Retrieval of total ozone quantity from high resolution infrared spectra : influence of spectroscopic and physical parameters

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In this work, we present the results obtained for total ozone quantity (TOQ) from Jungfraujoch observatory spectrometer using 3 different spectral regions.

The spectrometer is a University of Liège FTS with a resolution power of 0.0025 cm^{-1} and typical S/N ratio larger than 1500. The spectra cover the region from 1900 to 3500 cm^{-1}.
In principle the use of isolated lines is perfect, as all the spectroscopic parameters are known, as well as their temperature dependence, that is to say position, intensity, halwidth and ground energy level. The three band are given in the next table I, as well as their band centers and the band strength given in cm^{-1}/molecule.cm^2. We note that the ratio of intensities is roughly a factor 10 or 50,

ν_0	$v'_1v'_2v'_3$	$v_1v_2v_3$	S_{band}
2705.2391	111	000	0.243×10^{-19}
2110.7843	101	000	0.124×10^{-17}
3046.0882	003	000	0.131×10^{-18}

permitting to cover different zenith angles, but which makes simultaneous retrieval not very easy. The line positions and intensities for $\nu_1+\nu_2+\nu_3$, $\nu_1+\nu_3$, $3\nu_3$ are given respectively in references 1, 2,3, as well as ground energy levels. The air broadening coefficients are given in reference 4 and pressure shifts in reference 5. We derived TOQ by least square fitting between observed and calculated transmittances. The calculated transmittance uses Voigt function, using Whiting expression modified by Oliveiro and Longbothum and the atmosphere is divided in 30 layers in which Pressure (P) and Temperature (T) are considered as constants (reference 6). P and T have been obtained by soundings during the same day as the recording spectra.
We show in figure 1 to 5 the examples of fits which have been obtained in the different spectral regions. For each of these fits the TOQ is given in Dobson units.
The influence of different spectroscopic parameters of the retrieved TOQ has been tested :

* Line strength S : retrieved TOQ is of course inversely proportional to S.
* Halfwidth : we have plotted in figure 6 the value of T.O.Q. with respect to α for two different spectral regions.

* n coefficient, defined by $\alpha(T)=\alpha(T_0)\cdot\left(\frac{T_0}{T}\right)^n$. The results are the following, for the 3040 cm^{-1} and with $\alpha = 8410^{-1}$ cm^{-1} atm^{-1}.

n= 0.75 → T.O.Q. = 323
n = 1.3 → - = 344

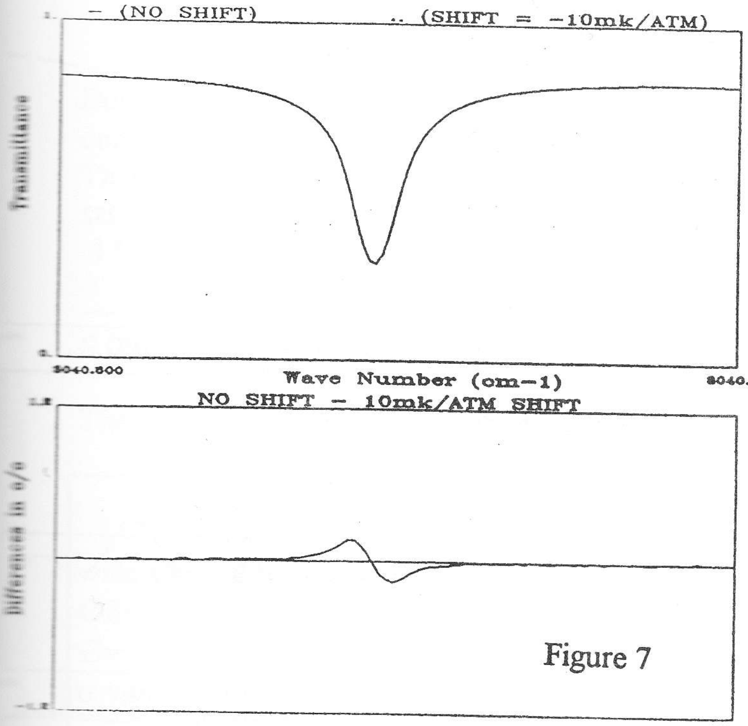


Figure 7

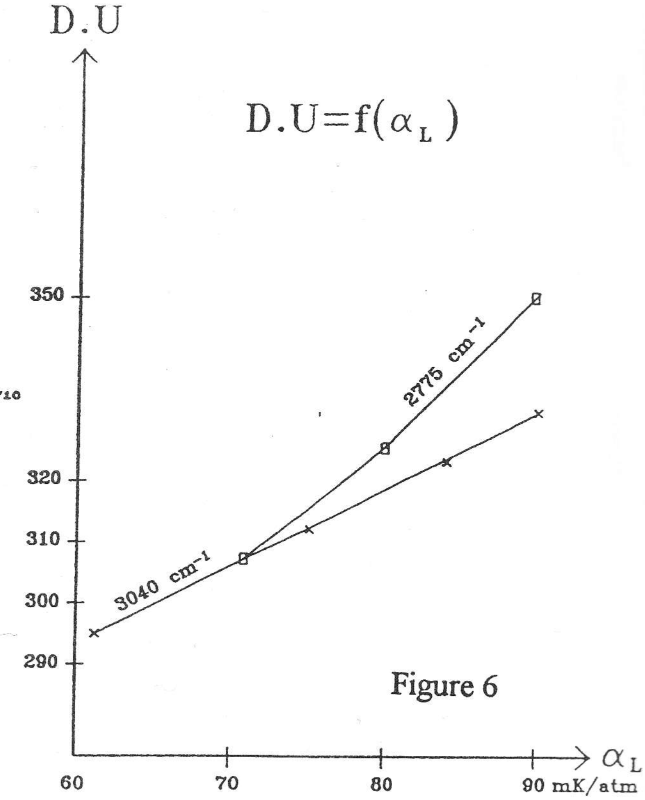


Figure 6

*For the pressure shifts we have plotted in figure 7 the differences (in %) between spectra calculated with $\Delta\nu = -10.10^{-3}cm^{-1}.atm^{-1}$ and $\Delta\nu = 0$

All these results are summarized in table II, part A.

A. Spectroscopic parameters

1.υ	→	0 %	position
2.S	→	4 %	line strength
3.α	→	1 %	halfwidth
4.Δν	→	0 %	pressure shift
5.n	→	2 %	variation of α
Total		7 %	

In table II, part B, we have estimated the errors coming from instrument function, that is to say the determination of zero level of transmittance and of the apparatus function.

B. Instrument

1.	0% transmittance	#3%
2.	Apparatus function	#2%

To estimate the influence of geophysical parameters we have tested the influence of a systematic variation of 3°C on T.O.Q., for the 3 different spectral regions (part. C).

C. Geophysical parameters

1.Temperature. For 2775 and 3040 cm^{-1} regions (lower state energy of 17.6 cm^{-1} and 50.64 cm^{-1} respectively, we have found :

$\Delta T = +3°C \rightarrow \Delta DU = +1.8$ %

For $\nu_1+\nu_3$ (E" = 447 cm^{-1}), we have found

$\Delta T = +3°C \rightarrow \Delta DU = -3$ %

2.Shape of the O_3 vertical distribution

Difficult to estimate Order : 2 %

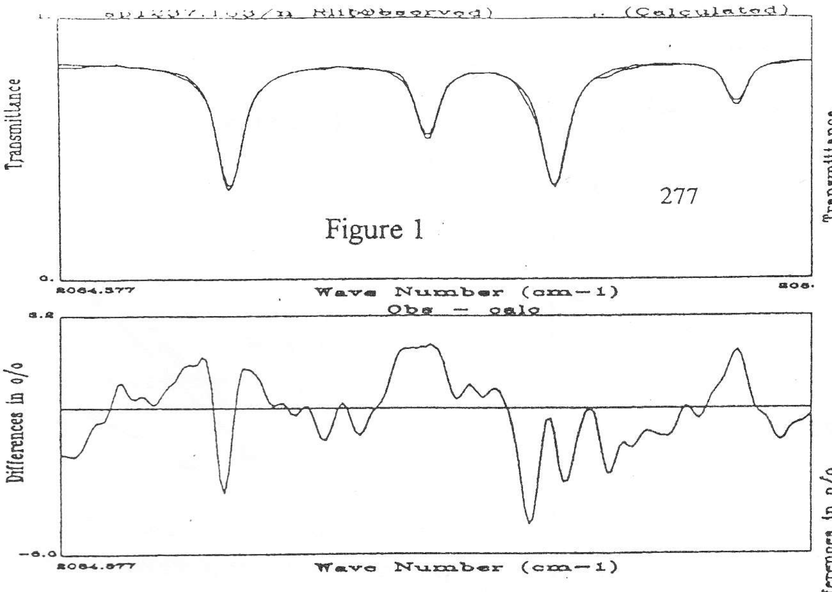


Figure 1

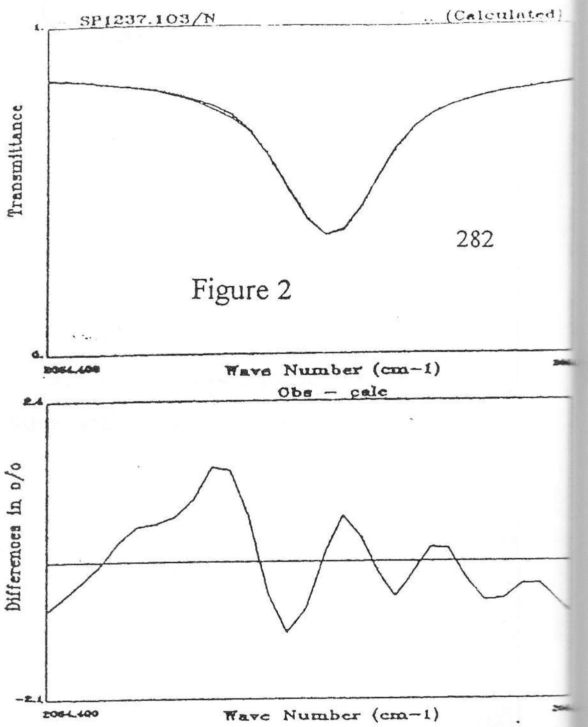


Figure 2

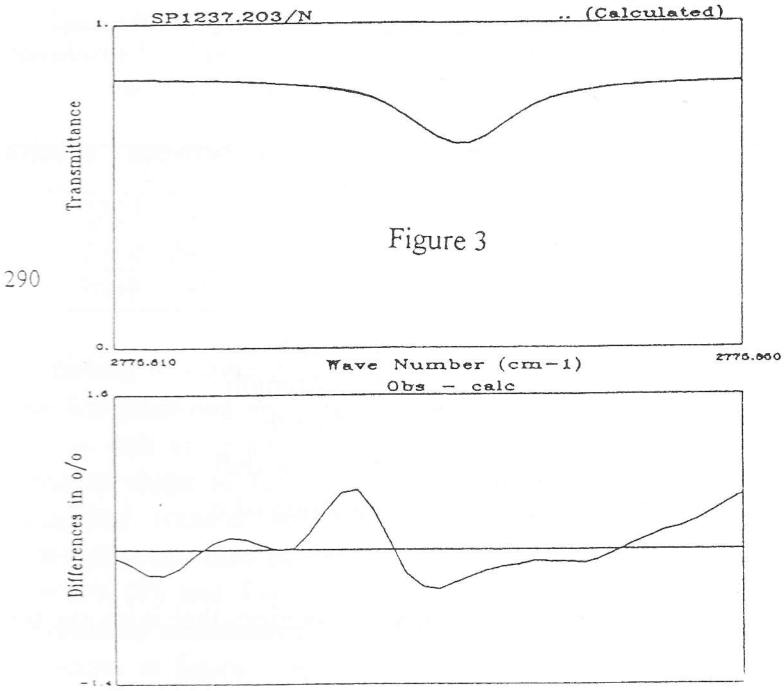


Figure 3

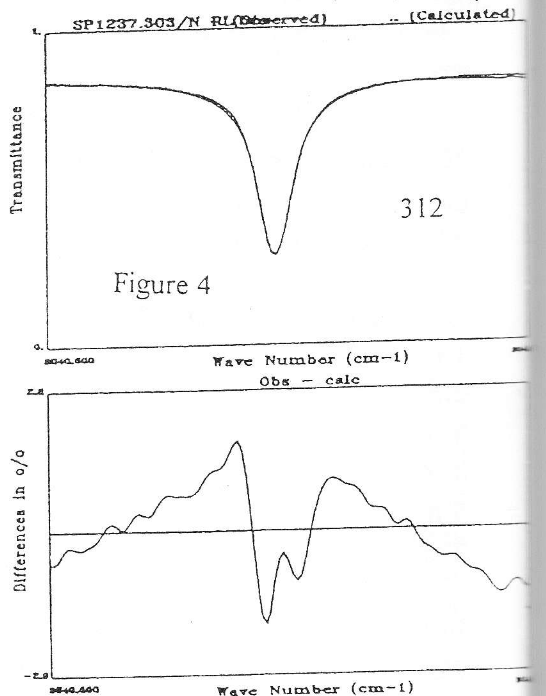
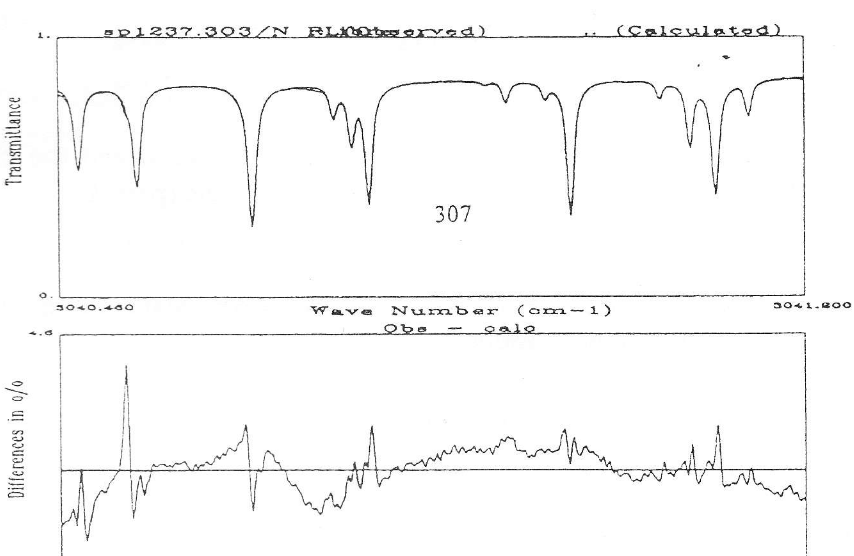


Figure 4

Figure 5



But the final error of T.O.Q. is not the sum of the three A, B and C parts, as many of these errors are correlated (T,n,α) or have the same effect (ex : S and 0% transmittance).
Then we finally estimate the theoretical maximum error of absolute total ozone quantity as :

$$\underbrace{4\,\%}_{S,0\%} \quad + \quad \underbrace{1\% + 2\,\% + 2\,\%}_{\alpha,n,T,\ \text{shape}} = 9\,\%$$

The experimental final results obtained from the different fits are summarized in table III.

	Results					
	2080 ($\nu_1+\nu_3$)		2775	($\nu_1+\upsilon_2+\nu_3$)	3040	($3\nu_3$)
	wide spectral region (wsr)	1 line	wsr	1 line	wsr	1line
Øfixed	256	277		287	300	
Øvariable	277	**282**		**290**	307	**312**
α variable		293				
		282 ± 11		290 ± 5		312 ± 12
		CONCL.	**295 ± 17 DU**	**6 %**		

Results
They are given for the 3 different spectral regions, covering a large spectral region or the best single line of this region. We let the radius of aperture of FTS free to have the best fit and then the final results are 282 ; 290 and 312 Dobson Units corresponding to 295 ±17 Dobson unit. These results are in the range of theoretical error : 9 %.

Conclusion : We believe that there are two points which can lead to a better ozone retrieval : one is concerned with absolute determination of intensity where the goal is to have a real 1% accuracy ; the second is to have a better knowledge of instrumental apparatus function (including zero level transmittance). In this case, we may expect a final retrieval of T.O.Q. better than 4 %.

References

1 The 3.6 µm region of ozone. Line positions and intensities
M.A. Smith, C.P. Rinsland, M. Devi, J.M. Flaud, C. Camy-Peyret, A. Barbe, Journ. of Mol. Spectr.,1990, 139 p 171-181
2 Intensities and self broadening coefficients of O_3 in the 5 µm region
J.J. Plateaux, S. Bouazza, A. Barbe, Journ. of Mol. Spectr.,1991, 146, p 314-325
3 The 3.3 µm region of ozone. Line positions and intensities
C. Camy-Peyret, J.M. Flaud, M. Smith, C. Rinsland, M. Devi, J.J. Plateaux, A. Barbe, Journ. of Mol. Spectr.,1990, 141, p 134-144
4 Nitrogen and oxygen broadening coefficients of ozone
S. Bouazza, A. Barbe, J.J. Plateaux, L. Rosenman, J.M. Hartmann, C. Camy-Peyret, J.M. Flaud, R. Gamache, Journ. of Mol. Spectr.,1993, 157, p271-289
5 Pressure shifts of O_3 broadened by N_2 and O_2,
A. Barbe, S. Bouazza and J.J. Plateaux, Applied Optics, 1991, Vol.30, n°18, p 2431-2436.
6 P. Marché, Thesis, Reims, 1980

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