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THE EXCITATION OF O_2 IN AURORAS

Prepared by D. C. CARTWRIGHT
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Laboratory Operations
THE AEROSPACE CORPORATION

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FOREWORD

This report is published by The Aerospace Corporation, El Segundo, California, under Air Force Contract No. F04701-71-C-0172.

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Approved

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Space Physics Laboratory

Curtis D. Williams

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Project Officer

ABSTRACT

Newly measured electron impact cross sections for excitation of the a $^1\Delta_g$ and b $^1\Sigma_g^+$ electronic states of O_2 have been employed to predict the absolute volume emission rates from these states under auroral conditions. A secondary electron flux typical of an IBC II nighttime aurora was used and the most important quenching processes were included in the calculations. The new excitation cross sections for the a $^1\Delta_g$ and b $^1\Sigma_g^+$ states are more than an order of magnitude larger than previous estimates, and lead to correspondingly greater intensities in the atmospheric and IR-atmospheric band systems. The calculated intensity ratios of the volume emission rates of 7621A and 1.27μm to that for 3914A are smaller than obtained from aircraft observations and recent rocket experiments.

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CONTENTS

TABLES

FIGURES

I. INTRODUCTION

Very intense emission of 1.27 μm radiation has been detected from auroras in both aircraft and rocket experiments, the magnitude of which greatly exceeded that predicted by using the previously available electron-impact excitation cross sections. Although Llewellyn et al., (1969) saw only a small enhancement during the NASA Airborne Auroral Expedition, Noxon (1970a) measured intensities of 1.27 μm which lead to the "energy-available paradox" in that the emissions are stronger than can be explained by the same excitation source that produces the 3914A radiation from N_2^+. Schiff et al., (1970) and Megill et al., (1970) have reported auroral rocket observations of 1.27 μm emissions for which the measured intensities also lead to the "energy-available paradox" as based on the intensity of the 3914A radiation.

New electron-impact cross sections for excitation of the a $^1\Delta_g$ and b $^1\Sigma_g^+$ states have recently been obtained (Trajmar et al., 1971) which are more than a factor of 30 greater than the previous values. In this paper, these new excitation cross sections, along with the measured secondary electron spectrum and recently reported quenching rates, are used to determine what fraction of the measured oxygen emissions can be attributed to direct electron impact excitation, and their volume emission rates relative to that for 3914A.

II. EXCITATION AND QUENCHING OF a $^1\Delta_g$ and b $^1\Sigma_g^+$

A. Transition Probabilities and Quenching Coefficients.

The two excited electronic states of O_2 arising from the (core) $3\sigma_g^2\ 1\ \pi_u^4\ 1\ \pi_g^2$ electron configuration, are respectively 0.977 and 1.63 eV above the ground vibrational level of the ground electronic state. Figure 1 is a schematic diagram of the first two vibrational levels for the X $^3\Sigma_g^-$, a $^1\Delta_g$ and b $^1\Sigma_g^+$ electronic states of O_2. In it are given the band origin wavelengths for the more important transitions in the Infrared Atmospheric, Atmospheric and Noxon band systems, the natural lifetimes for the two excited states, and the quenching species of importance at auroral altitudes for each excited state. The spectroscopic data used to generate the potential energy curves and corresponding Franck-Condon factors for the three electronic states are those discussed by Albritton et al., (1972). For transitions connecting these three electronic states, only the lowest two vibrational levels of each are important because all three states have nearly the same internuclear distance. The lifetime of the a $^1\Delta_g$ state was taken to be $3.9 \times 10^{+3}$ sec (65 min) as determined by Badger et al., (1965). A lifetime of 12 seconds for the b $^1\Sigma_g^+$ state (Zipf, 1969) was used to determine the transition probabilities for the b $^1\Sigma_g^+ \rightarrow$ x $^3\Sigma_g^-$ (atmospheric bands) band system and the results of Noxon (1961) used to determine the same for the Noxon bands. The transition probability for emission of 3914A radiation from N_2^+ was determined by using the recent lifetime results of Head (1971).

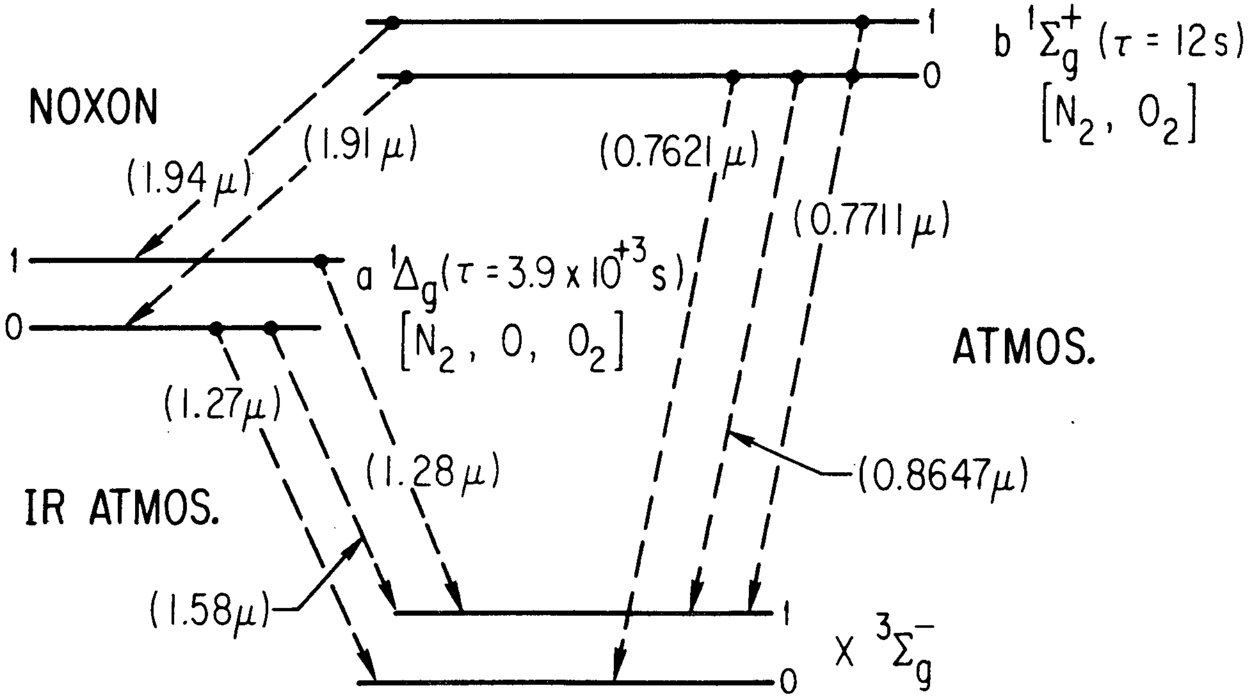

Figure 1. Schematic diagram for the lowest two vibrational levels of the first three electronic states of O_2. Indicated are some of the transitions connecting the various levels for the three different band systems, the natural lifetimes of the two excited states, and the most important quenching species at auroral altitudes.

The quenching rates used for this study are summarized in Table 1. The deactivation rates of a $^1\Delta_g$ by N_2 and O_2 were taken from Clark and Wayne (1969a) and Wayne (1969); those by O and N taken from Clark and Wayne (1969b). The quenching rates assumed for b $^1\Sigma_g^+$ by N_2 and O_2 were taken from Noxon (1970b) but no rates for quenching by O and N could be found. If only upper limits for a particular quenching species were given, that value was used in the calculations.

The atmospheric model used in these calculations correspond to the Model A atmosphere of Sharp (1970) which is essentially the 1965 CIRA model atmosphere at all altitudes except that it is richer in atomic oxygen below 120 km (Sharp, 1970).

B. Excitation Cross Sections

In Figure 2 are shown the total cross sections for elastic scattering (right hand ordinate) and for excitation of the a $^1\Delta_g$ and b $^1\Sigma_g^+$ states (left hand ordinate) obtained by Trajmar et al., (1971). The experimental values are given by the different symbols indicated with the corresponding error bars. The solid curves represent a best estimate to the shape of the cross sections which would pass through the datum points and are the cross sections used in these calculations. The open squares are the recent measurements of Linder and Schmidt (1971), from threshold to 4 eV, which are in excellant agreement with the cross section values used in these calculations. The curve labeled K in the figure is an estimate for the a $^1\Delta_g$ excitation cross section based on preliminary data by Konishi et al., (1970). Also shown in the figure is a previous estimate for the a $^1\Delta_g$ excitation cross section made by Watson et al., (1967) (curve marked by W) and previously used by Stolarski and Green (1967) to estimate auroral intensities of the O_2 emissions. Their cross section is more than an order of magnitude

TABLE I

Quenching rates for O_2 a $^1\Delta_g$ and b $^1\Sigma_g^+$

Species	$k_M(a\ ^1\Delta_g)$ [cm^3-sec^{-1}]	$k_M(b\ ^1\Sigma_g^+)$ [cm^3-sec^{-1}]
N_2	$\leq 1.1 \times 10^{-19}$	2.0×10^{-15}
O_2	2.4×10^{-18}	1.5×10^{-16}
O	$\leq 1.3 \times 10^{-16}$	-
N	3.0×10^{-15}	-

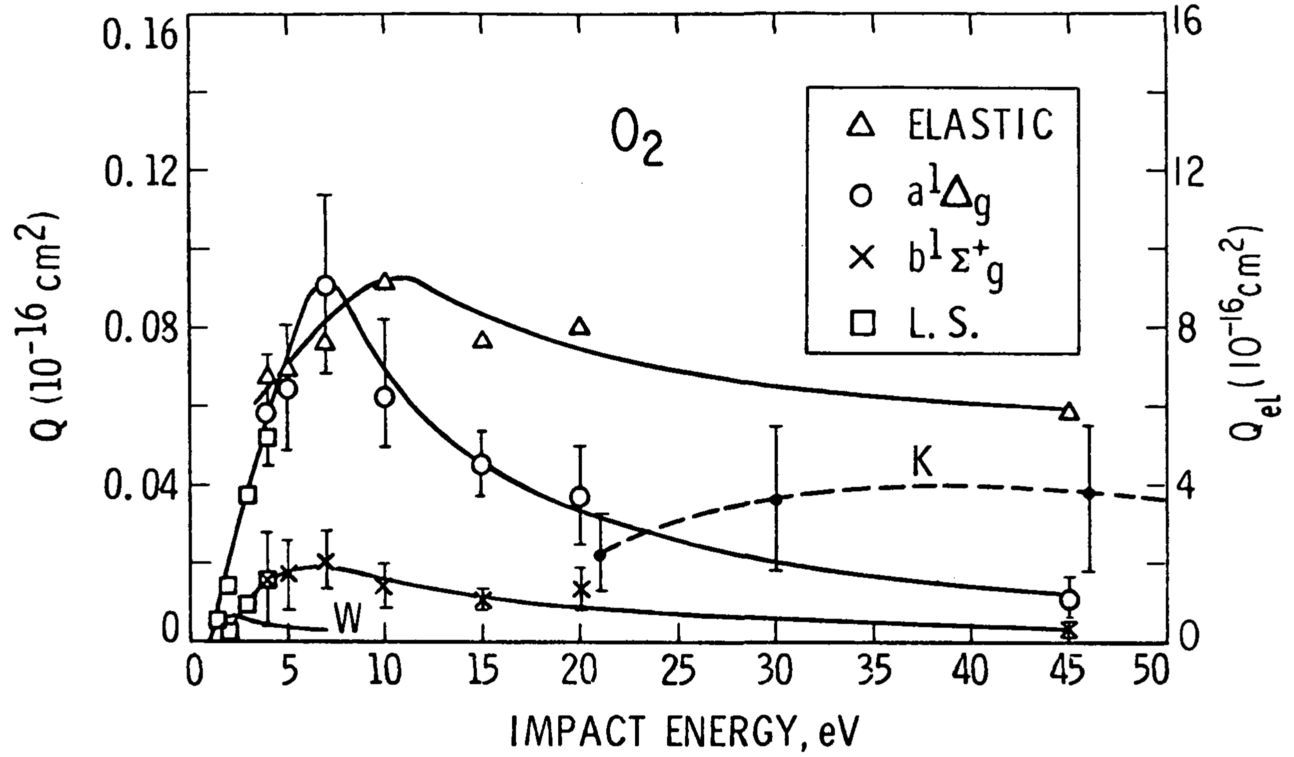

Figure 2. Integral cross sections for excitation of a $^1\Delta_g$ and b $^1\Sigma_g^+$ by electron impact as a function of incident energy from Trajmar, et al. (1971). The left ordinate is for the inelastic cross sections, the right one is for the elastic cross section. The data points are as indicated in the block in the upper right of the figure; the squares are the results of Linder and Schmidt (1971). The preliminary results of Konishi et al. (1970) are shown as the dashed curve and the semi-empherical estimate of Watson et al. (1967) is labeled as W.

smaller than that obtained by Trajmar et al., (1971) at their respective maxima. The b $^1\Sigma_g^+$ integral cross section estimated by Watson et al., (1967), although not shown in Figure 2, is also correspondingly smaller than that used in this work. It is noted that the new O_2 excitation cross sections are not only considerably larger than previously believed, but reach their maximum values at energies significantly farther above threshold than is usually the case for exchange excitation. The cross section used to describe the excitation of 3914A was taken from the recent work by Borst and Zipf (1970).

The "secondary" electron spectrum used to calculate the excitation rates was taken to have three components of the form

$$f(E) = f(E_o) \left(\frac{E_o}{E}\right)^m \text{(electrons cm}^{-2}\text{ster}^{-1}\text{eV}^{-1}\text{)} \qquad (1)$$

The three components correspond to the three different electron energy regions in the auroral electron spectrum discussed by Rees (1969). The magnitude of the electron spectrum was re-normalized to Pfister's (1967) flux at 10 eV in order to correspond to an IBC II aurora. The following sets of parameters were used: $1 \leq E(eV) \leq 100$ eV, $m = 3.2$, $f(10 \text{ eV}) = 1.6 \times 10^{+7}$; $100 \leq E(eV) \leq 1$ keV, $m = -1.0$, $f(100 \text{ eV}) = 1.0 \times 10^{+4}$; 1 keV $\leq E(eV) \leq \infty$, $m = 1.11$, $f(1 \text{ keV}) = 1.0 \times 10^{+5}$. A secondary electron spectrum of this form should provide a realistic estimate of the excitation of 3914A radiation relative to the low-lying electronic states of O_2. In order to obtain a feeling for the importance of the lower energy electrons in the population of the O_2 states, a spectral index of $m = 2.4$ was also used for the lowest energy portion of the spectrum.

III. RESULTS AND DISCUSSION

The equations of statistical equilibrium which describe the population and depopulation rates of electronic state α (a $^1\Delta_g$ or b $^1\Sigma_g^+$) are:

$$k^{x\alpha}_{v'o}\ n^x_o + \sum_\beta \sum_i A^{\beta\alpha}_{iv'}\ n^\beta_i = \left\{ \sum_\gamma \sum_r A^{\alpha\gamma}_{v'r} + Q^\alpha_{v'} \right\} n^\alpha_{v'} , \tag{1}$$

where $k^{x\alpha}_{v'o}$, $A^{\beta\alpha}_{v'v''}$, $Q^\alpha_{v'}$ and n^x_o are respectively the electron-impact excitation rate to state α, the Einstein spontaneous transition probability connecting states α and β, the quenching rate of state α, and the number density of the lowest vibrational level of the ground electronic state. The equations are relatively simple because only two vibrational levels of each state are appreciably populated and there is not a strong coupling between the two excited states.

The absolute volume emission rates predicted for the 1.27 μm, 7621A and 3914A emissions are shown in Figure 3 as a function of the altitude. The variation in the volume emission rates for 1.27 μm and 7621A caused by the variation in the spectral index of the lowest component ($m = 2.4$ to $m = 3.2$, but both having the same flux value at 10 eV) is shown by the shaded regions. Only the result obtained for the $m = 3.2$ case is shown for the 3914A emission because the corresponding effect due to the variation of m was quite small. As was expected, and is shown in the figure, such an appreciable change in the spectral index results in a significant change in the volume emission rates from O_2 and provides a measure of the sensitivity of the 1.27 μm and 7621A volume emission rates to the flux of very low energy ($E < 10$ eV) electrons.

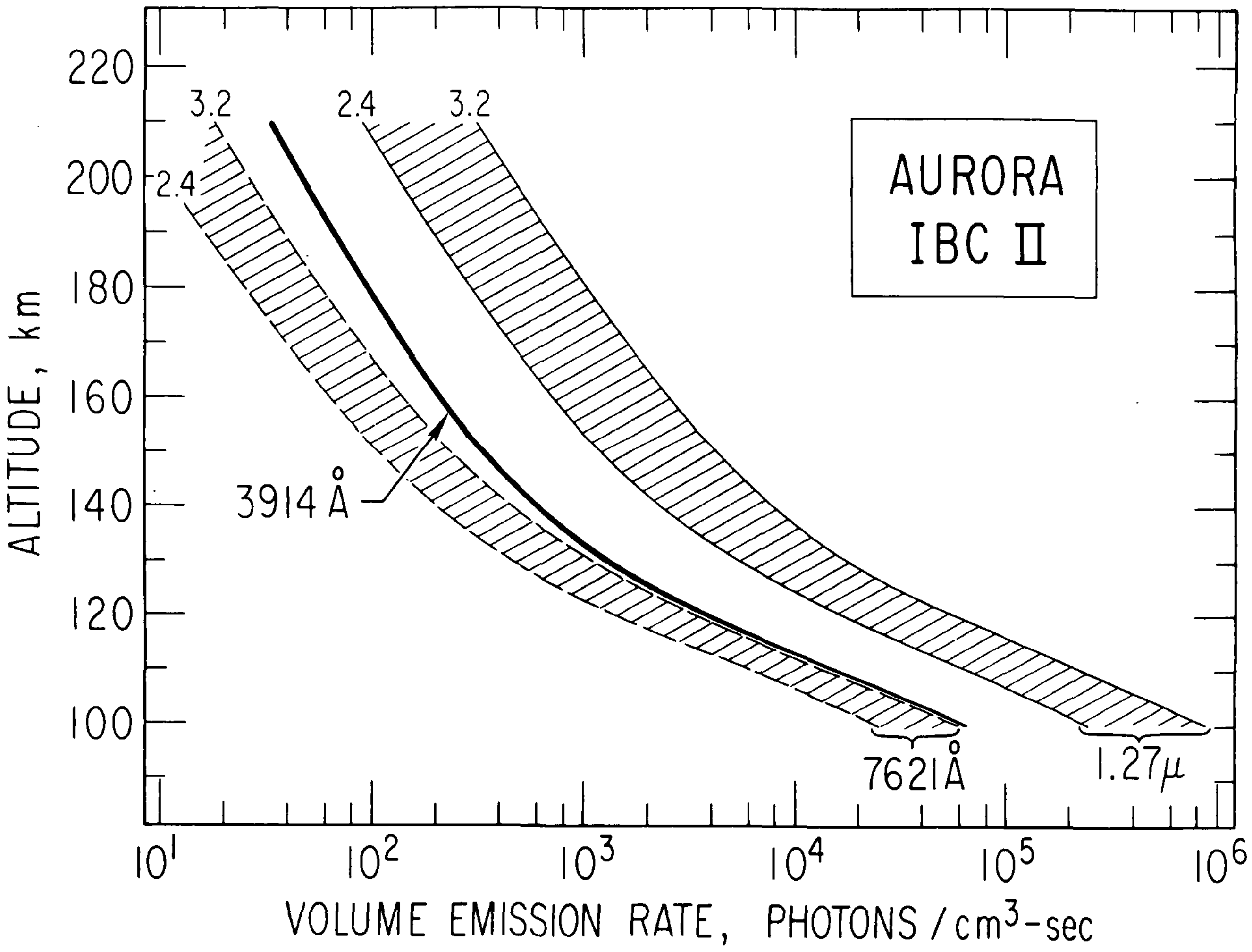

Figure 3. Predicted volume emission rates of 1.27 μm, 7621A, and 3914A radiation as a function of altitude for two different values of the spectral index for the lowest portion of the secondary electron spectrum (corresponding to an IBC II aurora).

The ratios of the volume emission rates for 1.27 μm and 7621A radiation to that for 3914A, for m = 3.2, are shown in Figure 4 as a function of altitude. The following definitions have been made: $R_1 = I(1.27\ \mu m)/I(3914A)$, $R_2 = I(7621A)/I(3914A)$, where I is the volume emission rate. Also shown are the corresponding ratios determined from recent auroral observations of these emissions from rockets and aircraft. For both the measured and the calculated ratios, the dashed curve is used to denote the ratio of the 7621A to 3914A volume emission rates and the solid curves, that for 1.27 μm to 3914A. The breadth of the horizontal lines denotes the range in the experimentally determined ratios. The lines labeled (LWVJ) and (NOXON) are respectively the airborne observations of Llewellyn et al., (1969) and Noxon (1970). Those labeled (MDBB) and (SHM) are the rocket observations of Megill et al., (1970) and Schiff et al., (1970), respectively. The location in altitude of the experimental ratios shown in Figure 4 do not correspond to the experimentally determined altitude but has been shown only for clarity in plotting the results. The predicted ratios involving 1.27 μm and 7621A are about a factor of 10 less than the observations except for the 1.27 μm to 3914A ratio inferred [Noxon, 1970; Megill et al., 1970] from the measurements of Llewellyn et al., (1969). The rocket measurements of Megill et al., (1970) provide the best basis for comparison of the predicted volume emission rates because they measured 1.27 μm, 7621A and 3914A emissions on the same rocket. Qualitatively, the predicted ratios agree with the preliminary results reported by Megill et al., (1970) for the altitude dependence of these ratios in that such dependence is not very strong. The preliminary results reported by Megill et al., (1970) were not converted to zenith intensities and it is possible that

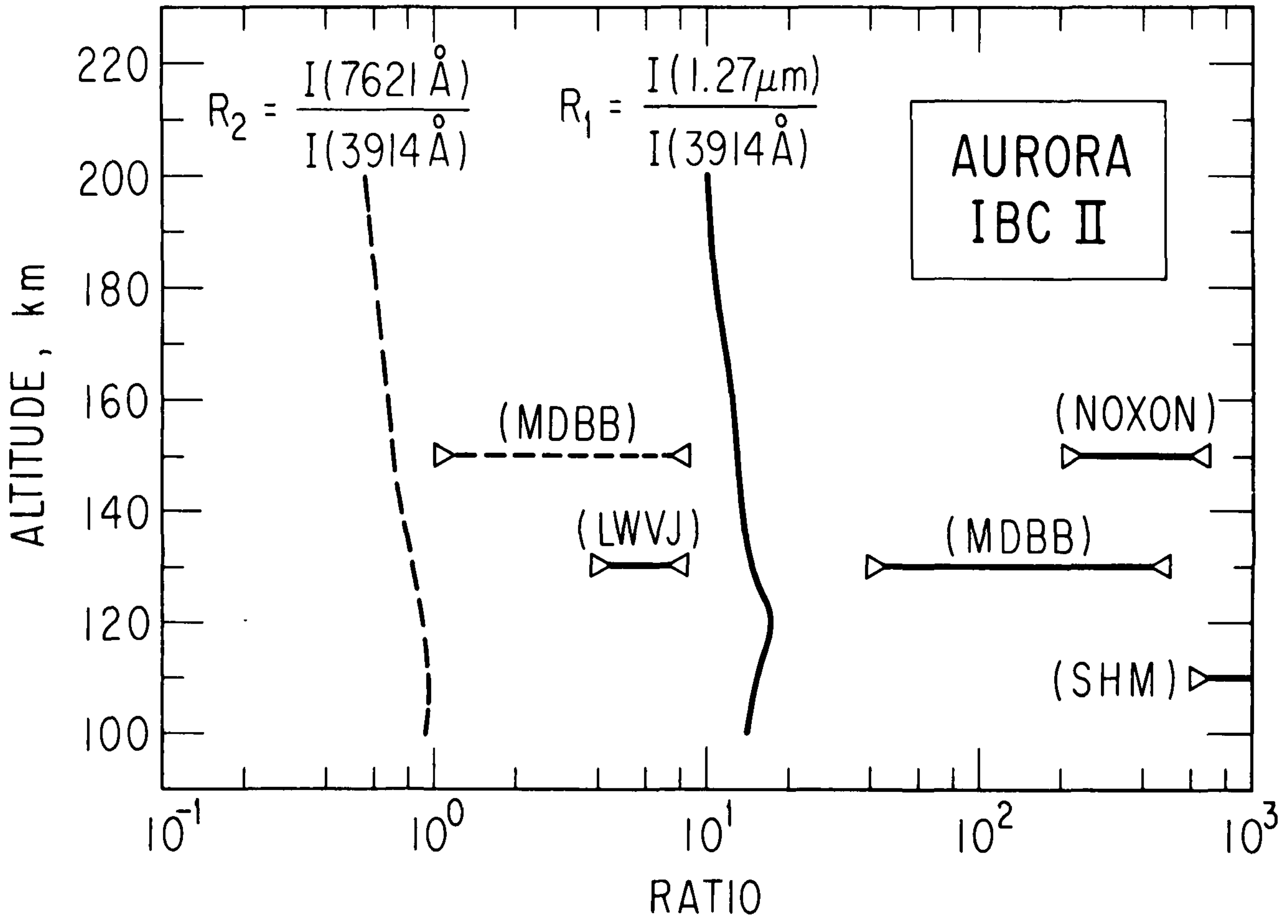

Figure 4. The ratios of the predicted volume emission rates shown in Figure 3 as a function of altitude. The dashed lines are for 7621A/3914A, the solid lines for 1.27 μm/3914A. The ratios determined from airborne and rocket observations are indicated: **LWVJ is Llewellyn**, et al. (1969); Noxon (1970a); **MDBB is Megill**, et al. (1970); and **SHM is Schiff**, et al. (1970).

such corrections to the raw data reported will reduce the measured intensities so as to be in better agreement with the predictions.

Another interpretation to the data of Megill et al., (1970) has been offered by Evans and Llewellyn (1971) [also see Megill et al., 1971] who suggest that the instruments of Megill et al., (1970) observed the nightglow layer rather than a true auroral enhancement. In any case, it is noted that the ratio of 1.27 μm to 3914A obtained from rocket experiments by Megill et al., (1970) and Schiff et al., (1970), as well as from the airborne observations of Noxon (1970a), is generally more than a factor of 10 greater than predicted. If these measured ratios are substantiated by future measurements it is clear that a mechanism other than secondary electron excitation is important in the population of the a $^1\Delta_g$ and b $^1\Sigma_g^+$ states of O_2.

There are a number of mechanisms other than secondary electron excitation which could contribute to the excitation rate for the a $^1\Delta_g$ and b $^1\Sigma_g^+$ states in auroras [Noxon (1970); Megill et al., (1970)]. It is also noted that since the a $^1\Delta_g$ and b $^1\Sigma_g^+$ states are imbedded energetically among the vibrational levels of the ground state, the population and depopulation processes of these vibrational levels in auroras may influence the population of the a $^1\Delta_g$ and b $^1\Sigma_g^+$ states. In addition, O_2 has a stable negative ion (Spence and Schulz, 1970) which appears to play a role in the vibrational population of X $^3\Sigma_g^-$ and may also be important in the population of the a $^1\Delta_g$ and b $^1\Sigma_g^+$ states under certain conditions. A complete treatment of the population of the a $^1\Delta_g$ and b $^1\Sigma_g^+$ states should therefore include the three electronic states formed from the ground electron configuration, the negative ion state, and their interconnection, when sufficient information becomes available to permit such a detailed analysis.

Finally, it is noted that to obtain a more accurate estimate of the volume emission rates below about 110 km, it is necessary to use a "secondary" electron spectrum whose magnitude decreases with decreasing altitude to account for the ultimate absorption of all the electron energy by the atmosphere.

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13. ABSTRACT

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14\.

KEY WORDS

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O_2 in auroras

Emission of 1.27 μm

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