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B E L G I S C H I N S T I T U U T V O O R R U I M T E - A E R O N O M I E

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## FOREWORD

This article will be published in the Journal of Geophysical Research.

## AVANT-PROPOS

Cet article sera publié dans le "Journal of Geophysical Research".

## VOORWOORD

Dit artikel zal verschijnen in de "Journal of Geophysical Research".

## VORWORT

Diese Arbeit wird in "Journal of Geophysical Research" herausgegeben werden.

# SIMULTANEOUS UPPER AIR COMPOSITION MEASUREMENTS BY MEANS OF UV MONOCHROMATOR AND MASS SPECTROMETER

by

M. ACKERMAN\*, P. SIMON\*, U. von ZAHN\*\* and U. LAUX\*\*

*\*Institut d'Aéronomie Spatiale de Belgique  
Bruxelles - Belgique*

*\*\*Physikalisches Institut, Universität Bonn  
53 Bonn - Germany (FRG).*

## *Abstract*

Molecular oxygen and nitrogen number densities in the altitude range 115 to 220 km above Sardinia were measured in two sounding rocket experiments (ESRO Payloads S84 and S90) in February 1972 by a combination of UV monochromators and mass spectrometers. The measured values agree closely with CIRA 1972 for the 120 km altitude region. At higher altitudes the O<sub>2</sub> profiles measured by UV monochromators indicate deviations from diffusive equilibrium with respect to the N<sub>2</sub> profile measured by the mass spectrometers.

## *Résumé*

Les concentrations de l'oxygène et de l'azote moléculaires ont été mesurées en Sardaigne dans le domaine d'altitude allant de 115 à 220 km lors de deux expériences par fusées-sondes (charges utiles ESRO S84 et S90) en février 1972. Des spectromètres ultraviolet et de masse ont été employé conjointement dans ce but. Les valeurs mesurées sont en accord avec le modèle CIRA 1972 à 120 kilomètres d'altitude. Plus haut les distributions de O<sub>2</sub> déduites par absorptiométrie dans l'ultraviolet sont en désaccord avec les distributions calculées à partir des valeurs pour N<sub>2</sub> obtenues par spectrométrie de masse dans l'hypothèse d'un équilibre de diffusion.

### *Samenvatting*

De concentratie van moleculaire zuurstof en stikstof werd bepaald in het hoogtegebied 115 tot 220 km boven Sardinië, door twee raketproeven (nuttige lading ESRO S84 en S90) in februari 1972. Hierbij werd gebruik gemaakt van een combinatie bestaande uit UV monochromatoren en massaspectrometers. De gemeten waarden komen goed overeen met CIRA 1972 voor een hoogte van 120 km. Bij grotere hoogten wijkt het gemeten O<sub>2</sub> profiel af van de diffusie evenwichtswaarden berekend aan de hand van het N<sub>2</sub> profiel, gemeten door de massaspectrometers.

### *Zusammenfassung*

Molekularsauerstoff und Molekularstickstoff Konzentrationen auf dem Höhegebiet von 115 zu 220 km wurden über Sardinia in zwei Raketexperimenten (ESRO Nutzlastungen S84 und S90) in February 1972, mit Hilfe UV Monochromatoren un Mass-Spektrometer gemessen. Auf der Höhe von 120 km stimmen die gemessene Werte gut mit CIRA 1972 ein. Oberhalb 120 km sieht man einen Unterschied zwischen die UV Monochromator O<sub>2</sub> Werte und die O<sub>2</sub> Diffusionsequilibrium Werte.

## INTRODUCTION

This report presents final results obtained from 2 sounding rocket experiments, ESRO payloads S84 and S90<sup>9</sup>. The experiments had two independent scientific aims which, on the other hand, could be pursued with the same instrumentation on board these payloads. One objective of our investigations was to obtain simultaneous observations of the thermospheric molecular oxygen content by means of two largely independent measuring techniques. These data were to be backed up, as far as possible, by measurements of additional atmospheric constituents in particular  $N_2$  in order to be able to crosscheck the density profiles and scale heights determined for the various constituents. The other objective of the experiments was to collect more detailed and quantitative information on the ultraviolet solar spectrum in the Schumann-Runge region where a considerable uncertainty about the solar fluxes exists. This paper deals with the results obtained from the thermospheric composition measurements whereas results with respect to the absolute solar flux measurements are being discussed in a separate paper by Ackerman and Simon (1973).

The two most important techniques for determination of the composition of upper air in the 100 to 200 km altitude region are in situ mass spectrometry and solar EUV and UV absorption measurements. Both methods have their merits and shortcomings, too. Because the shortcomings of the two techniques influence the derived data in different ways it appears reasonable to try to combine both techniques in one sounding rocket payload in order to allow extensive cross checks on absolute number densities and relative altitude profiles obtained from the two types of instruments. In fact, Hall *et al.* (1965) have argued in favor of such joint measurements of mass spectrometers and EUV monochromators as early as 1965.

Our personal interest in such correlated optical and mass spectrometer experiments was even more alerted by the results of a mass spectrometric investigation of upper air composition in the 150 km altitude region which we formed in December, 1966. Unexpected high  $O_2$  densities observed in the ion source of the mass spectrometer could only be explained by a considerable degree of recombination of O to  $O_2$  at the ion source walls (von Zahn and Gross, 1969). Such behaviour of atomic oxygen had not been noted before in rocket borne

mass spectrometers. It was hoped, therefore, that combined mass spectrometer and optical measurements of atmospheric O<sub>2</sub> would allow a distinction between ambient O<sub>2</sub> and molecular oxygen produced inside the ion source of the mass spectrometer by recombination of atomic oxygen.

### *INSTRUMENTS AND PAYLOAD*

Both payloads, ESRO S84 and S90, carried identical scientific instrumentation. It consisted of one UV monochromator of the Institut d'Aéronomie Spatiale de Belgique measuring the absolute solar flux values at the wavelengths 1216Å, 1450Å and 1710Å, one UV monochromator of the Meteorologisches Institut der Universität München measuring the absolute solar flux values in the wavelength range 1450Å till 2100Å, and a mass spectrometer of the Physikalisches Institut der Universität Bonn measuring absolute number densities of O<sub>2</sub>, N<sub>2</sub>, and Ar. All three instruments were mounted forward looking under the ejectable nose cone of a sun-stabilized Skylark payload as shown in Figure 1. The coarse and fine sensors for the two axis sun stabilization were mounted alongside the instruments (Figure 2) and mounted to the same baseplate as the instruments. Care was taken that after jettisoning of the payload split nose cone and the ion source cap the mass spectrometer source had a free field of view of  $2\pi$  about the forward direction.

The Brussels ultraviolet monochromator was essentially an Ebert type spectrometer with a fixed position grating. The image of the entrance slit at three wavelengths was selected by three exit slits uncovered in sequence by means of a sliding shutter. The purpose of this device was to reproduce easily at each scanning sequence of six seconds the same wavelength bandpasses. The details of the instrument have been described by Ackerman and Simon (1973). The three bandpass central wavelengths : 1216Å, 1450Å, and 1710Å were chosen at values of the oxygen absorption cross section such that absorption measurements would, for a significant period of time, overlap at two wavelengths while the increase or decrease of optical thickness was taking place during the flights. These features give their unique character to the measurement : the oxygen column densities deduced at one wavelength are controlled at an other one and the choice of three wavelengths leads to oxygen

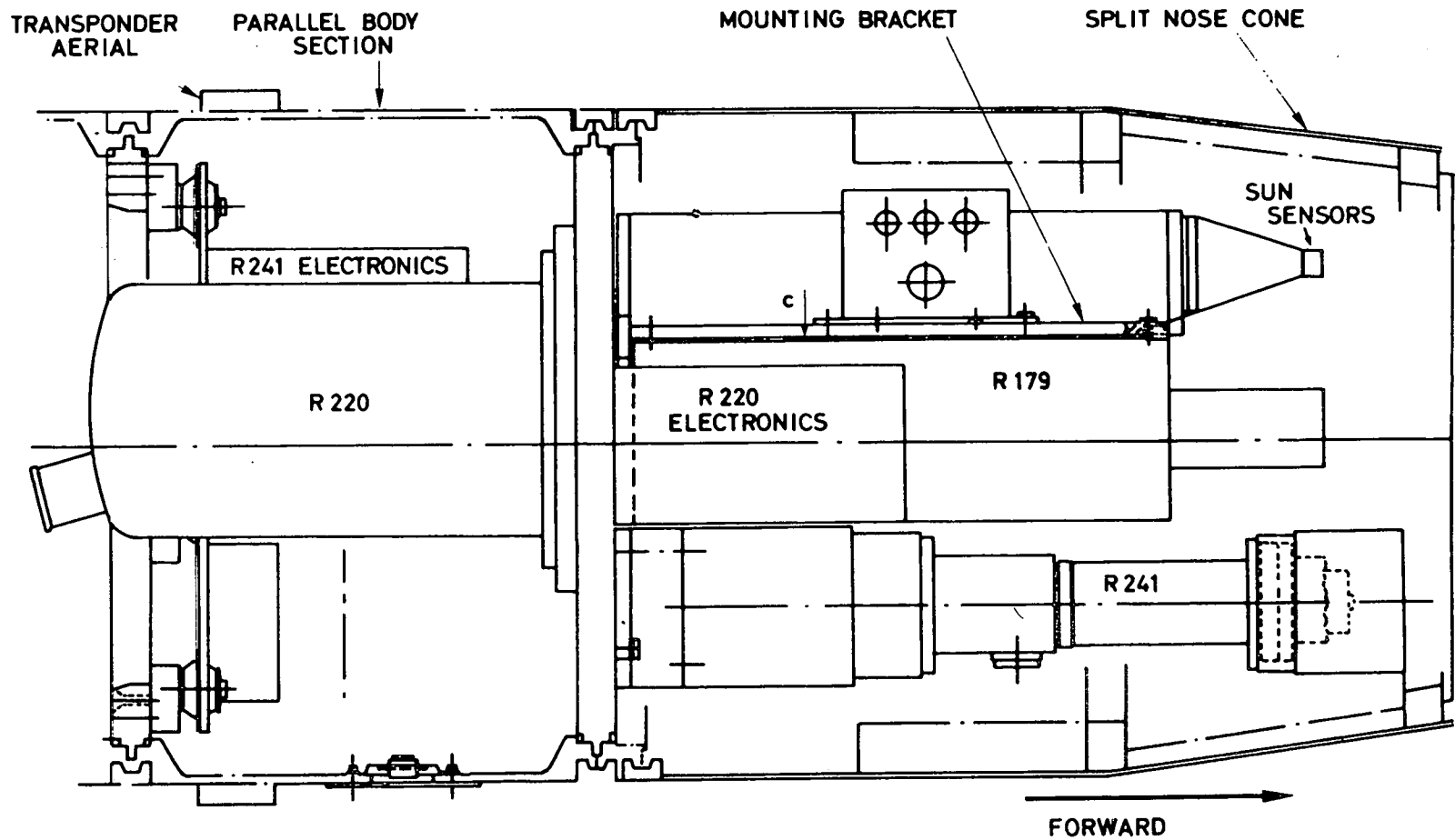


Fig. 1.- Cross section of the instrument bay in ESRO payloads S84 and S90 showing the Brussels UV monochromator (R220), the Munich monochromator (R179), the Bonn mass spectrometer (R241), and the sun sensors all mounted to a common platform under the ejectable nose cone. The mass spectrometer is shown with the ejectable ion source cap still attached to the instrument.

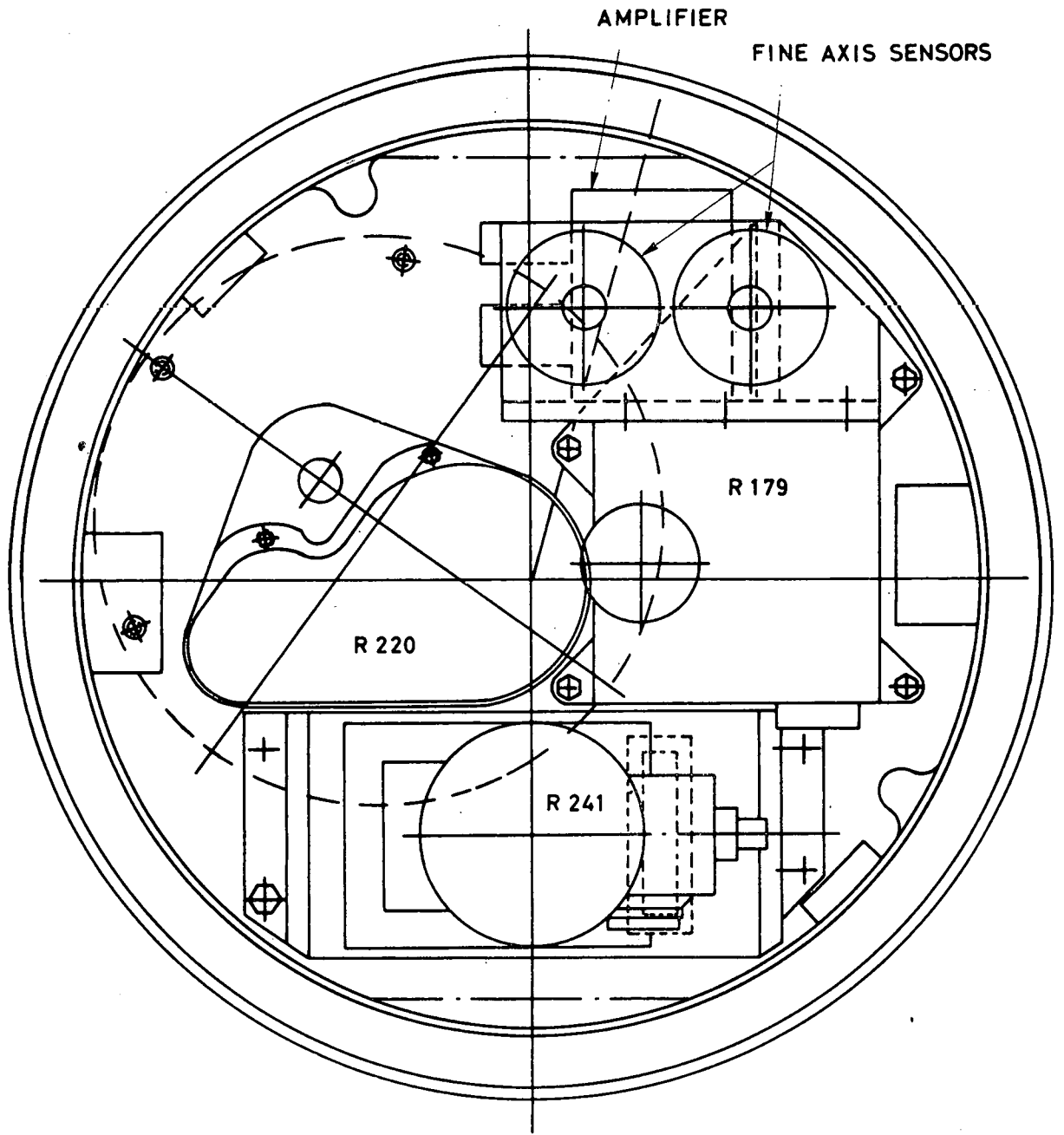


Fig. 2.- Front view of the instrument bay. All three instruments were mounted with the center line of their field of view being parallel to the axis of the sun sensors.



determinations over a wide range of altitude. In the case of the S84 flight measurements have been performed from 90 to 190 km at once, to our knowledge for the first time.

The Munich two channels ultraviolet spectrometer was designed to measure directly the difference in intensity of radiation with 2100Å and 1550Å (upleg of flight) and with 2100Å and 1450Å (downleg of flight). Because final results from this instrument are not available yet additional details of this experiment need not be discussed here.

The Bonn mass spectrometer employs a semi-open electron impact ion source, a monopole spectrometer as analyzing field, a three-fold ion detection system, and a multiplier operated in an analog mode. The instrument was an improved version of the spectrometer described by Bitterberg *et al.* (1970) and included the following new features:

- 1) The ion box, ion lens and total ion current monitor (see Figure 3) were made from solid gold in order to evaluate the influence of this material on the general performance of the ion source.
- 2) For evaluation of the design of a future satellite experiment this ion source carried two redundant filaments.
- 3) The instrument employed a threefold ion detection system (see Figure 3): The ions generated in the ion source are partly focused to the entrance orifice of the analysing field and partly collected by the total ion current monitor feeding the input of a linear electrometer (T-electrometer). The T-electrometer readings are thus related to the total ion flux leaving the ion source and a direct measure of the neutral density. Behind the analysing field the ion current passes through a grid system which collects about 50% of the ion current and feeds another linear electrometer (I-electrometer). The remaining ions enter the multiplier, become converted to electrons and amplified. The electron collector feeds a logarithmic electrometer (E-electrometer) with a range of 5 decades. The use we made of these three independent collectors will be outlined along with data reduction procedure.
- 4) Because of the spectrometer axis being parallel to the optical axis of the payload (thus allowing a two-axis stabilization system only) the ion source and analyzing field were directly facing into the sun. It was therefore a recognized danger that solar UV could

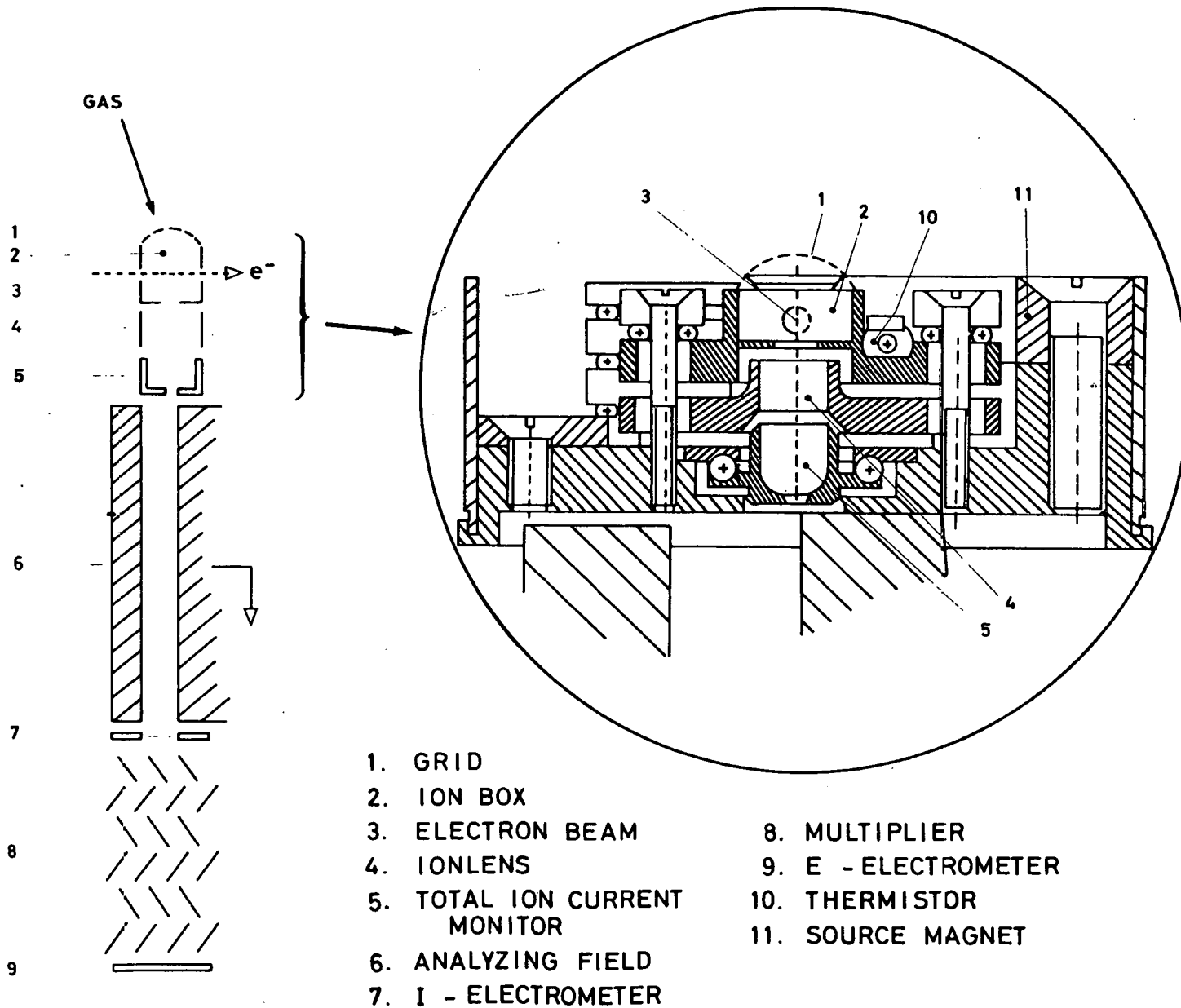


Fig. 3.- Schematic of the detector layout and cross section of the mass spectrometer ion source. The electron beam (3) is focused by a small magnet (11). The temperature of the ion box walls (2) is measured by means of a thermistor (10). See text for further explanations.

enter the multiplier and cause an increased multiplier background current. Therefore the multiplier was mounted off-axis from the analysing field, and additional baffles and shields were placed inside the spectrometer to block the direct access of UV light to the multiplier.

A mobile pumpstand provided us with the capability to perform a direct pre-flight calibration of the mass spectrometer sensitivity for nitrogen at the launch range a few days before the launch date.

### *FLIGHT PARAMETERS AND PERFORMANCE*

On February 28, 1972 both payloads were launched from the range of Salto di Quirra, Sardinia. The payloads reached altitudes of about 250 km and all systems including the sun pointing system worked quite well. A summary of flight parameters is given in Table 1.

During the S84 flight the sun was very close to the local horizon. For the UV monochromators this meant a large optical path length of solar radiation through the atmosphere thus shifting to comparatively high altitudes the ranges of useful absorption measurements at the three present wavelengths. For the mass spectrometer this provided two advantages : First after sun acquisition the payload maintained a horizontal attitude thus enabling the mass spectrometer to take data on the up- and downleg of the flight. Second due to this near horizontal attitude the angle of attack was almost the same for data points collected at a given altitude on up- and downleg. Figure 4 illustrates the history of the angle of attack throughout the flight above 100 km altitude.

Figure 5 indicates the quality of spectra obtained from the I-electrometer of the mass spectrometer. The example is taken from the downleg data of S84 showing clearly an ion current ratio  $I(16^+)/I(32^+) > 1$  at 116 km. Although this paper does not deal directly with the in-situ measurement of atomic oxygen we wish, however, to point out here that the large angle of attack of S84 at 116 km prevented any ambient atoms to cross the electron beam of the ion source without prior hitting an ion source surface. Thus the entire  $16^+$ -peak

TABLE 1.- Flight parameters of ESRO Payloads S84 and S90.

Parameter	S 84	S 90
Range	Salto di Quirra, Sardinia	
Geographic coordinates	9° 11' E : 39° 36' N	
Date of launch	February 28, 1972	
Local time of launch	0654 CET	1047 CET
Solar zenith angle at apogee	89.8°	52.8°
Apogee	242 km	251 km
Azimuth of trajectory	51° f.N	130° f.N
F <sub>10.7</sub> (one day before launch) <sup>+</sup>	143.0	143.0
F <sub>10.7</sub> (average Dez. 71-Apr. 72)	124.5	124.5
Kp (6 hours before launch)	3-	3-
T <sub>exosphere</sub> (from CIRA 1972)	913 K	1012 K
Mass spectrometer :		
Ejection of ion source cap	108 km	119 km
Electron energy in ion source	68 eV	80 eV

+ F values in  $10^{-22} \text{ W.m}^{-2} \cdot \text{Hz}^{-1}$  at 10.7 cm wavelength.

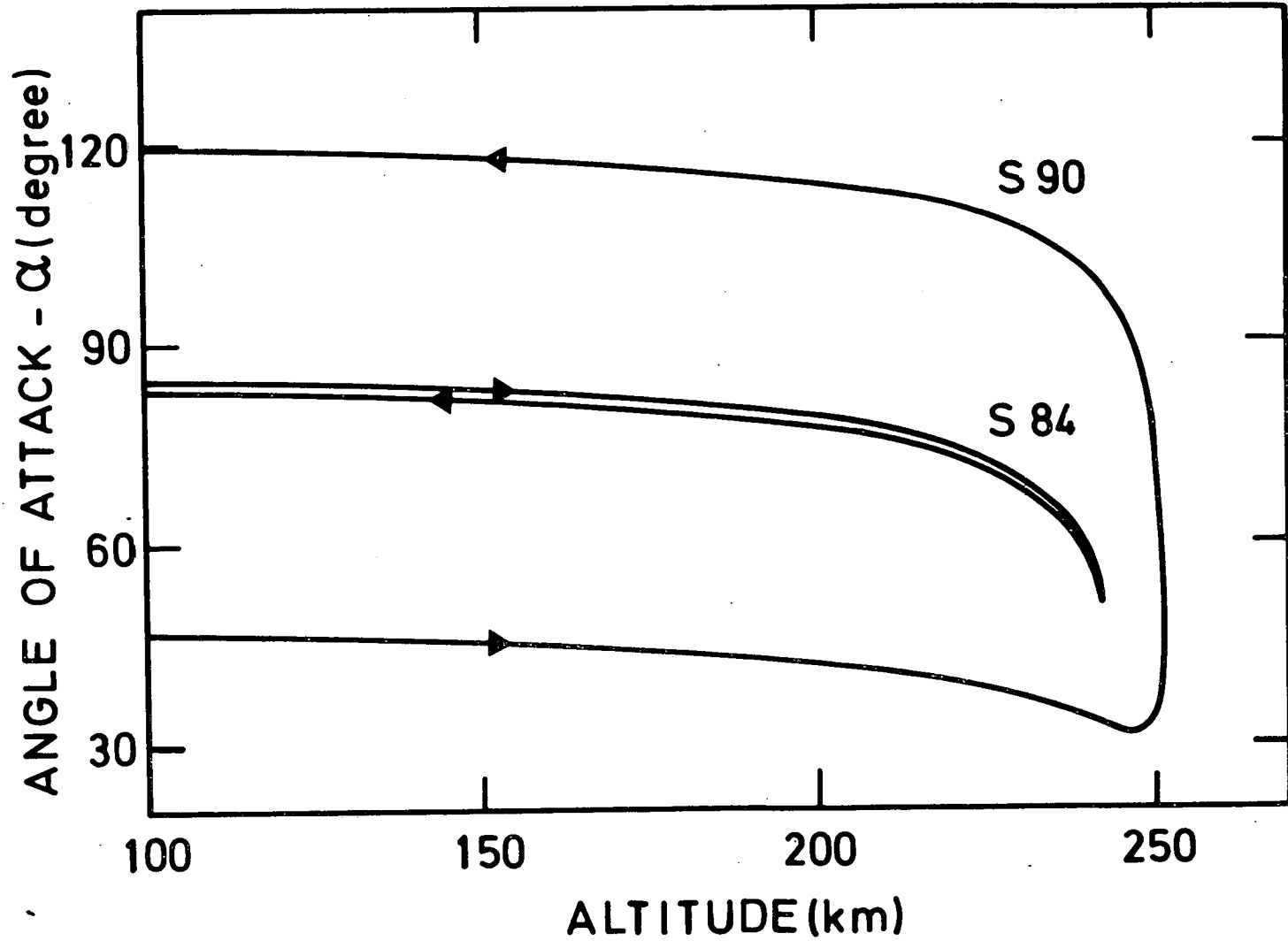
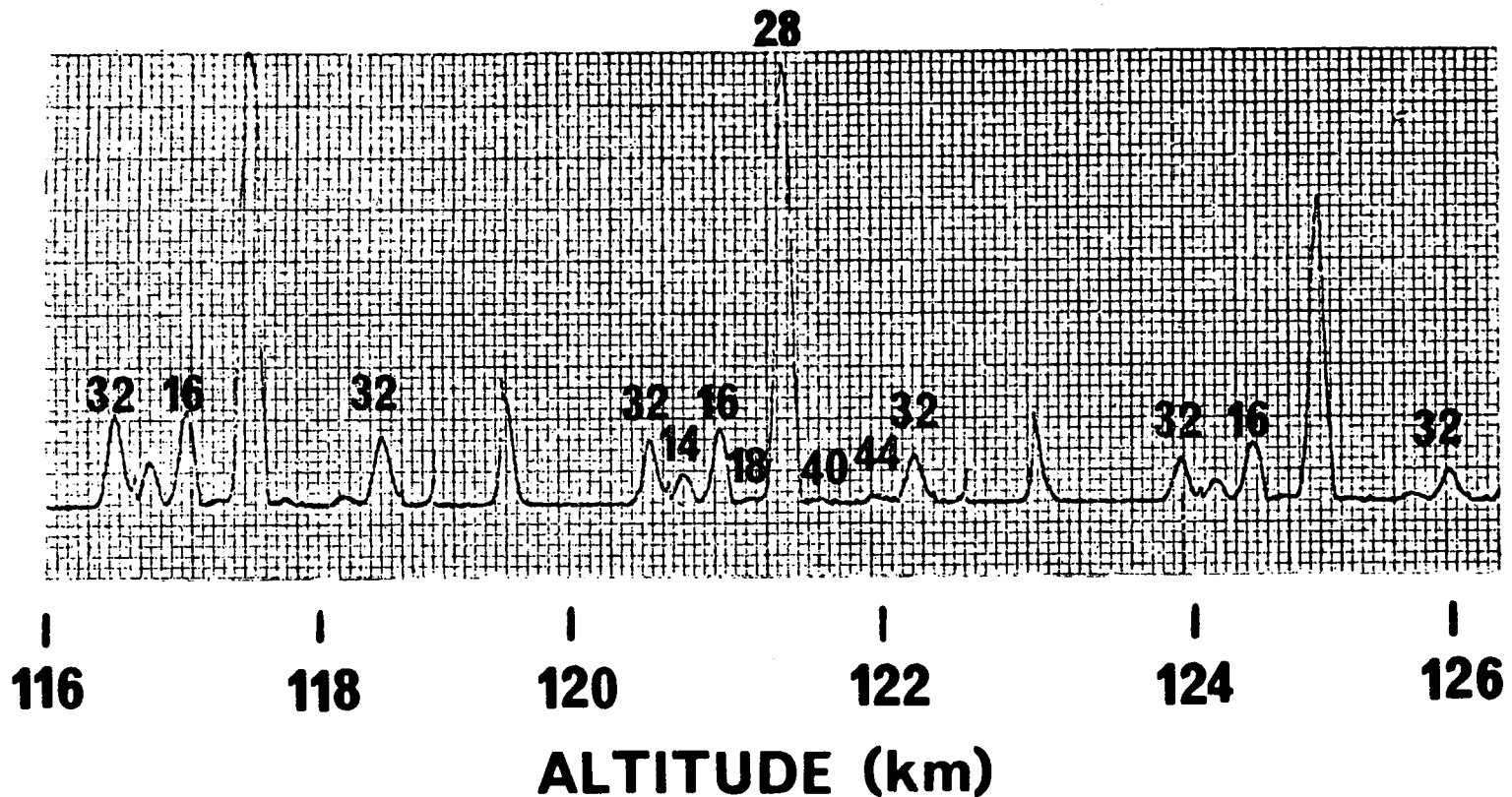


Fig. 4.- Angle of attack (= angle between payload axis and velocity vector) vs. altitude. Because the sun was close to the local horizon during the flight S84 the  $\alpha$  upleg and downleg profile fall almost on top of each other.

# ION-CURRENT SPECTRA S 84 (downleg)



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Fig. 5.- Programmed mass spectrum taken during the downleg of flight S84 at the I-electrometer (linear) of the mass spectrometer. Mass numbers are indicated in amu. Mass 32 was sampled twice as frequently as the other mass numbers. Note that the ratio  $16^+/32^+ > 1$  as low as 116 km although due to the angle of attack at this altitude most ambient O atoms must have undergone at least one wall collision before becoming ionized.

must originate from O atoms which have had at least one wall collision before ionization.

Unfortunately our attempts to prevent solar UV light from reaching the multiplier of the mass spectrometer proved ineffective. For both payloads upon jettisoning of the ion source caps a large, though steady background current appeared on the E-electrometer channels, which rendered them essentially worthless. Thus all the data presented below are taken from the T- and I-electrometers. Due to their lower sensitivity the N<sub>2</sub> data only reach up to 220 km and the O<sub>2</sub> data to 165 km.

### DATA REDUCTION

The monochromator appeared to not have been fully outgassed during the ascent. The photon flux measurements were only considered after stabilization of the signals observed in absence of absorption. This occurred at about 230 km altitude while the rockets were still ascending. On the downleg the signals decayed in sequence, first at 1450Å then at 1710Å and eventually at 1216Å. Using the intensity I<sub>0</sub>, in absence of atmospheric absorption, and the intensities I, when absorption was taking place, Beer's law

$$I = I_0 e^{-\sigma n_t}$$

was applied to determine the total number of oxygen molecules, n<sub>t</sub>, along the optical path. At 1450Å and 1710Å the values of absorption cross sections, σ, were taken from Ackerman (1971). They were weighted by taking into account the instrumental band passes and the relative variation of solar intensity with wavelength (Detwiler *et al.*, 1961). At 1216Å, the Lyman-α line shape and the variation of O<sub>2</sub> absorption cross section over its width were taken into account after Hall (1972).

The total amounts of molecules were then plotted versus altitude and the tangents to the curves yielded scale height values. These were combined with the solar zenith angle and with the earth geometrical parameters taken from Swider (1964) to determine number densities versus altitude. A new generation of scale heights was determined from these values

and reintroduced in the computation. The iteration was stopped after reaching stability. The so deduced number densities are represented in Figure 6 where smooth curves are drawn through the data points for the two flights. The curves are reproduced in Figure 7 for the sake of comparison with other data obtained by means of optical techniques.

In case of the mass spectrometers the data reduction involved the following standard steps: first conversion of measured ion currents into ion source densities through application of laboratory calibration data on the sensitivity (= ratio of ion current output over ion source number density) of the spectrometer for  $N_2$  and  $O_2$ ; second conversion of ion source densities to ambient number densities through application of the ram effect correction assuming negligible adsorption and chemical reactions of the constituents at the ion source walls (Hedin *et al.*, 1964).

The following details within our data reduction procedure appear noteworthy :

- 1) We had to make a choice between various calibration curves available in particular for the  $N_2$  sensitivity of the spectrometer. T- and I-electrometer both had independent calibration data obtained at the laboratory and at the launchsite. For both spectrometers we decided to keep unaltered the calibration data obtained for the T-electrometer at the launch-site. The other calibration data were adjusted so as to conform with this primary calibration curve whereby the ratio of  $N_2$  over  $O_2$  sensitivities at the I-electrometer was maintained.
- 2) At altitudes below 130 km the nitrogen number densities were calculated from the mass 14 peaks which height is more linear with ion source density than the mass 28 peaks.
- 3) For the S90 data a background correction was applied to the high altitude  $N_2$  data which brought the number densities down by 10% at 200 km. This correction was suggested by the observation of a noticeable mass 28 background on the downleg of the flight when the spectrometer was actually looking into the wake of the payload.

Further details of the analysis procedure for the mass spectrometer data are given by Laux and von Zahn (1974). The number densities for  $O_2$  and  $N_2$  so deduced from the mass spectrometer are shown in Figure 8 (S84) and Figure 9 (S90).



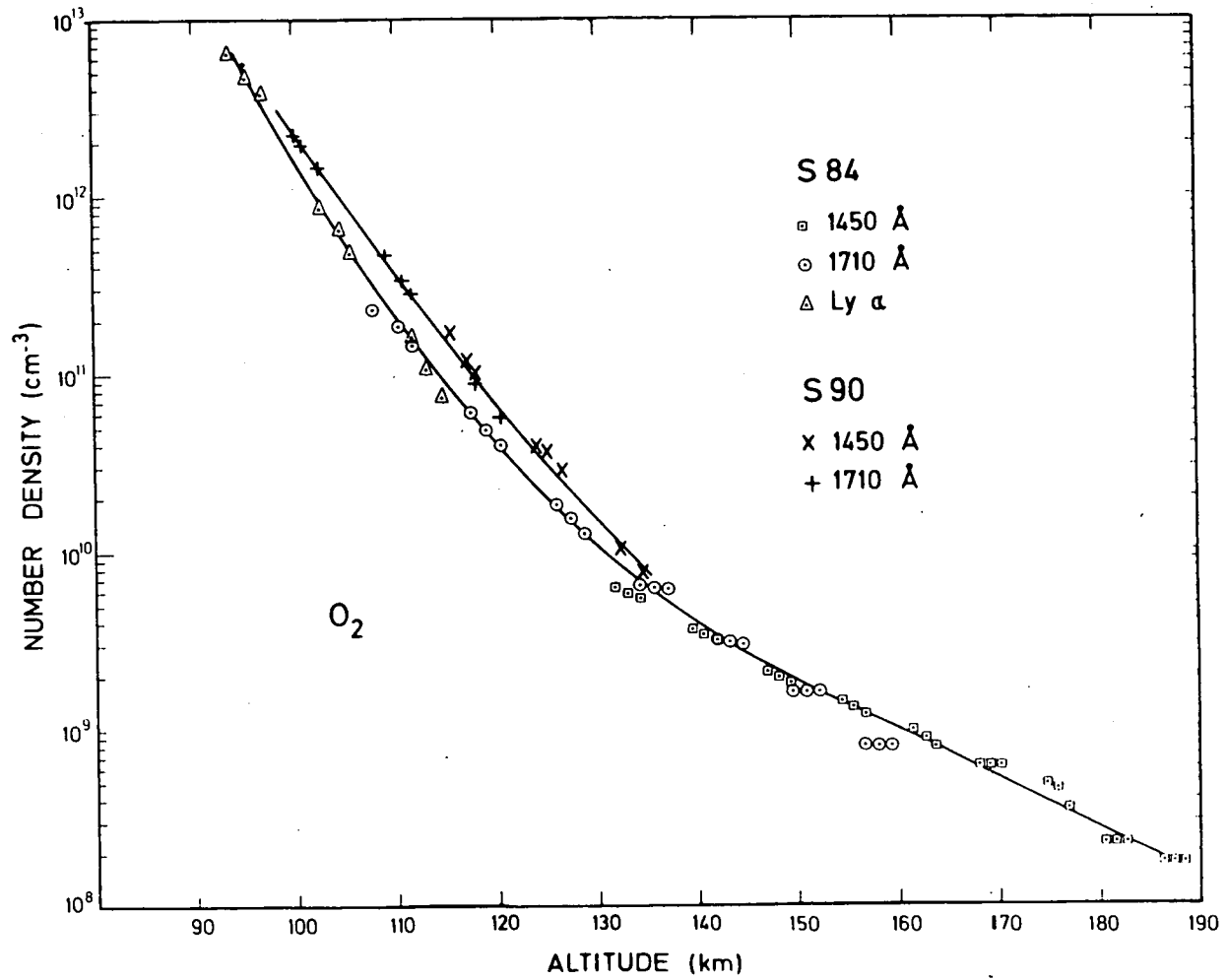


Fig. 6.-  $O_2$  number densities derived from the UV monochromator.

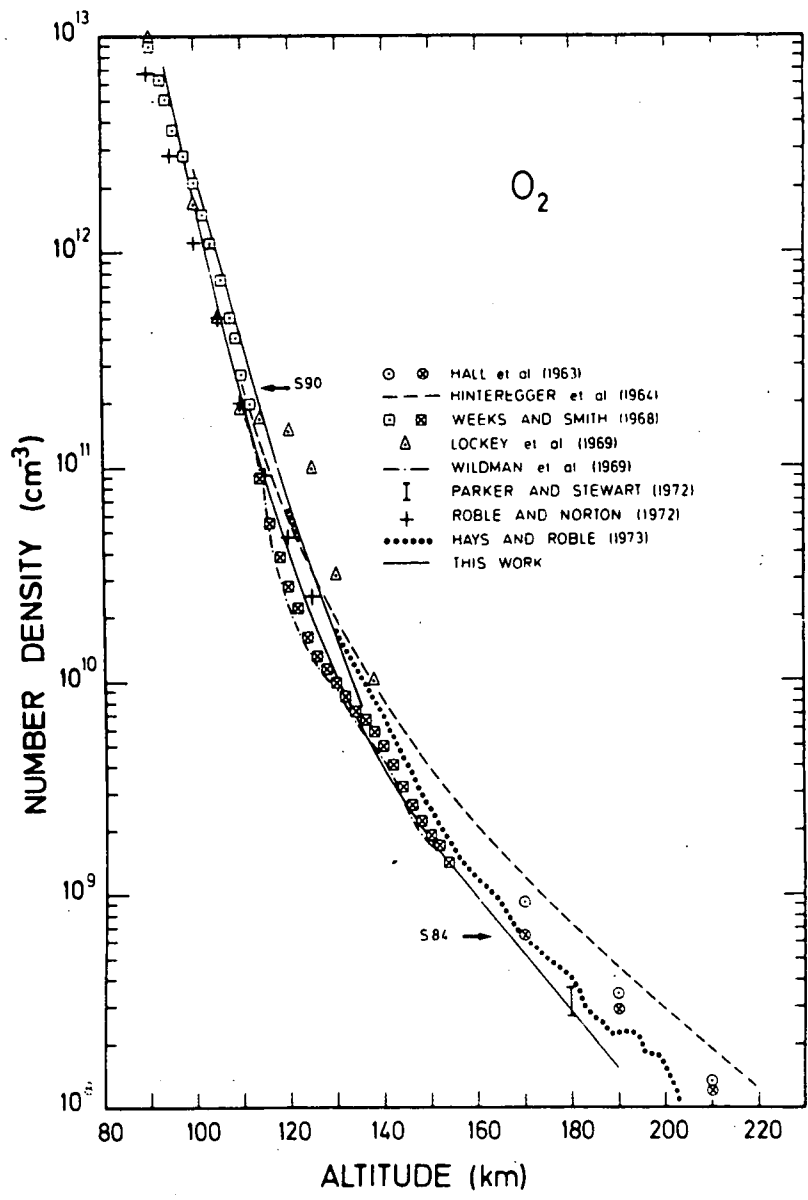


Fig. 7.-  $O_2$  number densities versus altitude from ultraviolet absorption data.

## DISCUSSION

We are quite satisfied with the agreement between the independent data obtained from the three wavelengths (Fig. 6) in case of the UV monochromator and the agreement between  $N_2$  and  $O_2$  densities obtained from the S84 upleg and downleg part of the flight (Fig. 8) in case of the mass spectrometer. We further note that at low altitudes (115 km for S84; 130 km for S90) the intercomparison of the absolute  $O_2$  number densities derived from the two different instruments yields quite good results (see Table 2). Last not least a comparison with previous experiments (Fig. 7) and a model atmosphere (Fig. 8 and 9) indicates a fair degree of conformity with possible geophysical variability in the state of the lower thermosphere accounting for the observed minor deviations.

A closer look, however, reveals a feature which deserves more consideration. Although the  $n(O_2)$  densities derived from the two different techniques at low altitudes agree it is evident that the gradients of the altitude profiles are different. This fact is more clearly shown in Figure 10 where the two data sets are compared directly for the flight which gave the largest altitude coverage. The difference amounts to a factor 1.7 at 160 km which we consider outside our calibration errors. The question then becomes which  $O_2$  profile come closer to the real atmospheric conditions? For the UV extinction measurement raising the  $O_2$  values in the 150 km region would require the assumption of lower absorption cross sections at both 1450Å and 1710Å.

It appears, however, rather unlikely that the cross sections used so far are so much in error to account for the whole observed variance. On the other hand, lowering the mass spectrometer  $O_2$  values could be justified by assuming that in fact additional  $O_2$  was produced inside the ion source by recombination of O into  $O_2$ . Using the appropriate CIRA 1972 O densities and taking into account the different ram factors for O and  $O_2$  one can calculate that of all incoming O atoms about 10% would have to recombine to  $O_2$  at the ion source walls to explain the difference between the mass spectrometer observations and the UV measurements. Although we do not wish to exclude this possibility we have to note the following: The  $O_2$  profile measured by the mass spectrometer comes closer to being in

TABLE 2.- Measured O<sub>2</sub> and N<sub>2</sub> Number Densities

S-84				S-90		
Altitude	n(O <sub>2</sub> ) (UV monochromator)	n(O <sub>2</sub> ) (mass spectrometer)	n(N <sub>2</sub> )	n(O <sub>2</sub> ) (UV monochromator)	n(O <sub>2</sub> ) (mass spectrometer)	n(N <sub>2</sub> )
km	cm <sup>-3</sup>	cm <sup>-3</sup>	cm <sup>-3</sup>	cm <sup>-3</sup>	cm <sup>-3</sup>	cm <sup>-3</sup>
115	9.50 x 10 <sup>10</sup>	9.75 x 10 <sup>10</sup>	7.20 x 10 <sup>11</sup>			
120	4.30 x	4.9 x	4.00 x	7.30 x 10 <sup>10</sup>		
125	2.10 x	2.74 x	2.45 x	3.30 x	2.8 x 10 <sup>10</sup>	2.6 x 10 <sup>11</sup>
130	1.10 x	1.65 x	1.57 x	1.60 x	1.6 x	1.65 x
135	6.40 x 10 <sup>9</sup>	1.04 x	1.05 x	8.10 x 10 <sup>9</sup>	9.7 x 10 <sup>9</sup>	1.05 x
140	4.10 x	6.93 x 10 <sup>9</sup>	7.2 x 10 <sup>10</sup>		6.2 x	7.0 x 10 <sup>10</sup>
145	2.70 x	4.75 x	5.1 x		4.15 x	4.85 x
150	1.90 x	3.33 x	3.7 x		2.78 x	3.4 x
155	1.35 x	2.38 x	2.76 x		1.9 x	2.5 x
160	1.00 x	1.72 x	2.08 x		1.35 x	1.9 x
165	7.40 x 10 <sup>8</sup>	1.26 x	1.58 x			1.46 x
170	5.40 x		1.22 x			1.15 x
180	2.80 x		7.35 x 10 <sup>9</sup>			7.3 x 10 <sup>9</sup>
190	1.4 x		4.55 x			4.8 x
200			2.89 x			3.33 x
210			1.85 x			2.4 x
220			1.19 x			1.77 x

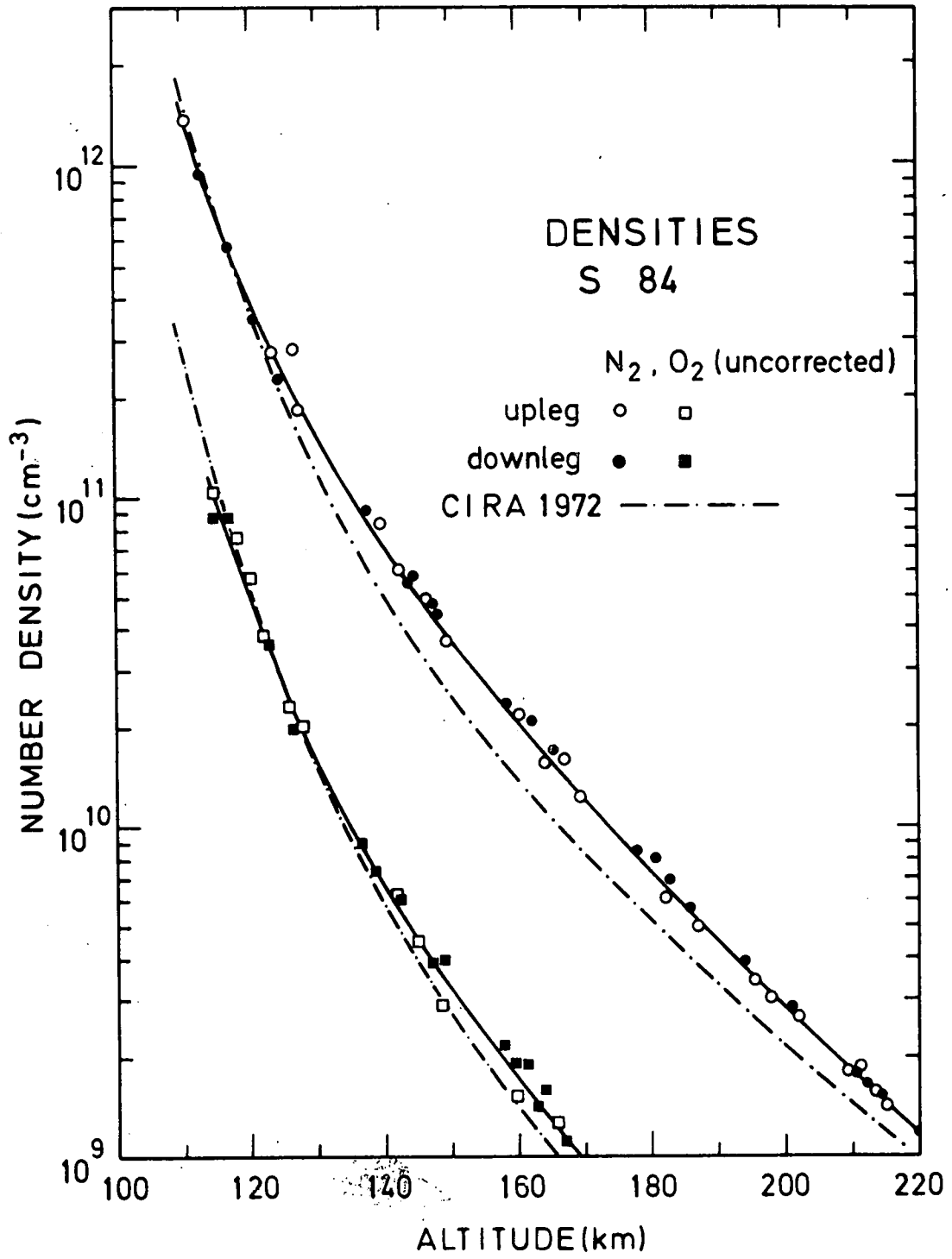


Fig. 8.- O<sub>2</sub> and N<sub>2</sub> number densities measured by the mass spectrometer during flight S84.

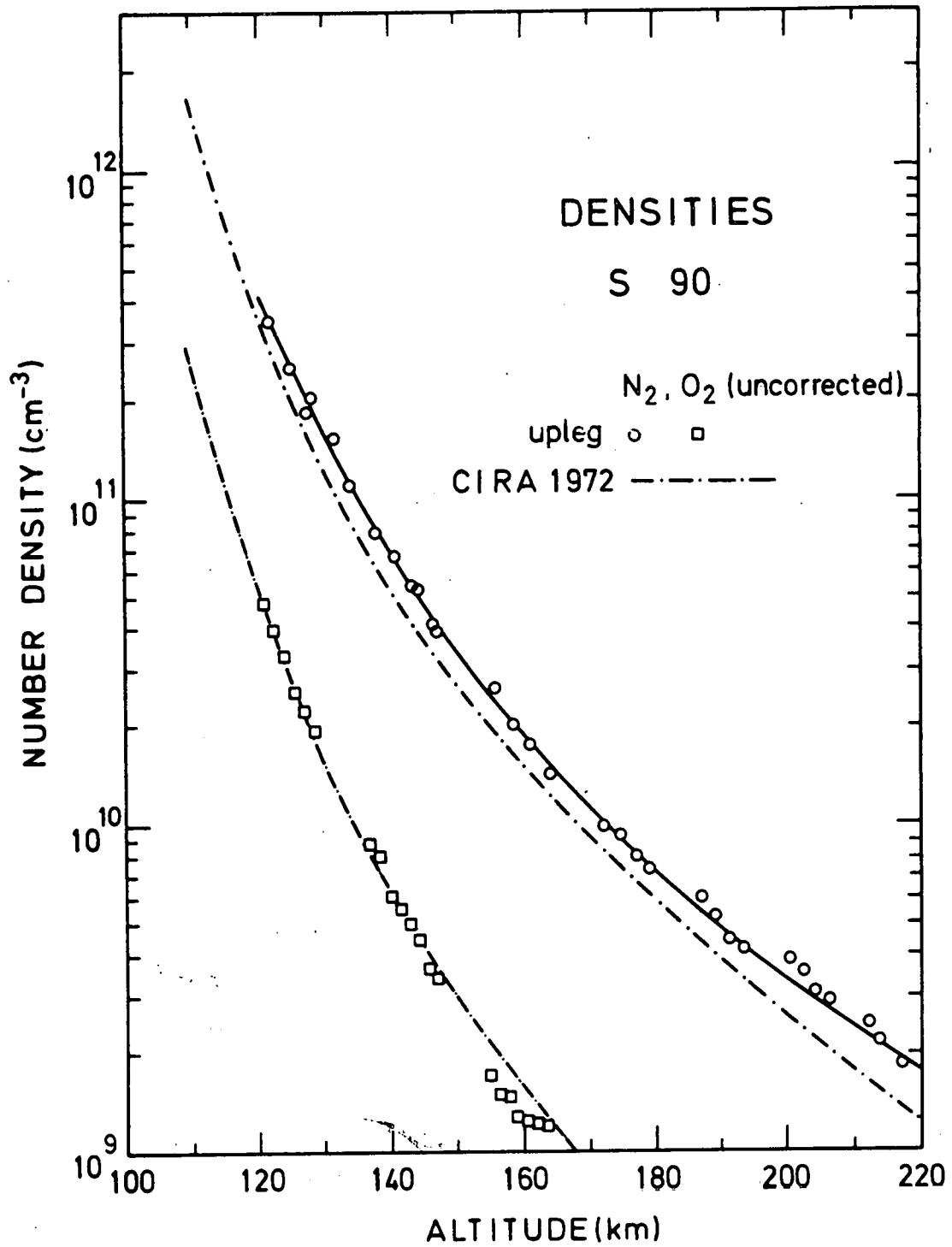


Fig. 9.- O<sub>2</sub> and N<sub>2</sub> number densities measured by the mass spectrometer during flight S90.

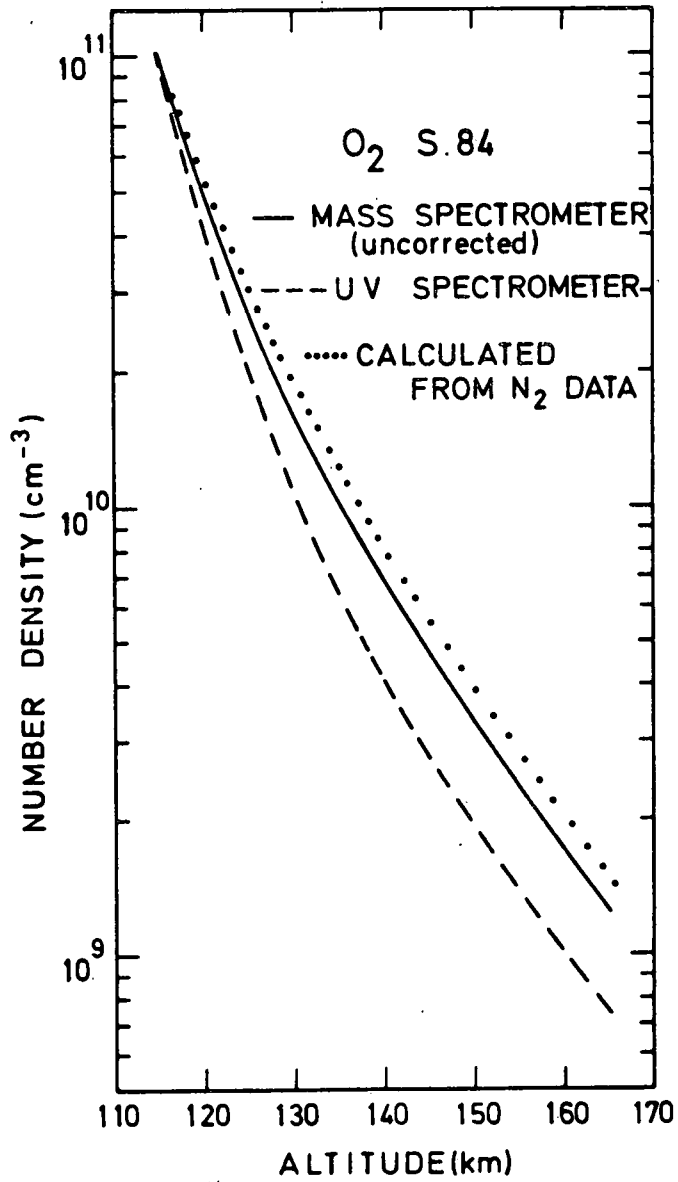


Fig. 10.- Comparison of final UV monochromator data and mass spectrometer data (uncorrected for possible recombination of ambient O into  $O_2$ ) on  $O_2$  number densities obtained from flight S84. The dotted line indicates a theoretical  $O_2$  profile which matches the 115 km altitude data of the mass spectrometer and follows higher up a distribution which is in diffusive equilibrium with the  $N_2$  profile measured simultaneously.

diffusive equilibrium with the simultaneously measured  $N_2$  profile than the UV absorption data. This comparison is indicated in Figure 10 where is shown a calculated  $O_2$  profile with  $n(O_2) = 9.75 \times 10^{10} \text{ cm}^{-3}$  at 115 km altitude and which is in perfect diffusive equilibrium with the measured  $N_2$  distribution. If we correct the measured  $O_2$  profile for possible contributions of the recombination of O to  $O_2$  it would move to lower values and thus further away from the diffusive equilibrium profile.

In summary we conclude that due to the quantitatively unknown recombination effects of O the mass spectrometrically measured  $O_2$  profile can only be considered an upper bound to the genuine ambient  $O_2$  distribution. On the other hand, we place considerable faith in the  $O_2$  profiles measured by the UV monochromators and the  $N_2$  profiles of the mass spectrometers. These profiles, however, can not be reconciled with the prevalence of diffusive equilibrium conditions. In case we attribute the deviation from the equilibrium conditions to the  $O_2$  distribution it would imply upward flow of  $O_2$ . This direction is in general accordance with the idea that photodissociation of  $O_2$  and dissociative recombination of  $O_2^+$  throughout the thermosphere must lead to an upward transport of  $O_2$  and corresponding downward transport of O.

#### *ACKNOWLEDGEMENT*

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