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SHORT PAPERS

UPPER LIMITS TO [O] IN THE LOWER THERMOSPHERE FROM AIRGLOW

William E. Sharp

Space Physics Research Laboratory/Atmospheric and Oceanic Science
The University of Michigan
Ann Arbor, Michigan 48109

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INTRODUCTION

A review of the measurements of the atomic oxygen densities in the lower thermosphere/upper mesosphere has been given by Offermann, *et al.*, (1981). This is for *in situ* determinations by various techniques. The data show a variation in the concentrations by over a factor of 10 at 120 km, a factor of 40 for the peak at about 95 km and much larger factors below this. Peak concentrations range from 6×10^{10} cm^{-3} to 2×10^{12} cm^{-3}. Within any one technique there are factors of 5 variations over altitude. Some of this variation can be due to time of day, season, and dynamics. However, the principal source of the variation is probably the differing measurement techniques.

The oxygen airglow emissions have long been discussed as well as used for the remote sensing of the oxygen concentrations. An example is the 5577A emission (Donahue, *et al.*, 1973; Wasser and Donahue, 1979). The difficulty here is being confident in the details of the production source. The recombining oxygen atoms are producing the airglow; however, there is some evidence to suggest that the mechanism may not be straight forward (McDade, *et al.*, 1982).

This note points out a means of estimating the upper limit to the oxygen atom concentrations based on the energetics of the recombination process and the radiation from the excited levels.

THE PROCESS

The recombination process can be described by two reactions:

$$O + O + N_2 \rightarrow O_2 + N_2 : K_1 \qquad (1)$$

$$O + O + O_2 \rightarrow O_2 + O_2 : K_2 \qquad (2)$$

The energy available in the association reaction is 5.11 eV or 8.2×10^{-12} ergs. While the loss rate of oxygen atoms is comparable for (1) and (2) (Campbell and Gray, 1973; Schofield, 1979), the efficiency for production of specific excited states in reaction (2) can be several hundred times that for reaction (1) (Kenner and Ogryzlo, 1980). The first assumption made is that some fraction of energy of (2) is lost by radiation and that the recombination energy of (1) is given to translational energy (heating). The relative concentration of N_2 to O_2 is about 4 and K_1/K_2 is about 1.60 between 85 km and 105 km. Thus, 6 out of 7 recombinations are with N_2 and this leads to heating of the mesopause region. If ε is less than unity, then a larger fraction of the recombinations can lead to heating.

The energy density available in the recombination is given by:

$$E = 8.2 \times 10^{-12} \times K_2 \times \varepsilon \times [O_2] \times [O]^2 \qquad (3)$$

or by rearrangement

$$[O] = \sqrt{\frac{E/\varepsilon}{8.2 \times 10^{-12} \times K_2 \times [O_2]}} = 4.2 \times 10^{21} \sqrt{\frac{E}{\varepsilon[O_2]}} \qquad (4)$$

$K_2 = 3 \times 10^{-33}$ cm^3 sec^{-1} at 300°K (Schofield, 1979). K_2 will assuredly be much larger at 200°K since K_1 increases by a factor of 2.3 (Campbell and Gray, 1973). This factor of increase is adopted for K_2.

A second assumption is that there is little quenching in this altitude region. A justification of this will be given below. Figure 1 illustrates the airglow emission rates typical for these altitudes. The solid lines represent values deduced from typical measurements (Witt, et al., 1979; Thomas and Young 1981). The bars in each profile represent the range of several reported measurements for each emission. It is suggested (Vallance Jones, 1973) that 98% of the IR Atmospheric emission is in the 0,0 band at 1.27μ with no evidence for emission from v'>0 and that 94% of the Atmospheric emission is in the 0,0 band at 7620Å with no evidence for emission from v'>0. There is evidence for auroral excitation of the v'>0 levels (Gattinger and Vallance Jones, 1974). The molecular emissions in figure 1, therefore, can represent the total for that state. In the analysis which follows use will be made of the typical as well as the upper bounds.

For each state there is the amount of energy to produce that state: O(^{1}S) requires 4.17 eV (6.7×10^{-12} ergs), A$^3\Sigma_u^+$ requires 4.8 eV (7.7×10^{-12} ergs), b$^1\Sigma_g^+$ requires 1.6 eV (2.5×10^{-12} ergs), and a$^1\Delta$g requires 1.0 eV (1.6×10^{-12} ergs). With this information we can reconstruct the data of figure 1 to give the energy density released in the radiative process. This is shown in figure 2 where typical profile and limits are retained. The dashed line in figure 2 represents the sum of the energy released. The upper limit to the energy released is given by the dot-dashed curve. Thus, in both cases the dominate amount of energy is released by the a$^1\Delta$g state.

It is clear that the only state for which the no quenching assumption needs to be examined is the a$^1\Delta$g state. When a currently recommended quenching rate for a$^1\Delta$g by O_2 (2×10^{-18} cm^{3}sec^{-1}; Anderson, 1976) is used, then about 15% of the emission is quenched at 80 Km and 6% is quenched at 90 Km. The other oxygen emissions would require 60% of the emmission to be quenched at 90 Km to substantially alter the conclusions. Studies have shown the quenching fraction to be considerably less for the Herzberg I (Thomas, 1981) and for the Atmospheric (Greer, et al., 1981) band systems.

The efficiency of a$^1\Delta$g production can be estimated in the following manner. The estimate makes no assumption about the particulars of the recombination process. It only considers the output of the process when two atoms recombine in the presence of a third body. The Herzberg I bands are produced with an efficiency of 0.025 at 200°K in the laboratory (Kenner and Ogryzlo, 1980). This is compared with theoretical estimates of 0.05 (Wraight, 1980; Smith, 1984). This is good agreement given the accuracies of both methods. The I.R. Atmospheric bands are calculated to be produced with an efficiency of 0.05 (Wraight, 1982, Smith, 1984). There are no laboratory results reported. The theoretical calculations suggest, then, that these two band systems should have the same intensity. However, from figure 1 it is clear that in the region of little or no quenching (above 96 km) the I.R. Atmospheric emission rate is 60 times the Herzberg I emission rate. This factor times the laboratory efficiency for Herzberg I gives an estimate for the I.R. atmospheric efficiency of 1.5. Using the theoretical Herzberg I efficiency an efficiency of 3.0 is found; however, 2.0 is the upper bound because only 2 molecules are present at the end of the reaction. It appears, therefore, that the efficiency to produce the I.R. Atmospheric emission is between 1.5 and 2.

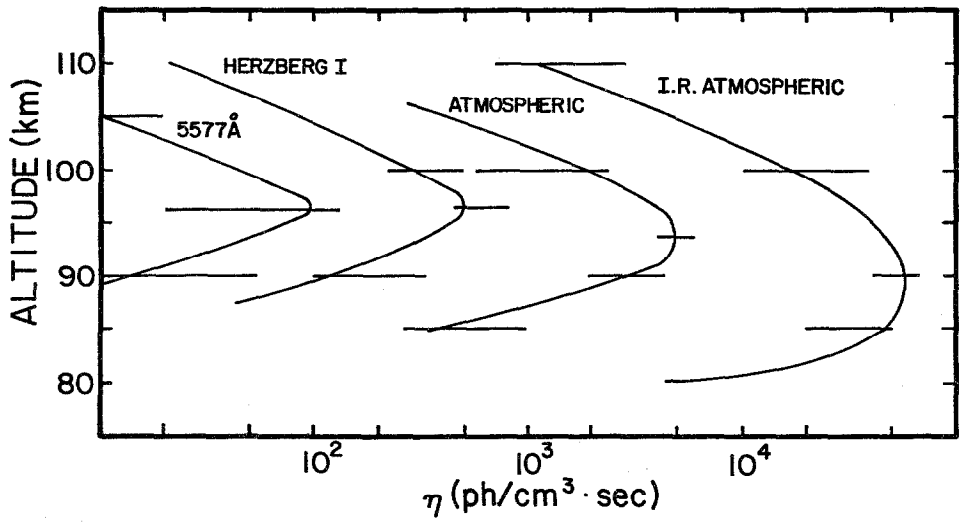

Fig. 1. Typical oxygen airglow volume emission rates. The solid lines are from particular measurements. The bars represent the spread among several measurements.

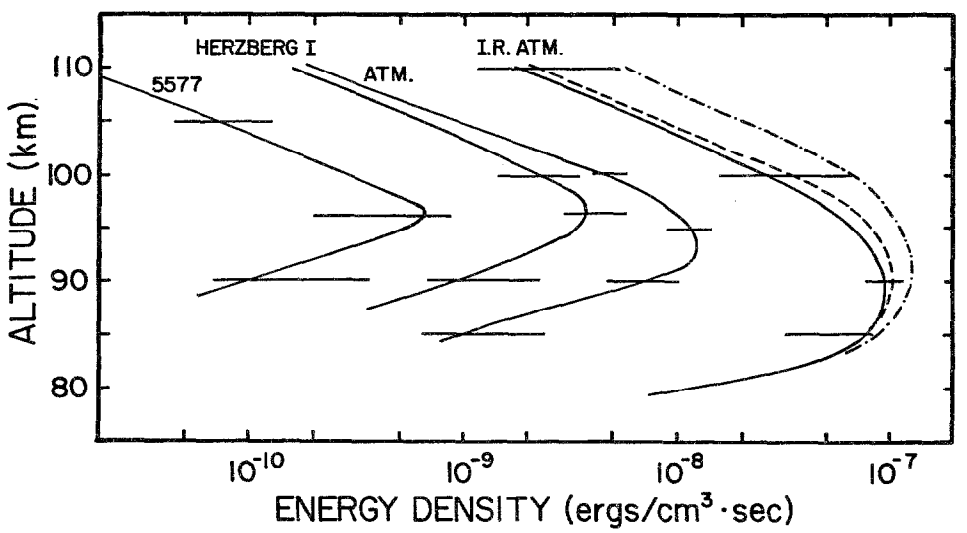

Fig. 2. The energy density released by the airglow emissions. See text.

Table 1 lists the atmospheric model used in estimating the [O] density from equation (4). The mean CIRA 1972 [O_2] reference atmosphere is used. The resulting [O] estimates are calculated using the data from figure 2 and efficiencies of 1.5 and 2.

TABLE 1: [O] estimates

H (Km)	[O_2] cm^{-3}	[O] cm^{-3}		
		Typical (ε=2.0)	Limit (ε=2)	Typical (ε=1.5)
85	5.3 (+13)	1.5 (+11)	1.6 (+11)	1.7 (+11)
90	1.6	2.4	2.7	2.8
95	5.5 (+12)	3.8	4.2	4.2
100	2.0	3.7	5.6	4.3
105	7.0 (+11)	3.2	4.9	3.8
110	2.8	2.5	3.9	2.9

read 5.3 (+13) as $5.3 \times 10^{+13}$

DISCUSSION

Table 1 indicates that the [O] densities at the peak of the profile will generally not excede 5.5×10^{11} cm^{-3} and will usually be less than 4×10^{11} cm^{-3}. This is in marked contrast to many published measurements of the peak density (see review by Offerman, et al., 1981). We suggest that the large values are clearly in error because of instrumental and/or measurement problems. We don't rule out that dynamics can cause some variations in concentrations (Frederick, 1978).

This study also suggests that the recombination process of oxygen atoms with O_2 through whatever path produces over 1.5 oxygen molecules in the $a^1\Delta g$ state. Such an investigation of this efficiency is currently underway in the laboratory (Slanger, private communication, 1984).

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