough estimate for $k_{\rm O_2}/k_{\rm O}$ is 0.1. At 300 km the density of O is about 1.2×10^9 cm⁻³, that of O₂ about 1.2×10^7 cm⁻³ giving $P(O_2(b^1\Sigma_g^+))/P(O(^1D)) \simeq 10^{-3}$. The production of $O(^1D)$ for the conditions of interest is about 2.8×10^3 cm³ s⁻¹ and $P(O_2(b^1\Sigma_g^+)) \simeq 2.8$ cm³ s⁻¹. This mechanism falls more than an order of magnitude short of what is required.

Another scheme is a reaction with atmospheric metastables. The two that dominate at this altitude are O(¹D) and N(²D). No other species would appear to have the density required to produce the emission. Vallance Jones and Gattinger (1974) have speculated that the rate constant for the reaction

$$N(^{2}D) + O_{2} \rightarrow N + O_{2}(b^{1}\Sigma_{a}^{+})$$
 (5)

may be $\simeq 1 \times 10^{-12}$ cm³ s⁻¹. This reaction must compete with

$$N(^{2}D) + O_{2} \rightarrow NO + O \tag{6}$$

which has a rate of $\simeq 1 \times 10^{-11}$ cm³ s⁻¹ (Vallance Jones and Gattinger, 1974). This rate constant requires a density of 4×10^6 cm⁻³ at 300 km to make this process work. This would be several times higher than the 1×10^5 cm⁻³ given as typical by Torr and Torr (1982). The typical density would require a rate of 4×10^{-11} cm³ s⁻¹. However, this would give about twice the $O_2(b^1\Sigma_g^+)$ density at 200 km, which would destroy the good agreement between theory and measurements there. Unless the number densities of N(2 D) at around 300 km are considerably enhanced near solar maximum, this cannot provide the additional source.

Another avenue is the possibility of some sort of ionneutral interaction. This usually takes the form of a charge exchange but perhaps some fraction may excite $O_2(b^1\Sigma_a^+)$. The main ionic species at these altitudes is O+ which can appear in two forms that can transfer energy to O_2 , $O^+(^2P)$ and $O^+(^2D)$. The transition $O^{+}(^{2}P^{-2}D)$ emits a photon with an energy of 1.69 eV (7320 Å) making it only 0.07 eV out of resonance with the (0-0) transition of O_2 (7620 Å). However, the number density of O⁺(²P) at 300 km is only 250-300 cm⁻³ which would require a rate coefficient of $\simeq 1.4$ $\times 10^{-8}$ cm³ s⁻¹. O⁺(²D) has a density an order of magnitude higher and requires a rate $\simeq 2 \times 10^{-9}$ cm³ s^{-1} . The charge exchange between $O^{+}(^{2}D)$ and O_{2} has been estimated to be $\simeq 1 \times 10^{-9}$ cm³ s⁻¹ [Torr and Torr (1982)]. The rate for production of $O_2(b^1\Sigma_q^+)$ by this process seems to require a rate coefficient larger than that for charge exchange which is unlikely for this type of reaction. The emission of $O_2(b^1\Sigma_a^+)$ at high altitudes cannot be adequately explained by the processes described here.

SUMMARY

The (0-0) and (1-1) bands of the O_2 atmospheric system were observed with the Fabry-Perot interferometer on the DE-2 satellite. The band brightness was estimated by using the instrument as a low sensitivity photometer. The observed brightness was found to be in accord with commonly accepted theory for the production of $O_2(b^1\Sigma_g^+)$, which is energy transfer of $O(^1D)$ between 140 and 250 km. However, the scale height is significantly different. Above 250 km the theory and measurements become increasingly dissimilar. This suggests an additional source is needed for the O_2 atmospheric band emission, one which becomes increasingly important at higher altitudes. The mechanism has not been identified in the work.

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