Sixth Workshop "Solar influences on the magnetosphere, ionosphere and atmosphere"

A method of determination of the atmospheric O_2 extinction spectrum

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26–30 May 2014, Sozopol, Bulgaria

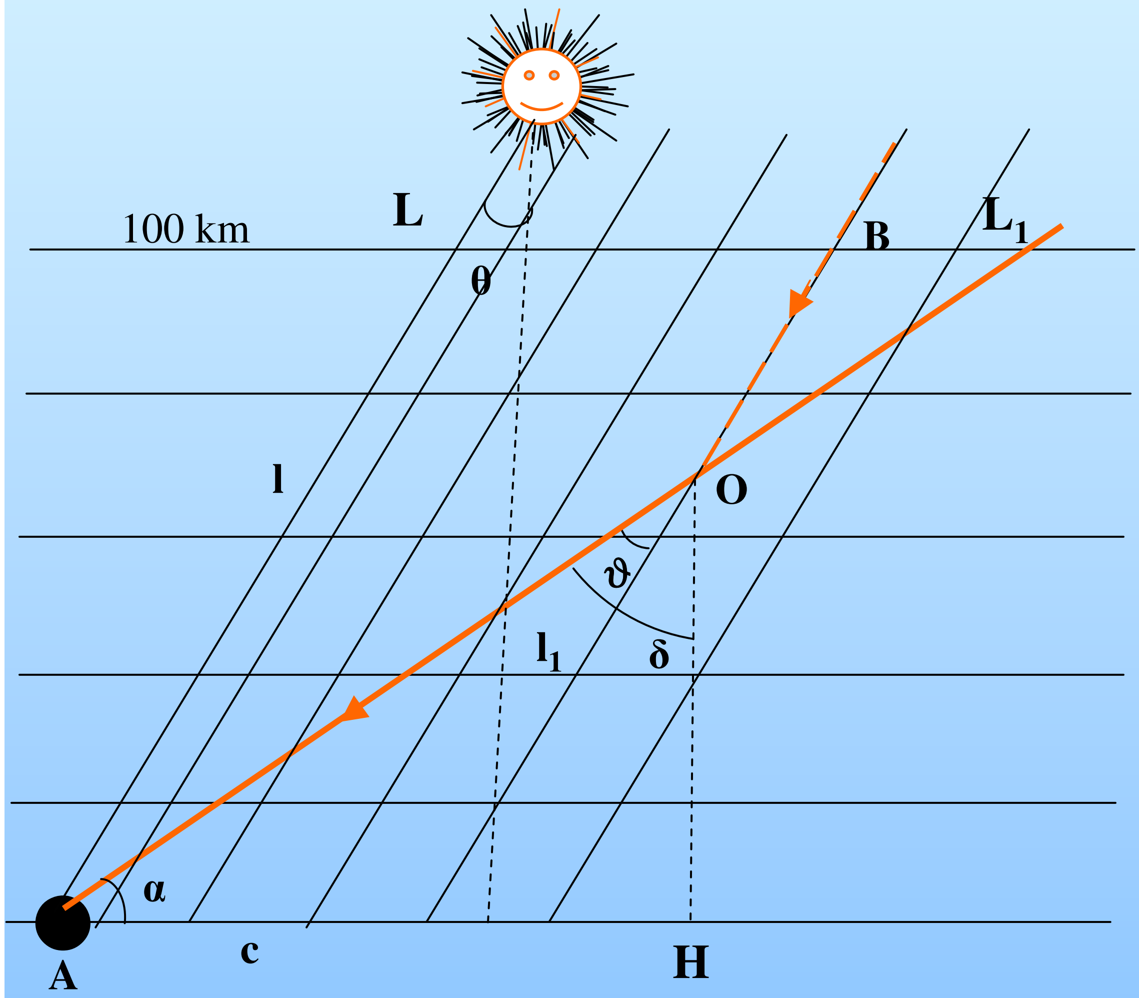
Molecular oxygen is one of the main atmospheric constituents and that's why its extinction bands are between the strongest ones in the observed solar spectrum.

A method to compute the extinction of the solar radiation by the atmospheric molecular oxygen was developed. Absorption and single scattering towards the observer were included in the calculations. The atmosphere was considered as plane parallel and divided into layers with equal thickness. A computation following the "line-by-line" method was applied for A (0,0) band of the oxygen atmospheric system.

This work has 3 basic **goals**:

- To optimize the computations;
- To make a theoretical estimate of the expected differences between the results obtained for different conditions;
- To examine ground based measurements of O_2 extinction and theoretical spectra computed for the same conditions.

Methods of computation



Principal scheme of the O_2 extinction computations assuming observation under angle α towards horizon. The calculations for every considered ray are divided into 3 parts: calculation of the absorption from the upper edge of the atmosphere to the layer where the ray crosses the direction of observation l_1 (point O), absorption and single scattering in the direction of observation l_1 in this layer and absorption of the obtained radiation from this layer to the Earth in the direction of observation under angle $\vartheta = 90^\circ - \alpha - \theta$.

Theory

The attenuation of the solar light in the atmosphere is due mainly to absorption and scattering. In the common case after the Bouguer law:

$$I(\lambda) = I_0(\lambda)\exp(-\tau(\lambda)/\cos\theta)$$

where $I_0(\lambda)$ is the flux with wavelength λ at the upper edge of the atmosphere, $I(\lambda)$ is the flux reached the Earth (or any other considered height) , θ is the zenith angle of the Sun, and $\tau(\lambda)$ is the optical depth.

$$\tau(\lambda) = \tau_R(\lambda) + \tau_a(\lambda) + \tau_g(\lambda)$$

$\tau_R(\lambda)$ is the Rayleigh optical depth, $\tau_a(\lambda)$ is the aerosol optical depth, and $\tau_g(\lambda)$ is the optical depth due to the gases absorption. Absorption optical depth at a height z is given by:

$$\tau(\lambda, z) = \frac{1}{\mu}\int_z^{\infty} n(z')\sum_J S_J\left[T(z')\right].f\left[n(z'),T(z'),\ldots\right]dz'$$

It depends on the vertical profiles of the concentration $n(z')$ and the temperature $T(z')$,on the air mass factor μ, and on the individual rotational lines intensities $S_J(T)$ and profiles f.

Theory

The molecular Rayleigh scattering at wavelength λ is:

$$I = I_0 \frac{8\pi^4\alpha^2}{\lambda^4 R^2}(1+\cos^2\vartheta)$$

where α is the polarizability of the molecule, R is the distance to it, and ϑ is the scattering angle. The Rayleigh scattering by a molecule can be defined as well by the total cross section $\sigma(\lambda)[cm^2)$:

$$\sigma(\lambda) = \frac{24\pi^3}{\lambda^4 N^2}\frac{(n_{(\lambda)}^2 - 1)^2}{(n_{(\lambda)}^2 + 2)^2} F_{k(\lambda)}$$

where $\lambda[cm]$ is the wavelength, $N[cm^3]$ is the molecular density, $n_{(\lambda)}$ is the refractive index, and $F_{k(\lambda)}$ is the King correction factor. The factor $(n_{(\lambda)}^2 - 1)^2 / (n_{(\lambda)}^2 + 2)^2$ is an effect of the local electrostatic field, known as Clausius-Mossotti or Lorentz-Lorenz factor, and it is proportional to N.

Theory

The King correction factor is defined by:

$$F_{k(\lambda)} = \frac{6+3\rho_n}{6-7\rho_n}$$

where ρ_n is the depolarization factor of the natural or non-polarized light taking into account the anisotropy of the non-spherical molecules.

The scattering cross section for λ>500 nm, where the examined O_2 bands lie, can be determined by

$$\sigma(\lambda) = A\lambda^{-(B+C\lambda+D/\lambda)}$$

where A=4.01061x10^{-28}, B=3.99668, C=1.10298x10^{-3}, D=2.71393x10^{-2}.

Scattered light per unit volume is characterized by the coefficient of total volume Rayleigh scattering $\beta[cm^{-1}]$. At height z' it is given by the formula:

$$\beta(\lambda, z') = N(z')\sigma(\lambda)$$

Then the Rayleigh optical depth at height z is defined by the integral:

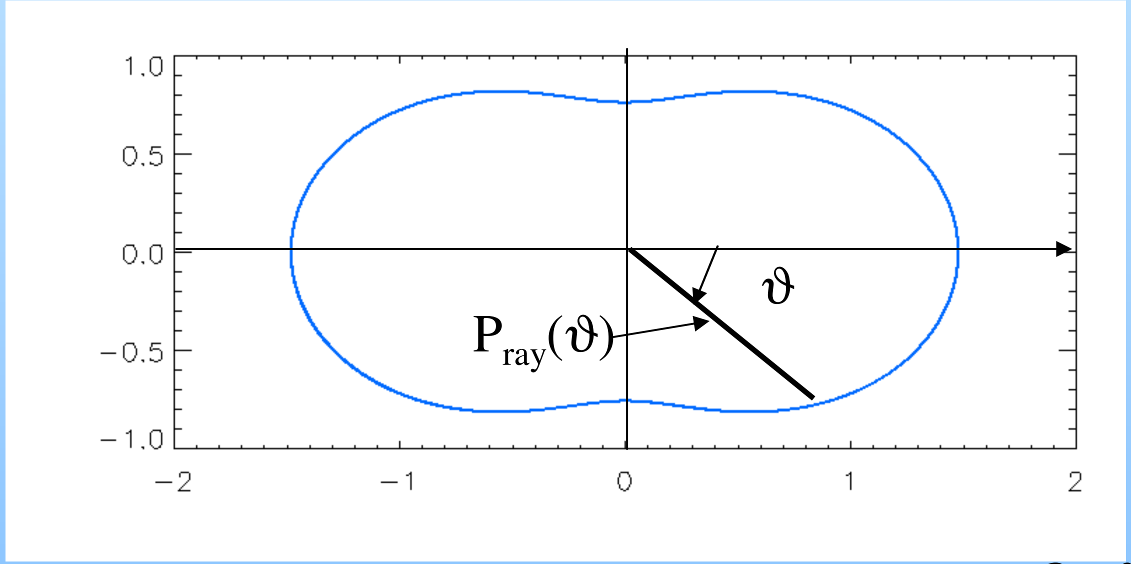
$$\tau(\lambda, z) = \int_z^{\infty} \beta(\lambda, z')dz'$$

Theory

The angular distribution of scattered light is described by the Rayleigh phase function:

$$P_{ray}(\vartheta) = \frac{3}{4(1+2\gamma)}\left[(1+3\gamma)+(1-\gamma)\cos^2\vartheta\right]$$

γ is defined by $\gamma = \dfrac{\rho_n}{2-\rho_n}$ where ρ_n is the depolarization factor.



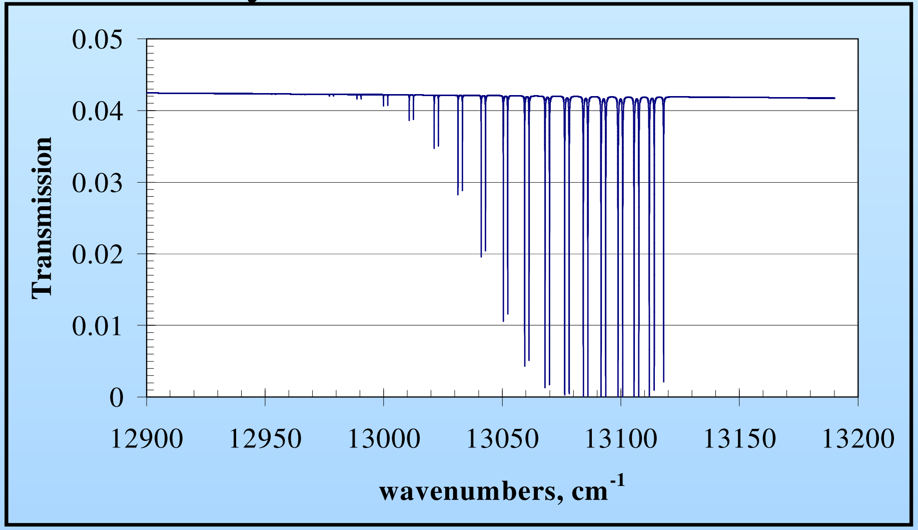
The angular coefficient of volume Rayleigh scattering is:

$$\beta(\vartheta,\lambda,z) = \frac{\beta(\lambda,z)}{4\pi}P_{ray}$$

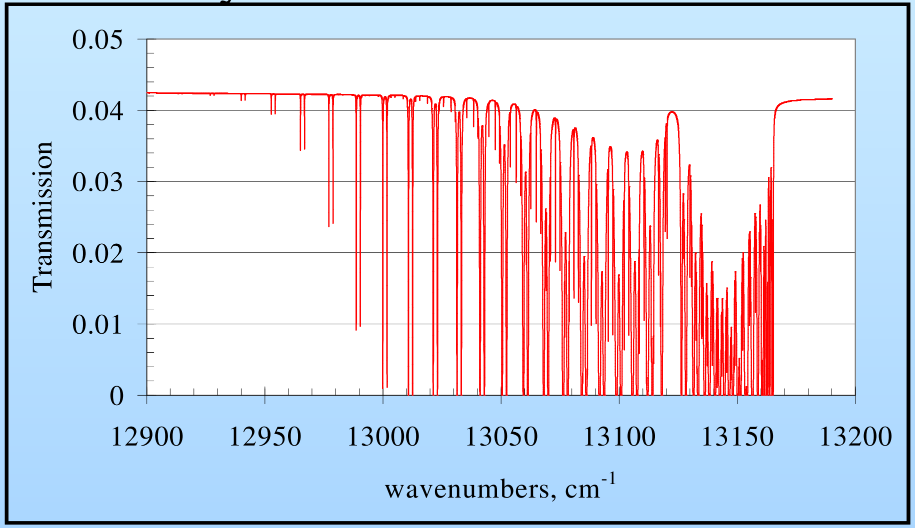
Computations

ZA=30°, obs. angle=50°

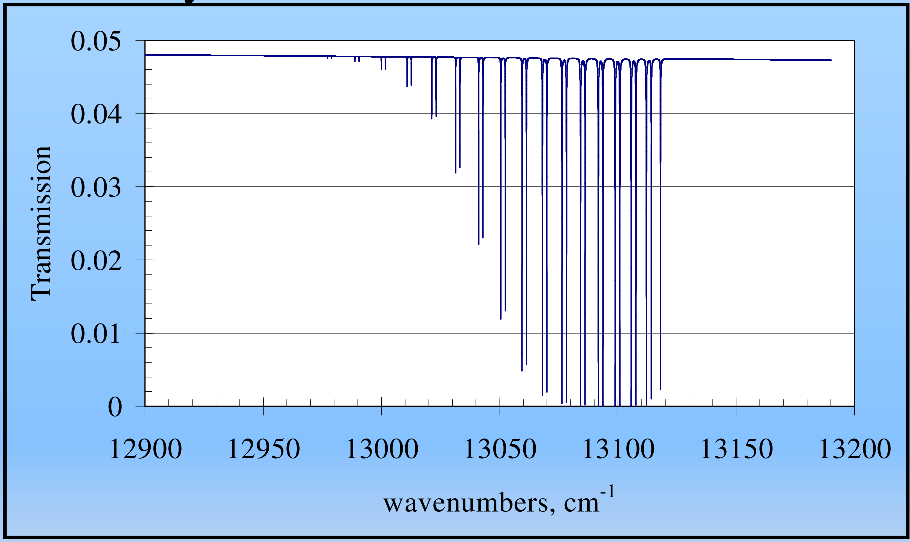
O_2 (0,0), P branch only
Layer thickness = 1 km



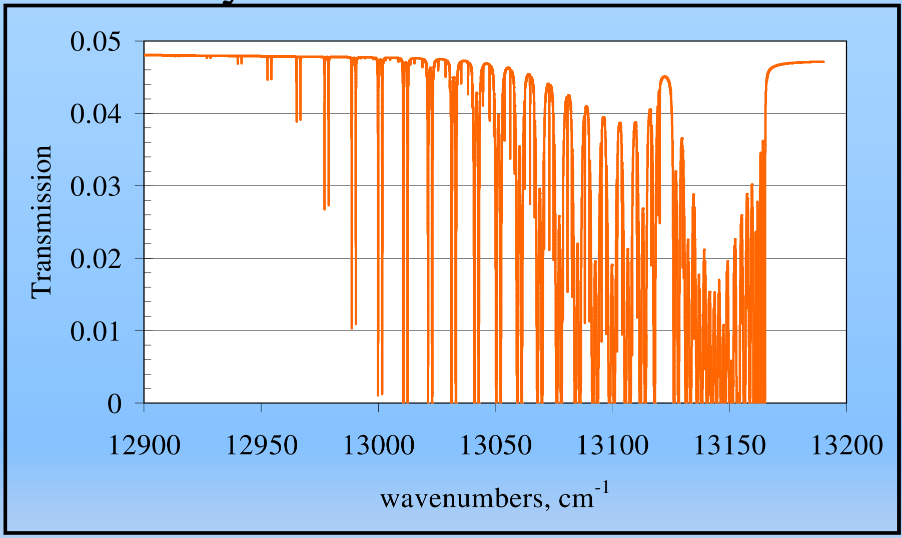
O_2 (0,0), whole band (P+R branches)
Layer thickness = 1 km



Layer thickness = 0.5 km



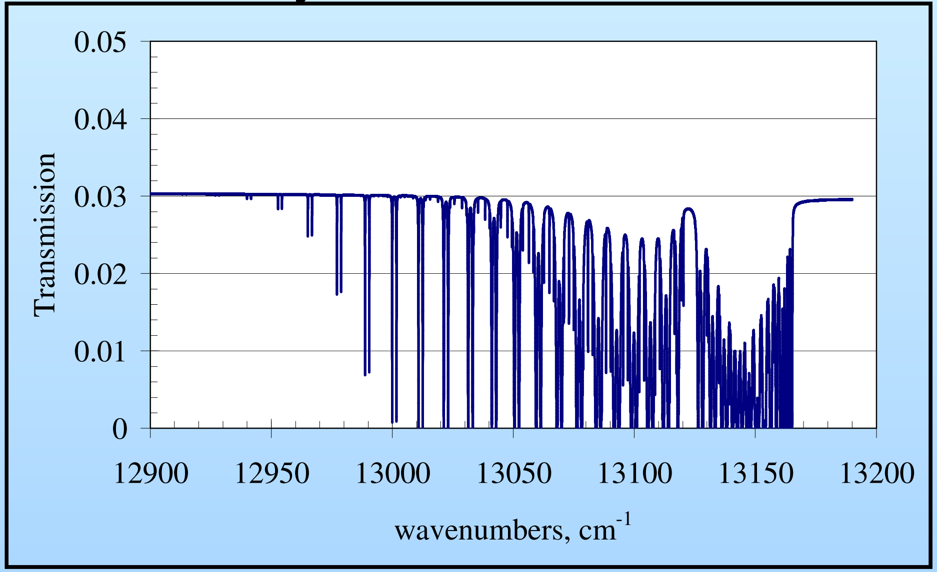
Layer thickness = 0.5 km



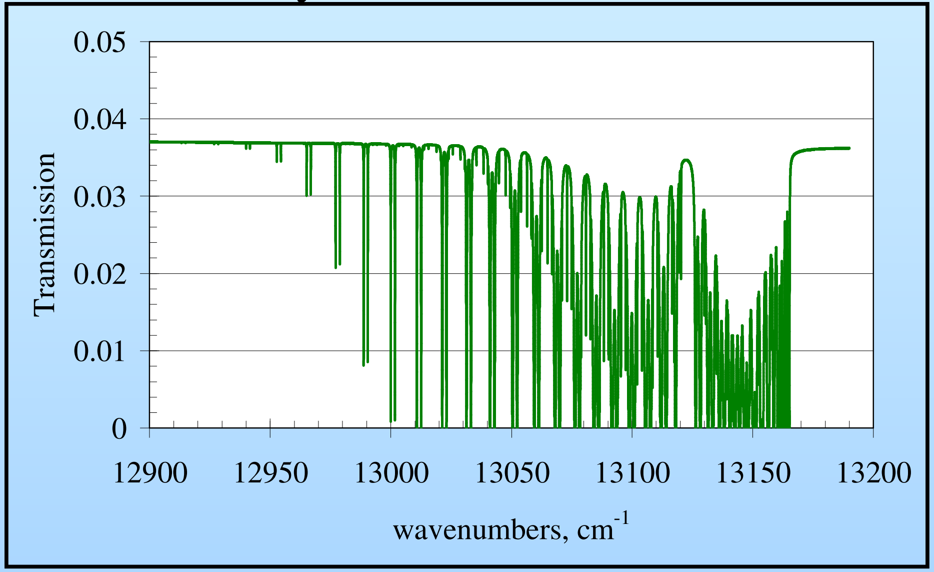
Computations

ZA=30°, obs. angle=50°, O_2 (0,0), whole band (P+R branches)

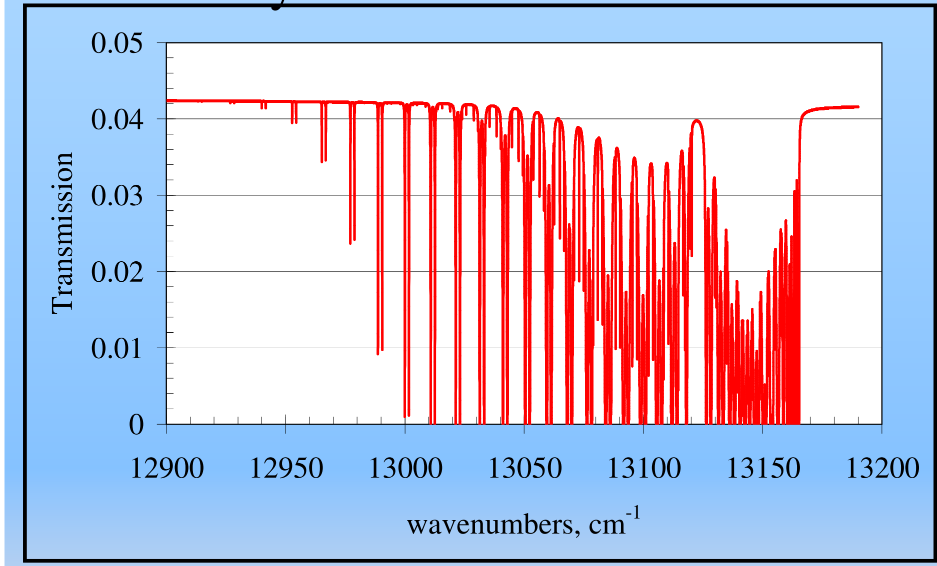
Layer thickness = 5 km



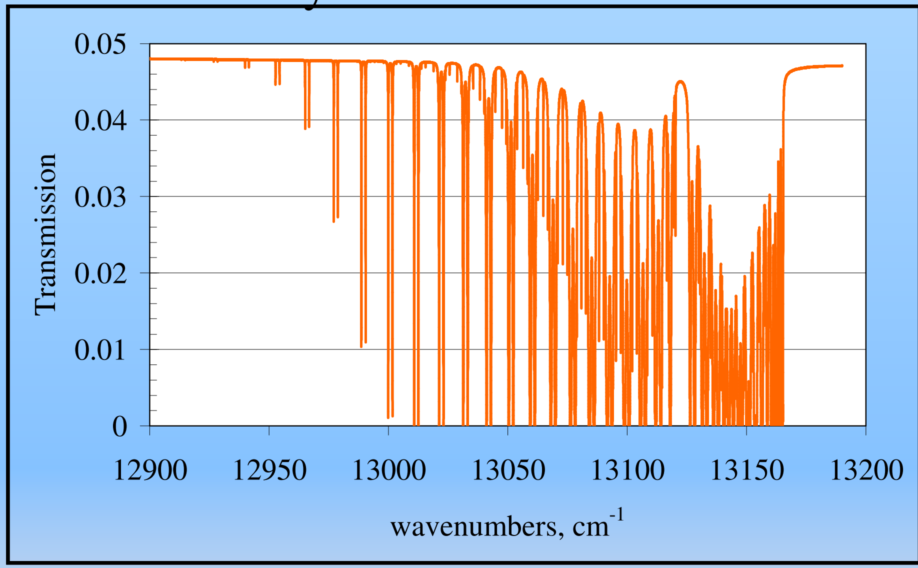
Layer thickness = 2 km



Layer thickness = 1 km



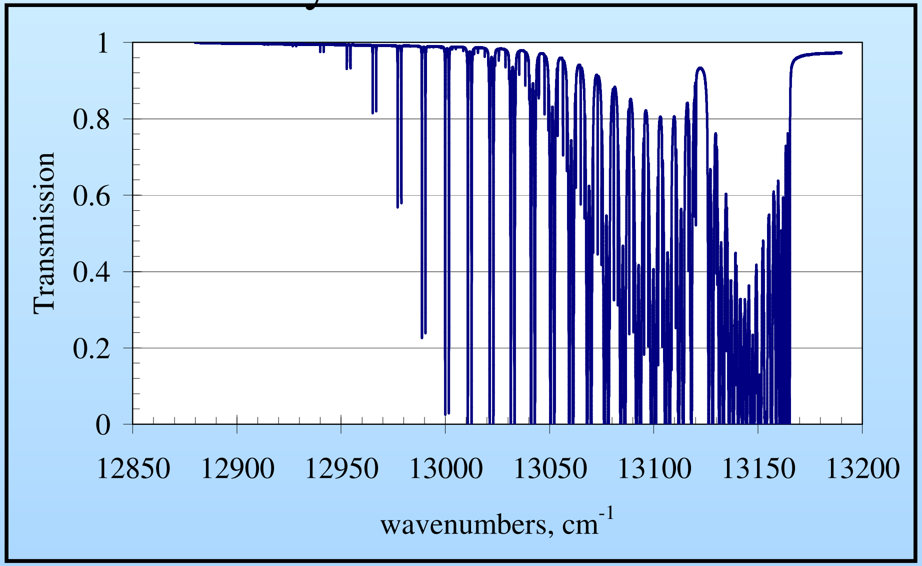
Layer thickness = 0.5 km



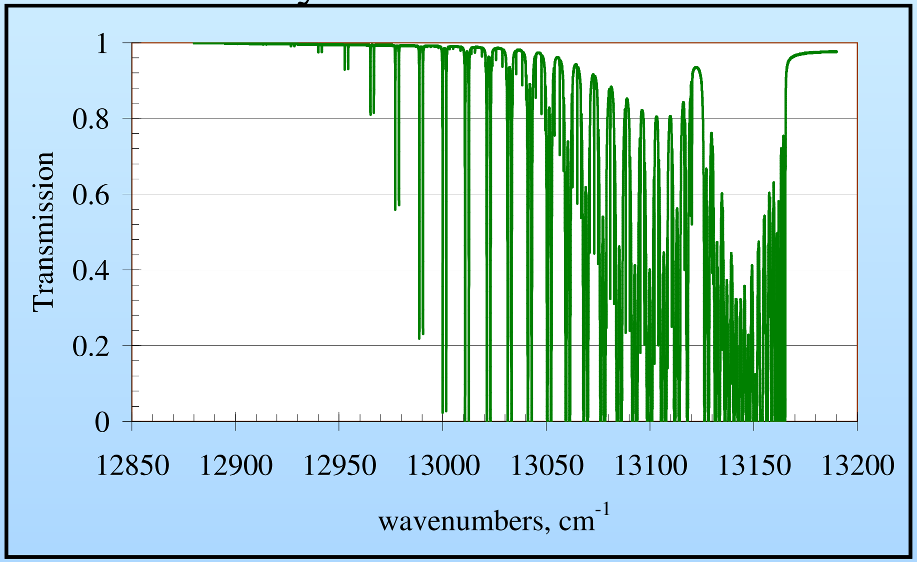
Computations

Normed O_2 (0,0) spectra, ZA=30°, observation angle=50°

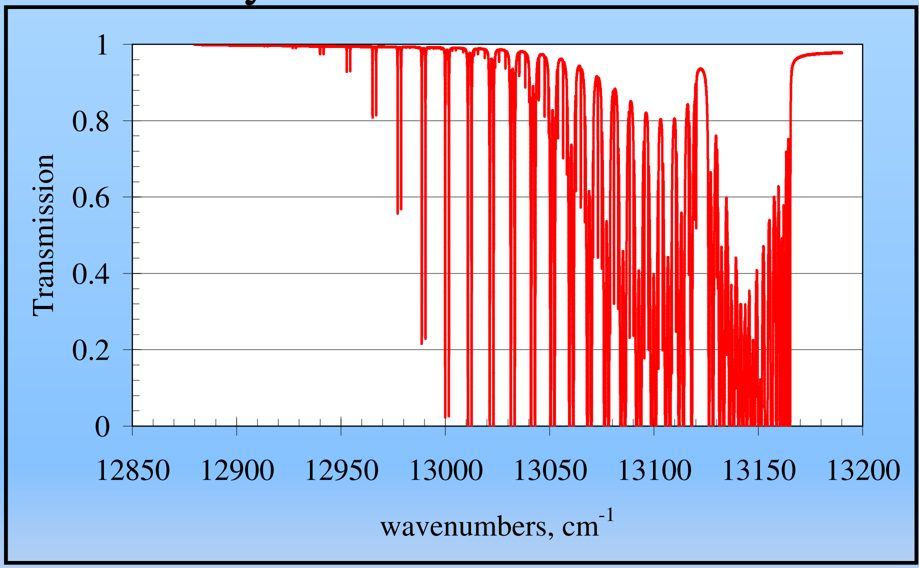
Layer thickness = 5 km



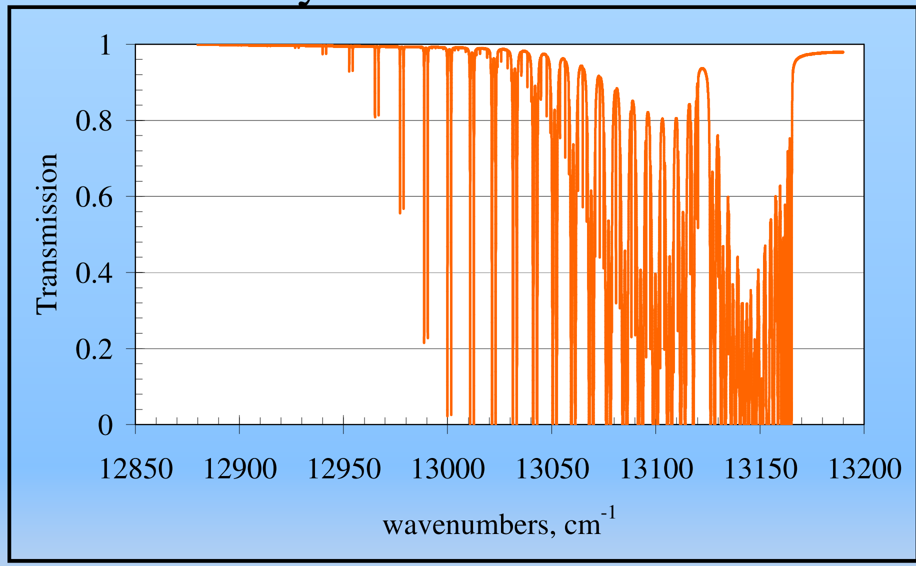
Layer thickness = 2 km



Layer thickness = 1 km

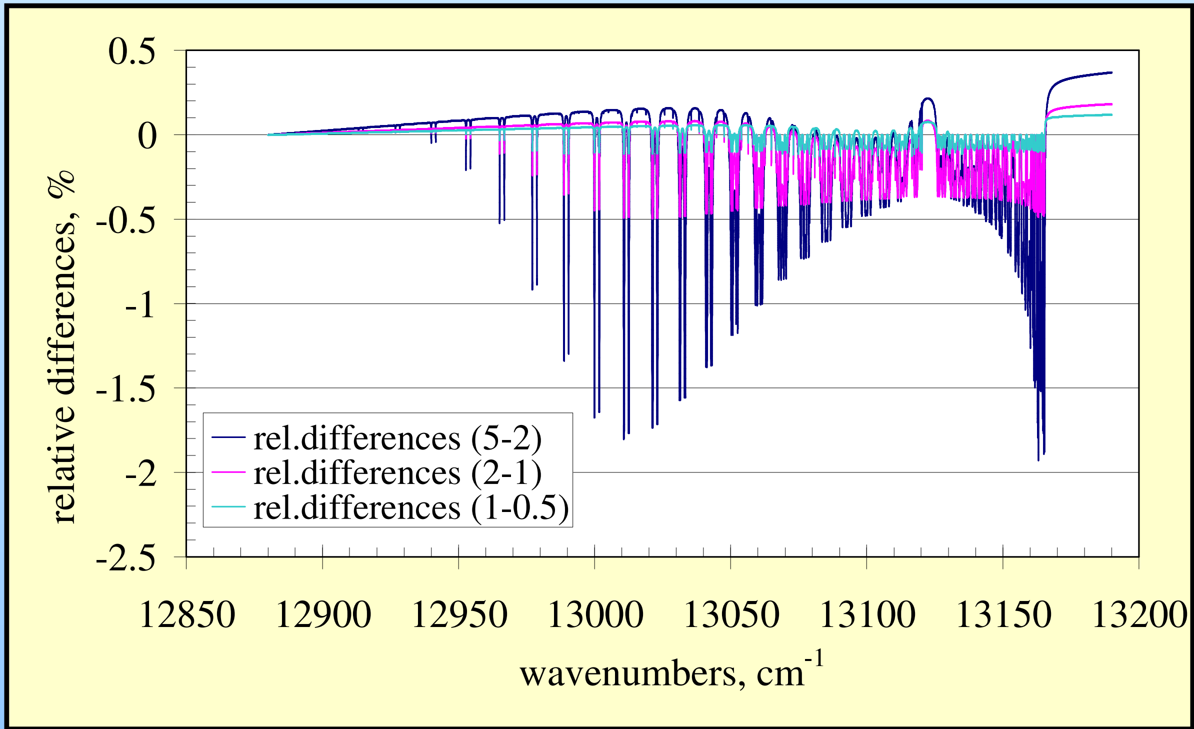


Layer thickness = 0.5 km



Computations

Relative differences, depending on the level thicknesses

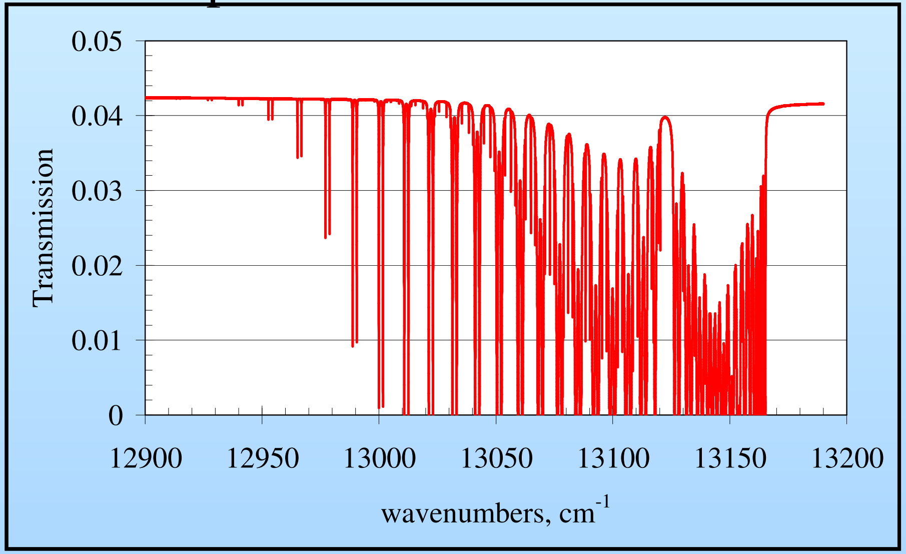


- For the computations, it is enough to use atmospheric layers with thickness 1 km.

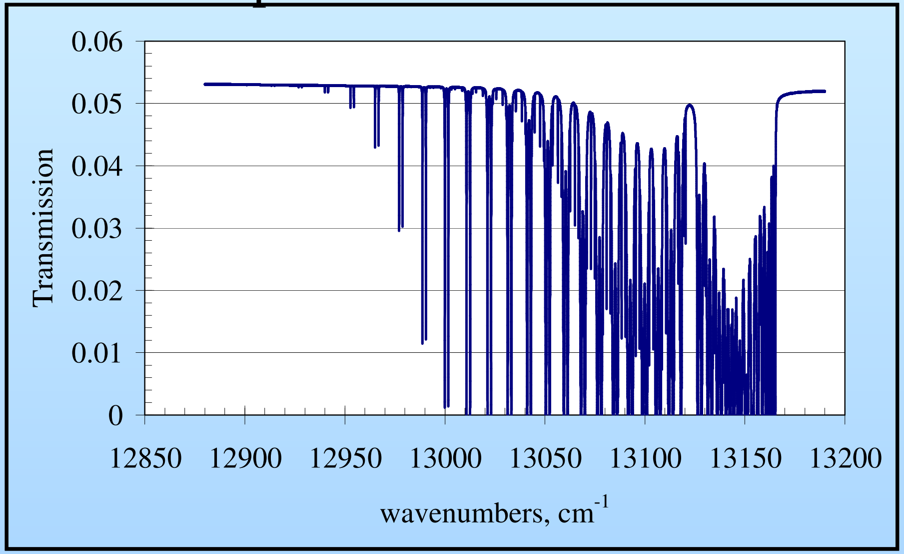
Computations

O_2 (0,0) extinction spectra, ZA=30°, observation angle=50°, layer thickness = 1 km

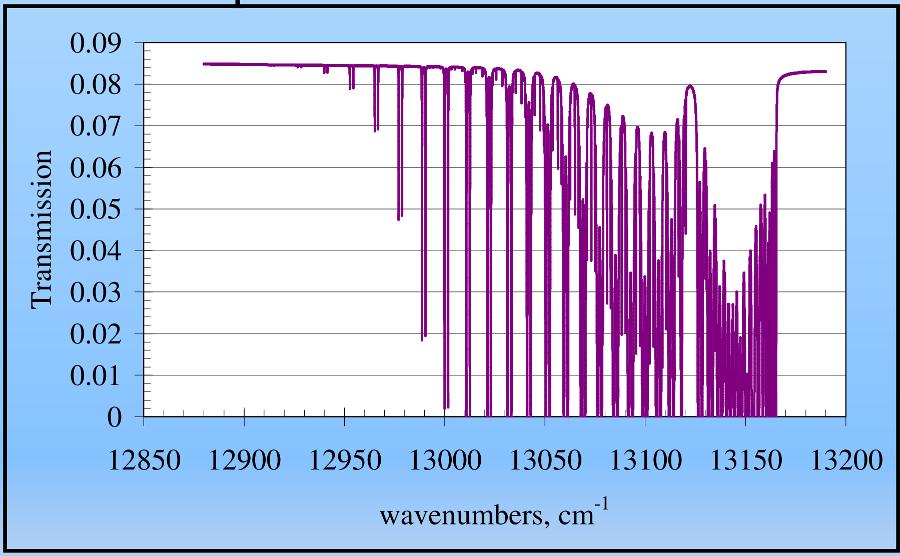
Atmosphere thickness = 100 km



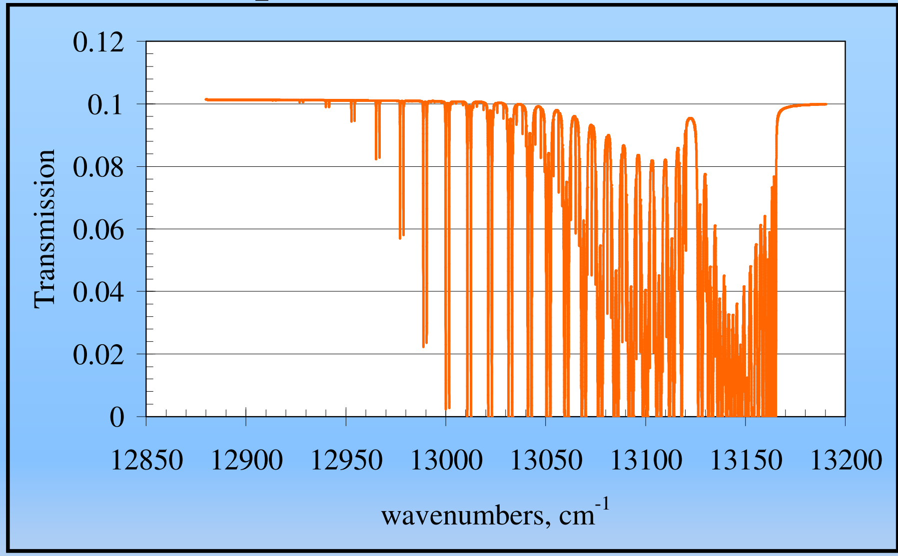
Atmosphere thickness = 80 km



Atmosphere thickness = 50 km



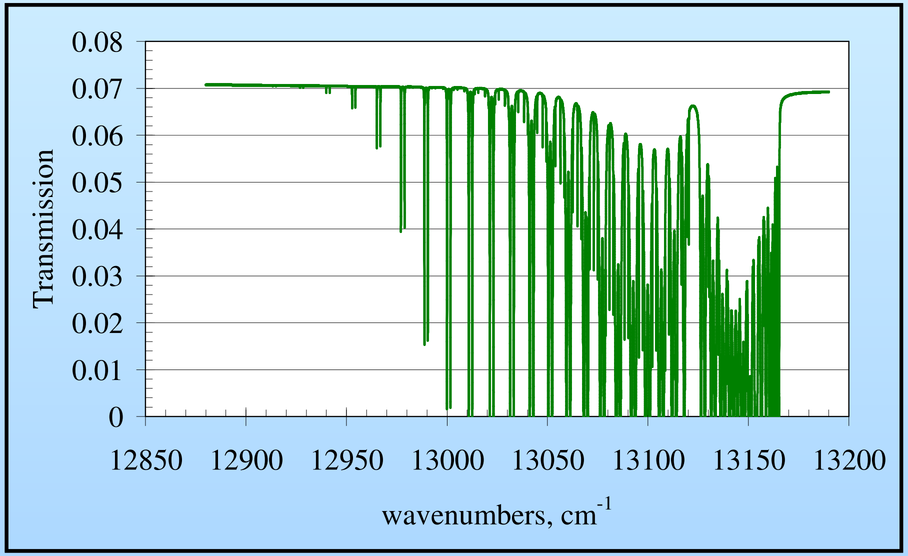
Atmosphere thickness = 40 km

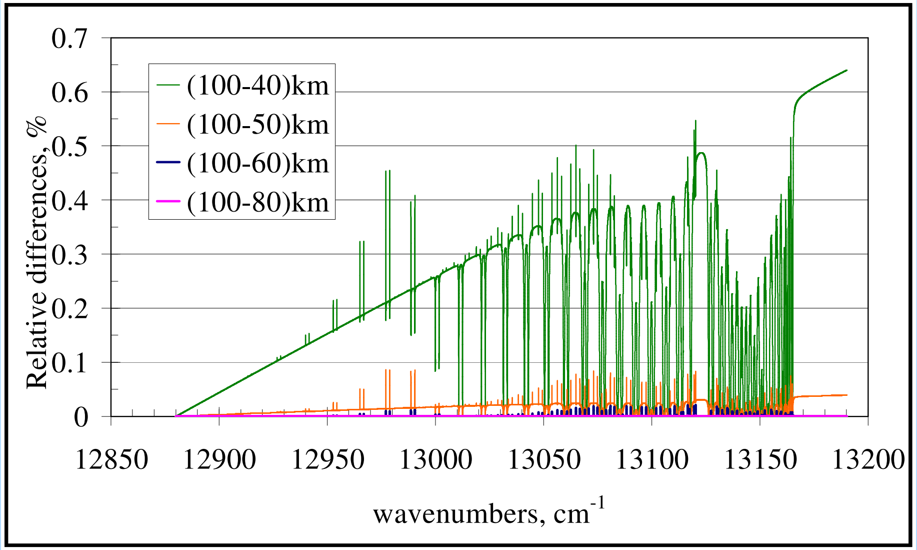


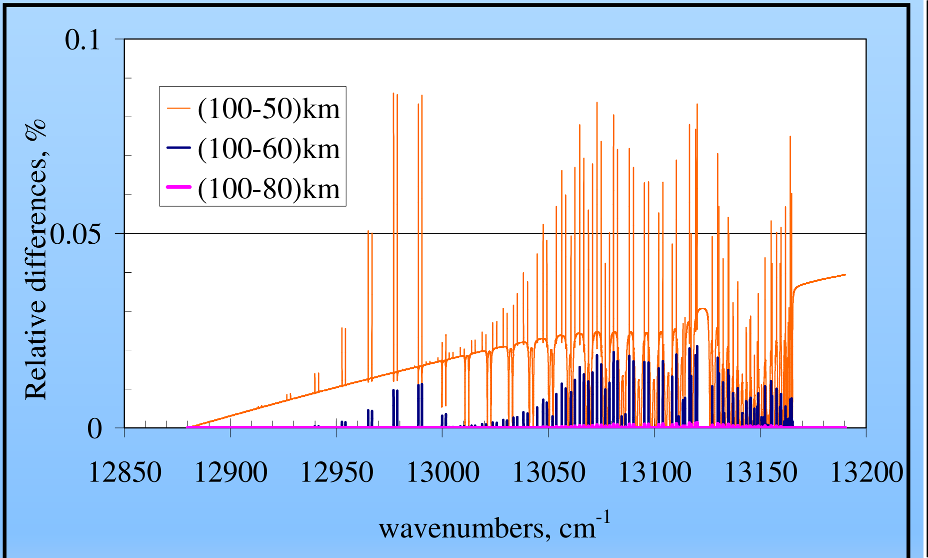
Computations

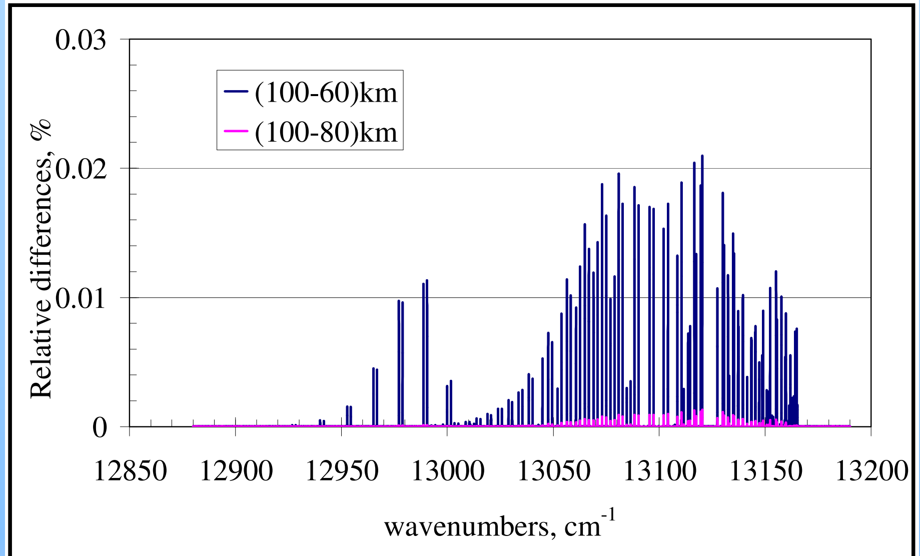
Relative differences, depending on the assumed atmosphere thickness

Atmosphere thickness = 60 km







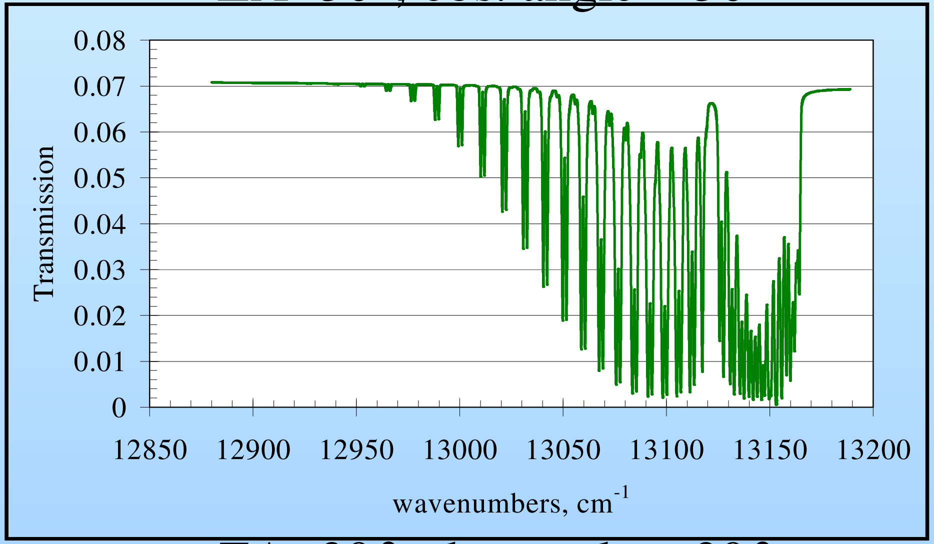


- For the computations, atmospheric upper limit at 60 km is sufficient.

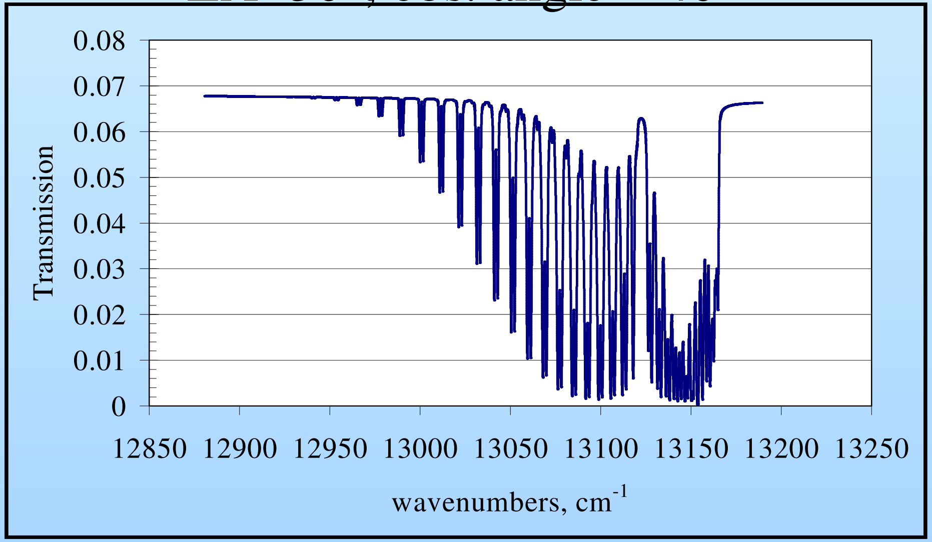
Computations

Computed O_2 (0,0) extinction spectra at ZA=30° and different obs. angles, layer thickness 1 km, atmosphere height = 60 km, convolved with a triangle function, half width=0.4 Ǻ

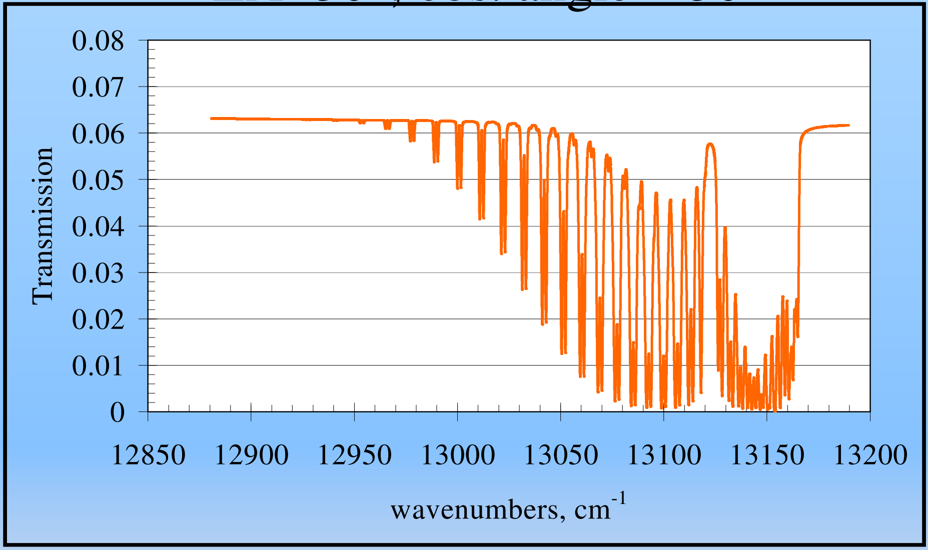
ZA=30°, obs. angle = 50°



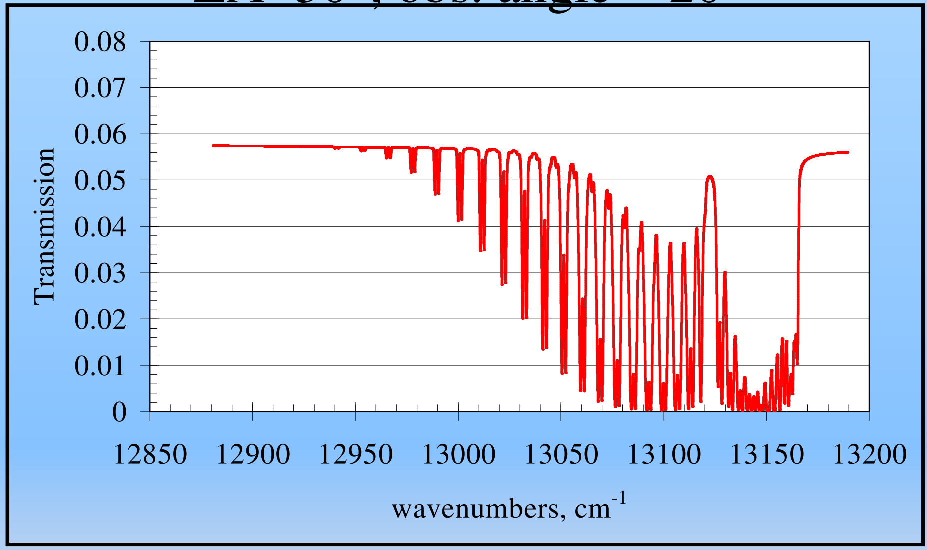
ZA=30°, obs. angle = 40°



ZA=30°, obs. angle = 30°

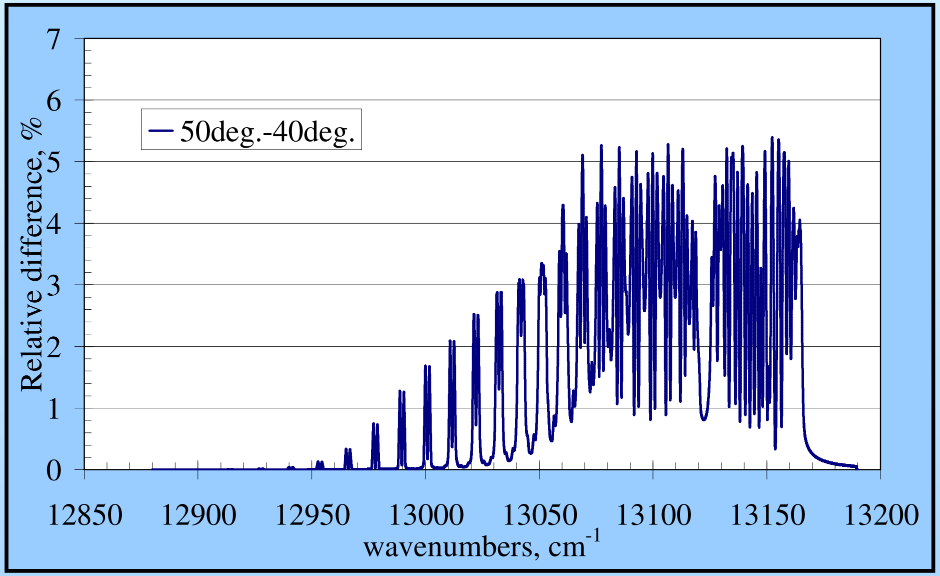


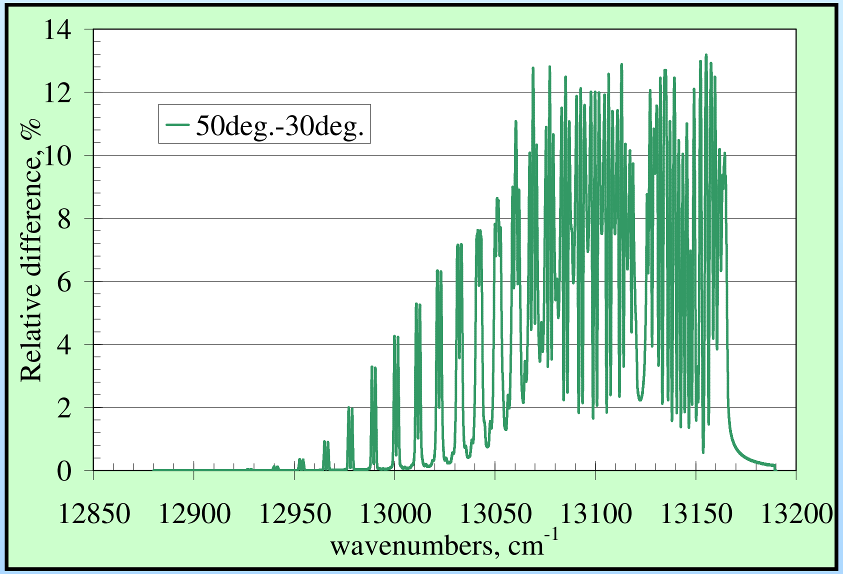
ZA=30°, obs. angle = 20°

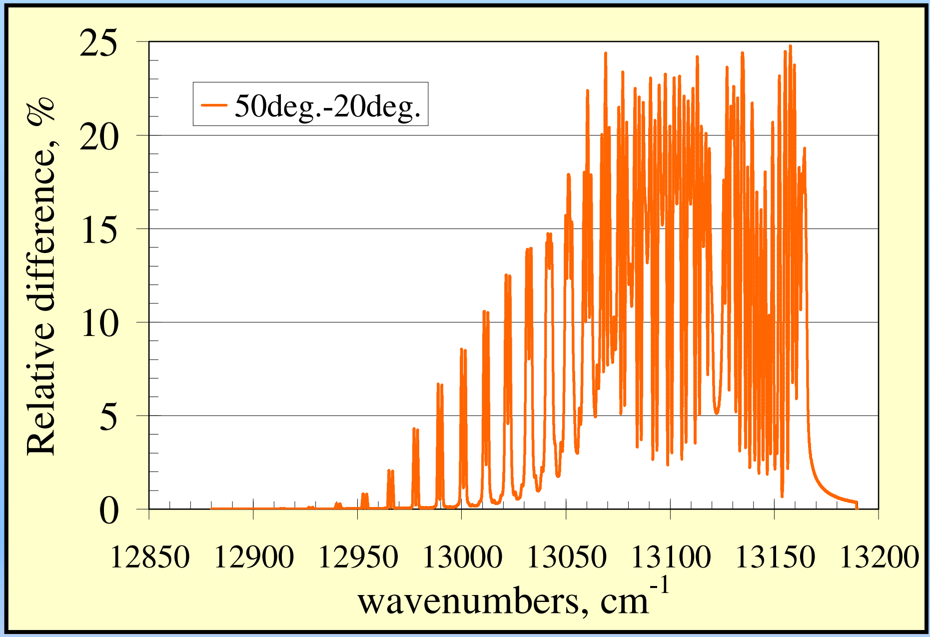


Computations

Differenses between the normed spectra





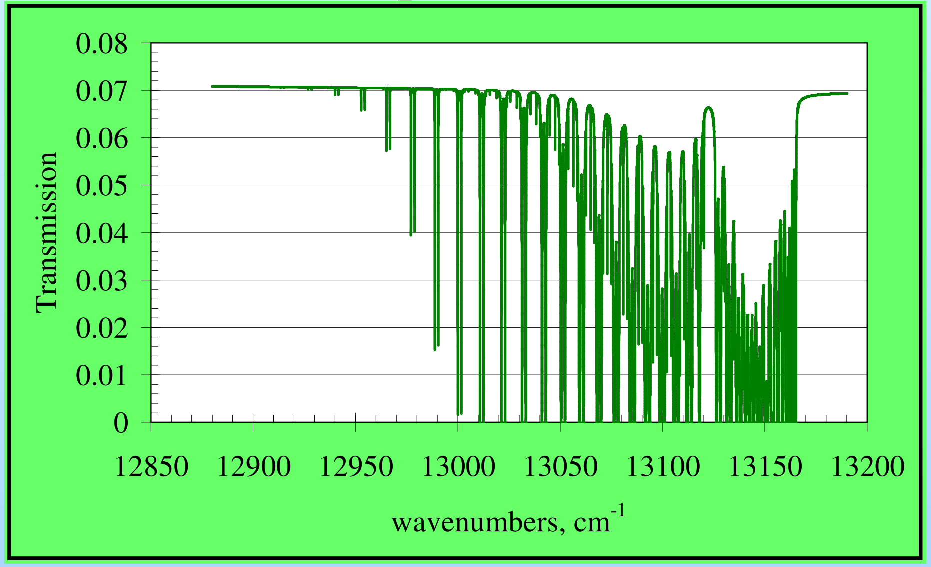


- The bigger differences are between the most intensive lines;
- The differences are bigger when the difference between the observation angles is bigger.

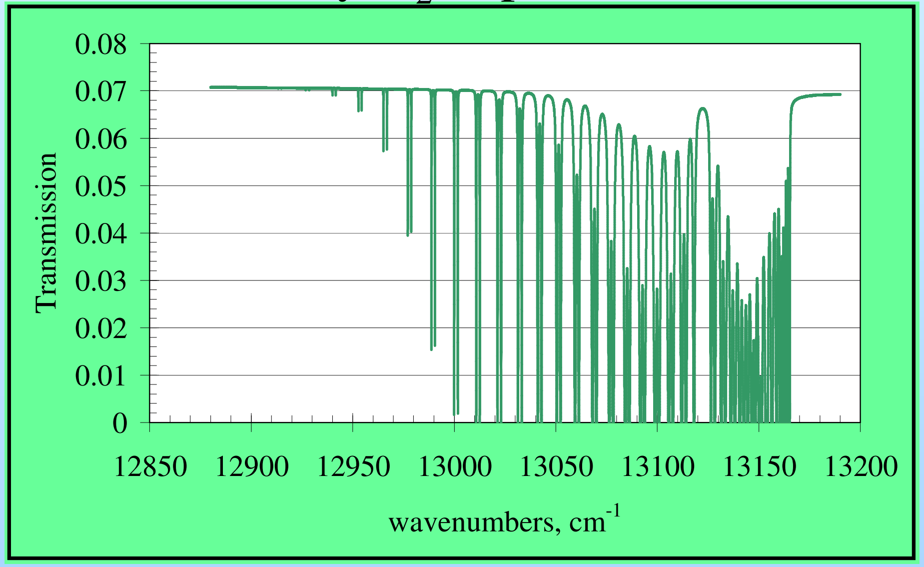
Computations

Computed O_2 (0,0) extinction spectra at ZA=30° and observation angle=50°

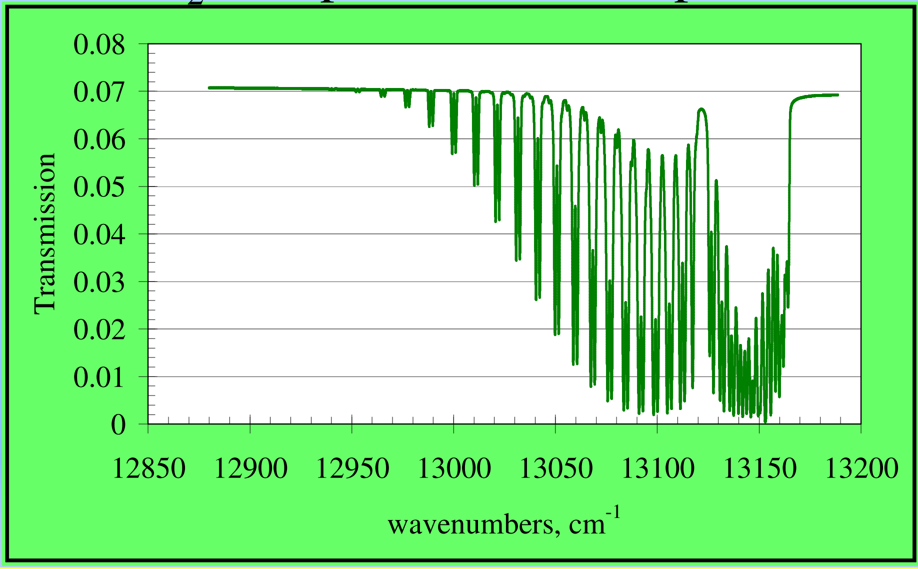
All O_2 isotopes



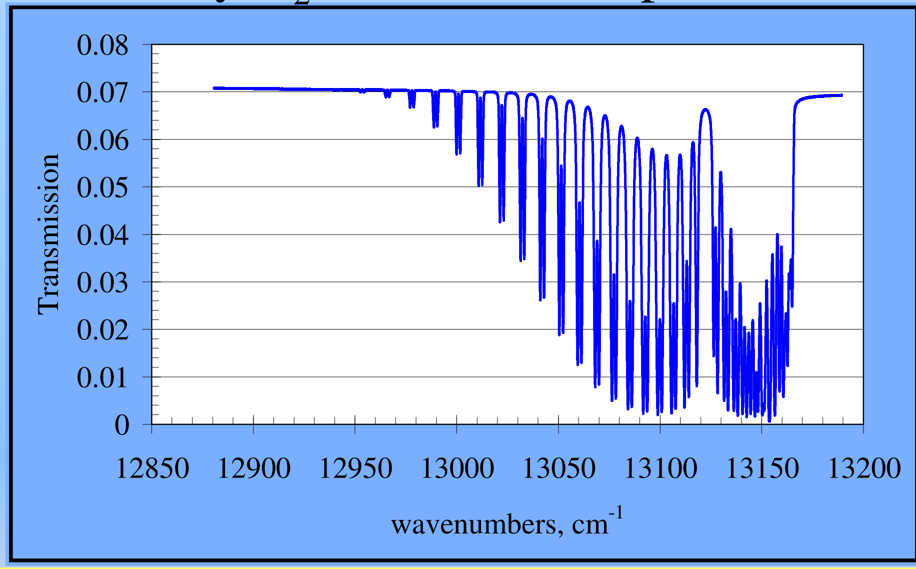
Only O_2^{16} spectrum



All O_2 isotopes, convolved spectrum



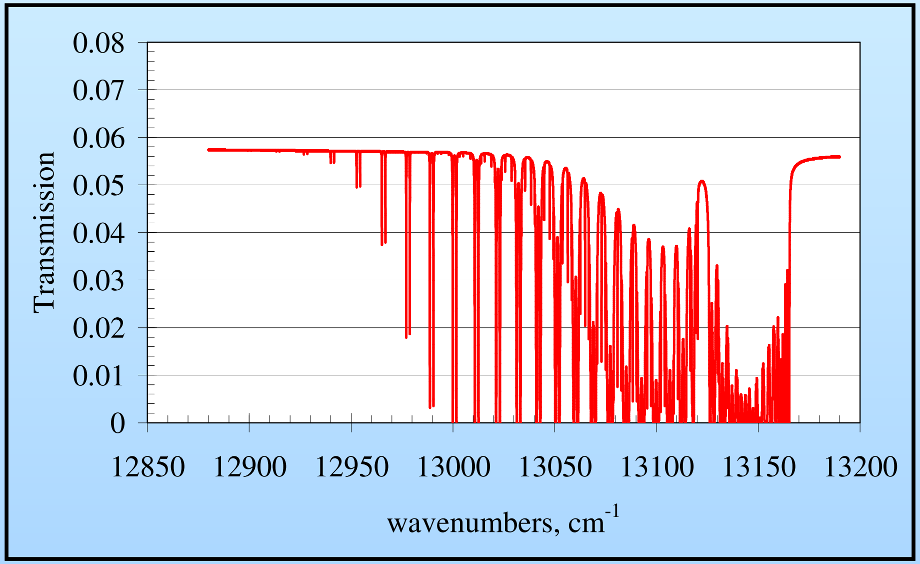
Only O_2^{16} , convolved spectrum



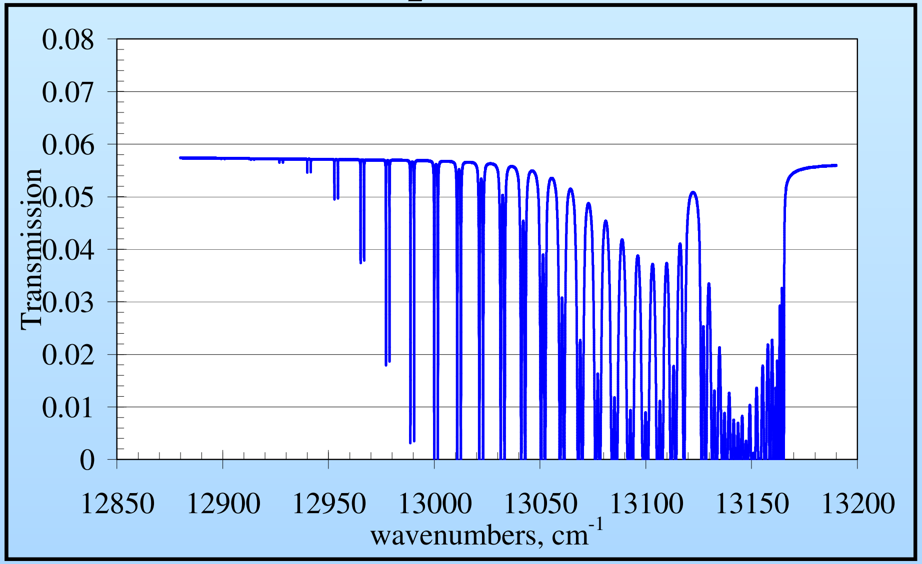
Computations

Computed O_2 (0,0) extinction spectra at ZA=30° and observation angle=20°

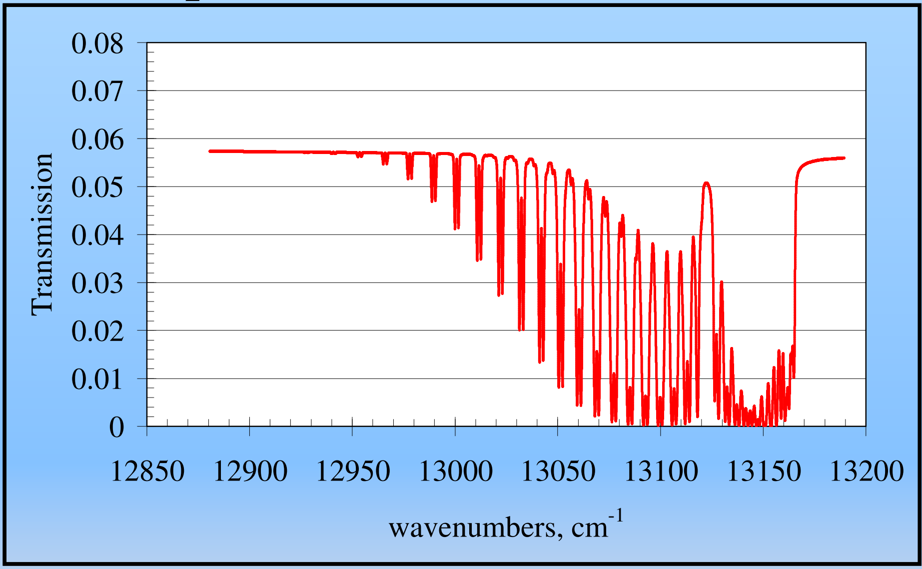
All O_2 isotopes



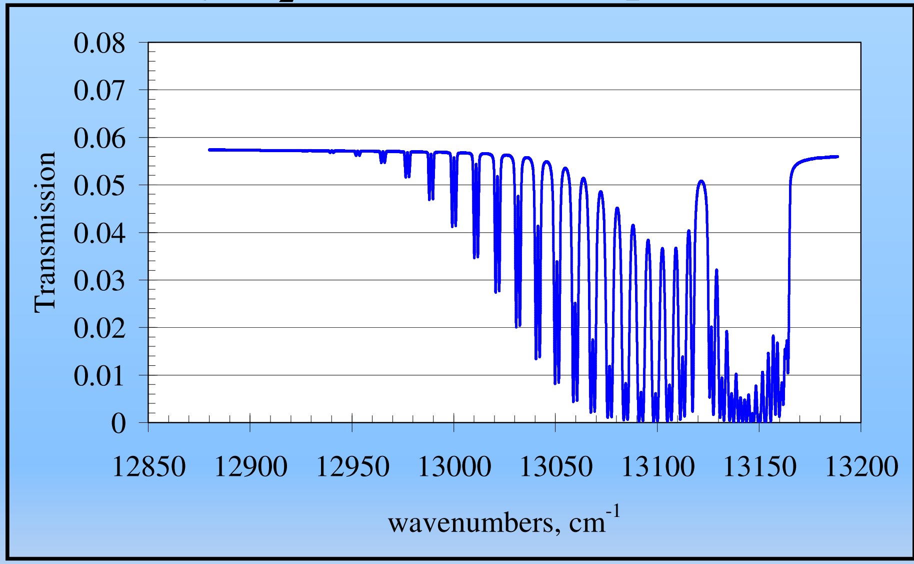
Only O_2^{16} spectrum



All O_2 isotopes, convolved spectrum

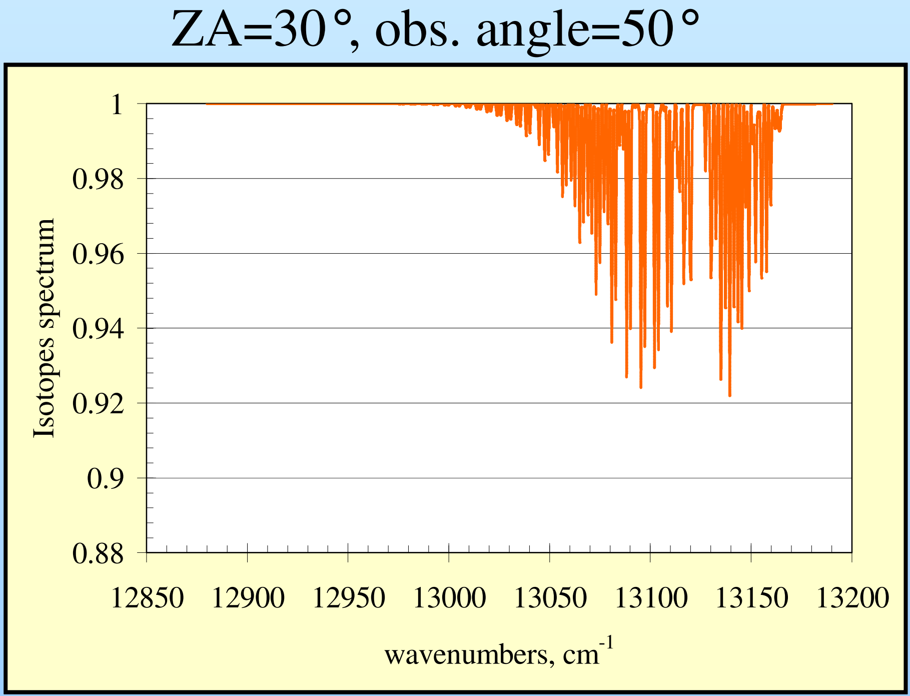


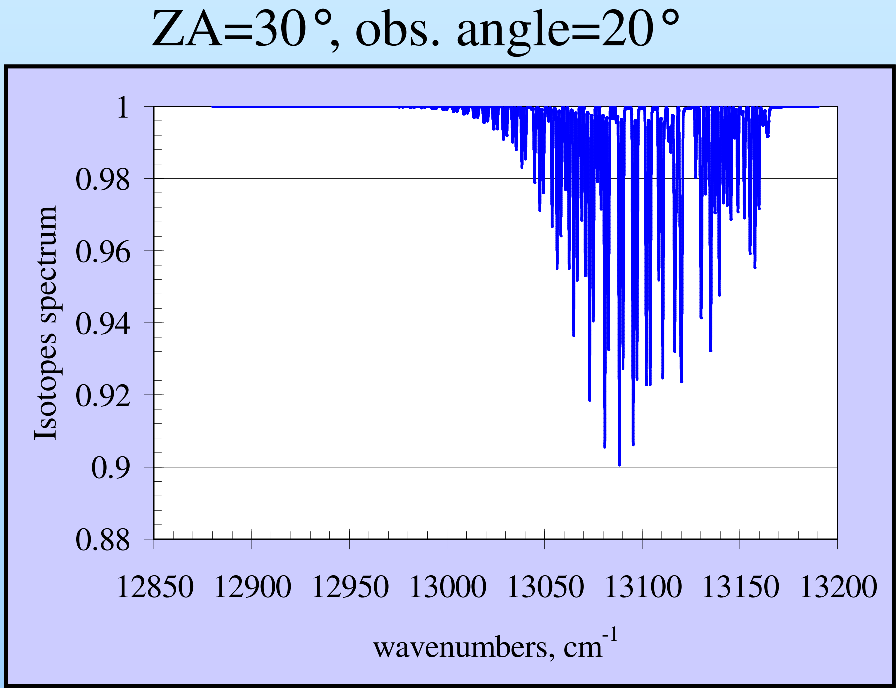
Only O_2^{16} , convolved spectrum



Computations

Isotopes spectra, obtained from the normed convolved spectra



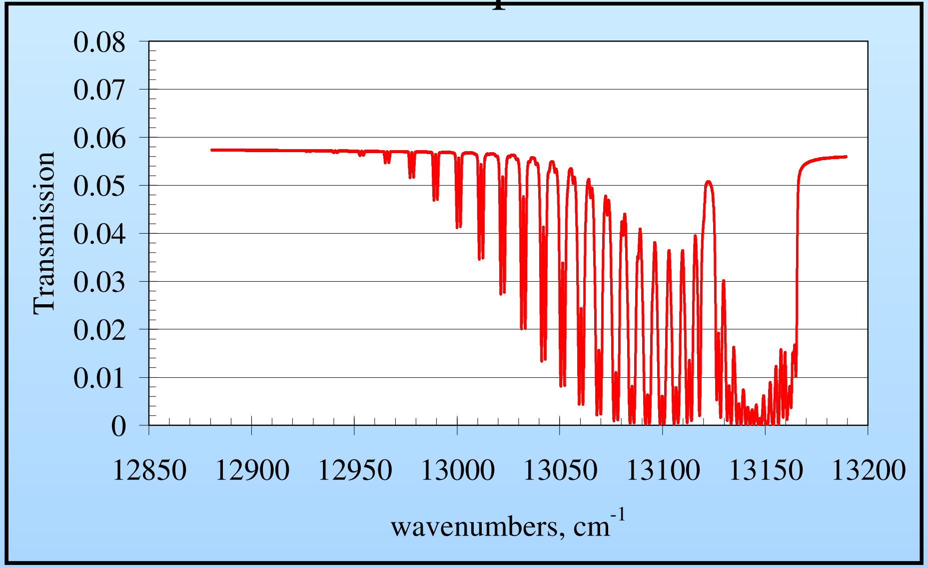


Isotopes lead to different contributions depending on the observation scheme, so they are to be included in the computations.

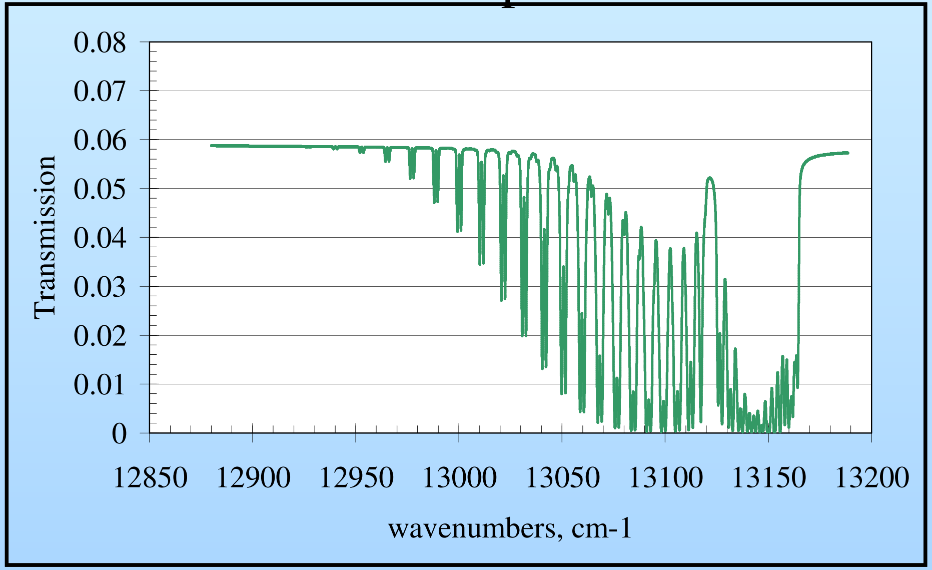
Computations

Convolved spectra, ZA=30°, obs. angle = 20°

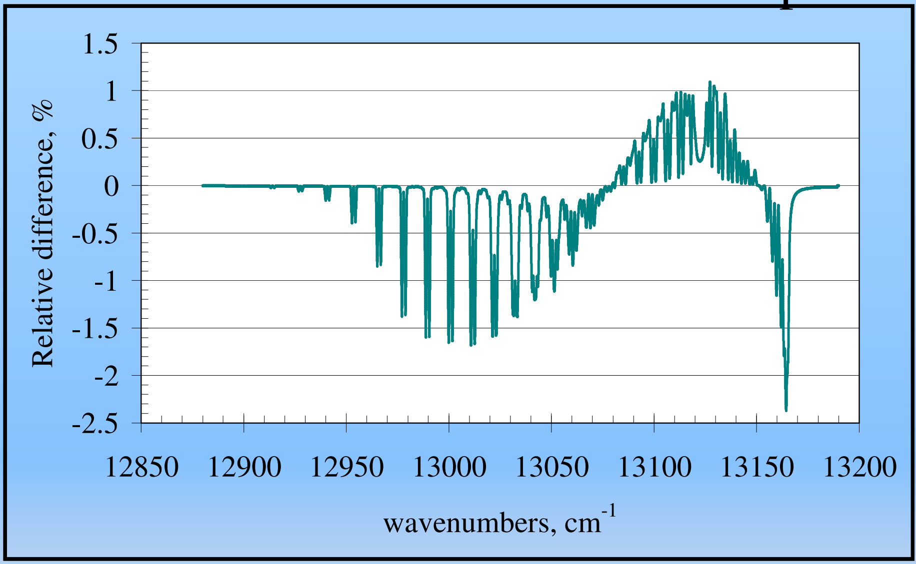
Mean temperatures



Summer temperatures

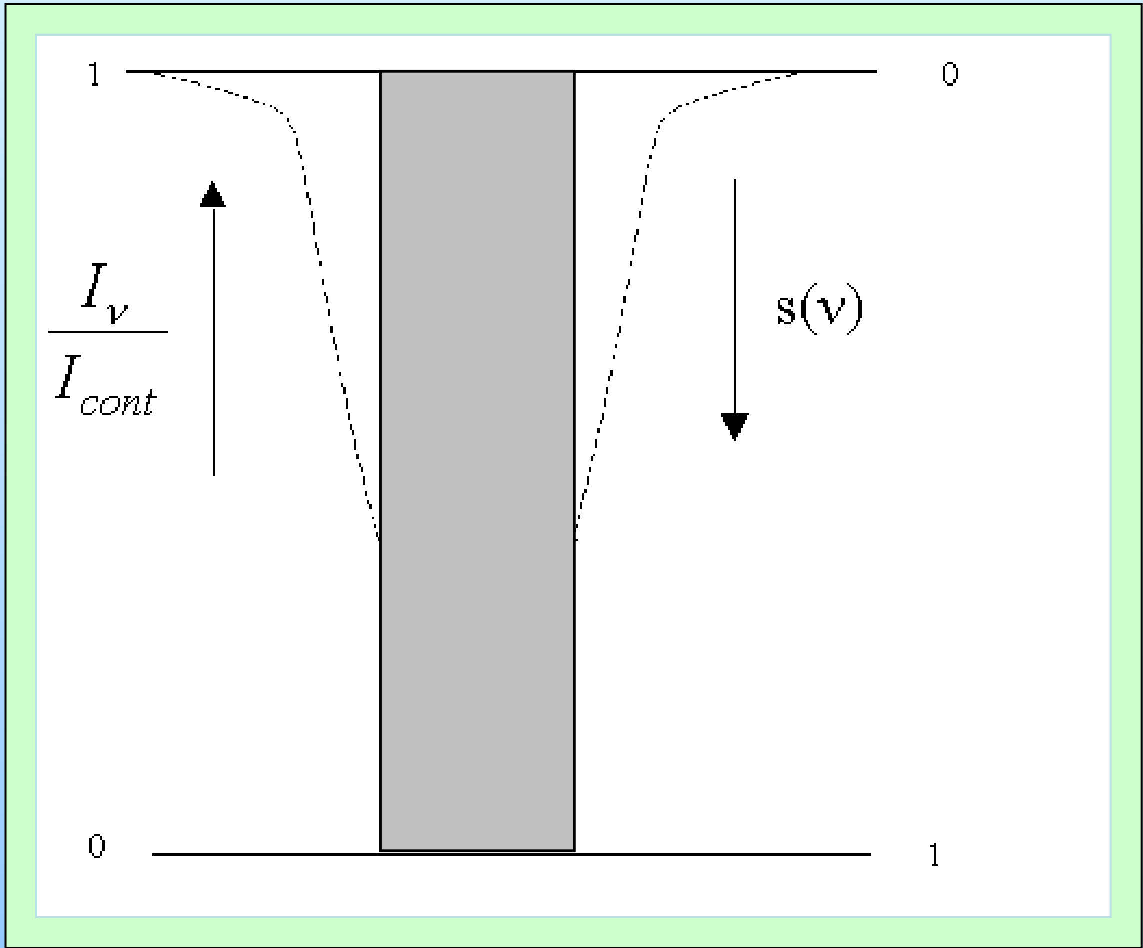


Relative differences between both spectra



- The convolution reduces the differences.
- The greatest differences are obtained between the medium lines, at the middle of the P-branch slope.
- The differences depend only slightly on the observation angle (x0.1%). They are greater at smaller obs. angles.

Equivalent width of the rotational lines.



$$W = \int_{line} s(\nu)\, d\nu = \int_{line} \frac{I_{cont} - I_\nu}{I_{cont}}\, d\nu$$

Equivalent widths and effective temperature

The equivalent width W_e of a rotational absorption line is a measure of the area of the line. It is connected to the absorption energy. In the case of strong absorption, the following dependence is obtained:

$$\ln\left(\frac{W_e}{S_{JJ}^{1/2}}\right) = const - \frac{B_0 hc}{kT_{eff}} \frac{J(J+1)}{2}$$

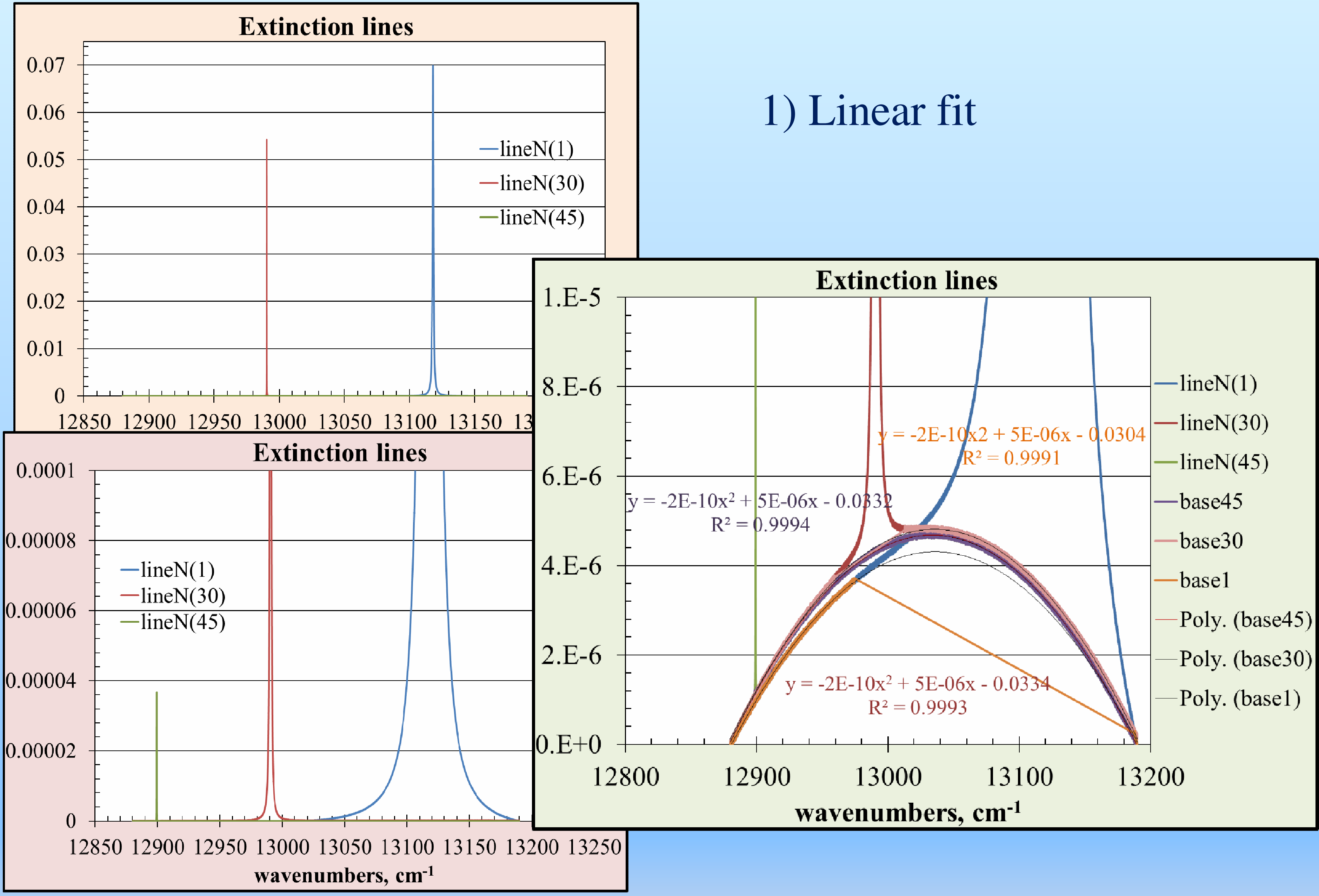
where S_{jj} is the line strength, J is the rotational quantum number of the lower level and T_{eff} is the effective temperature. T_{eff} is defined as:

$$T_{eff} = \frac{\int_0^\infty n(z)T(z)dz}{\int_0^\infty n(z)dz} = \frac{\int_0^\infty n(z)T(z)dz}{N}$$

The effective temperature represents the temperature which the gas would take, if the temperature was uniform along the whole length of the atmospheric column, saving the internal gas energy. It was obtained that T_{eff} corresponds to the temperature at 7 km of altitude of the standard atmosphere.

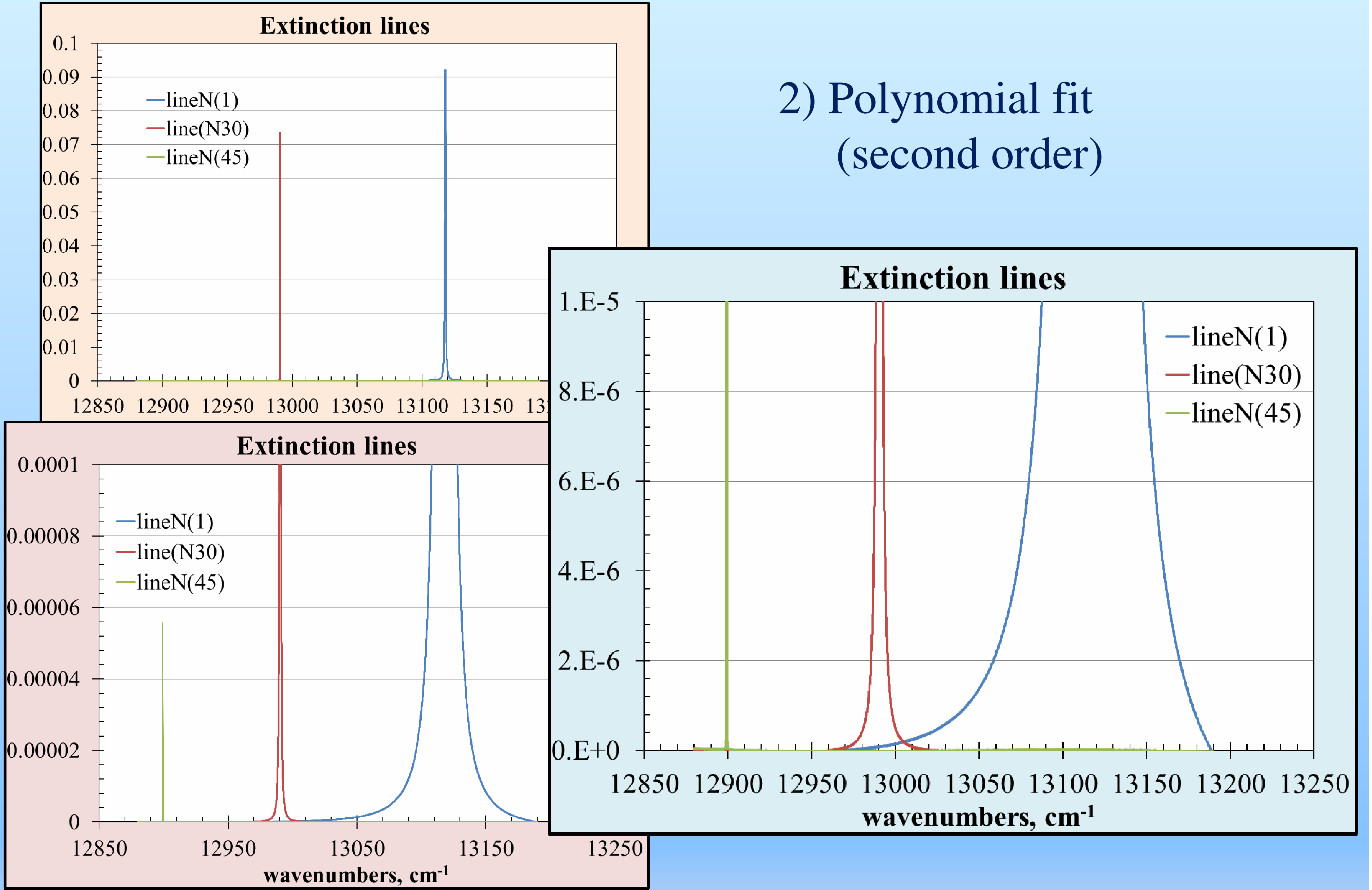
Baseline extraction

1) Linear fit



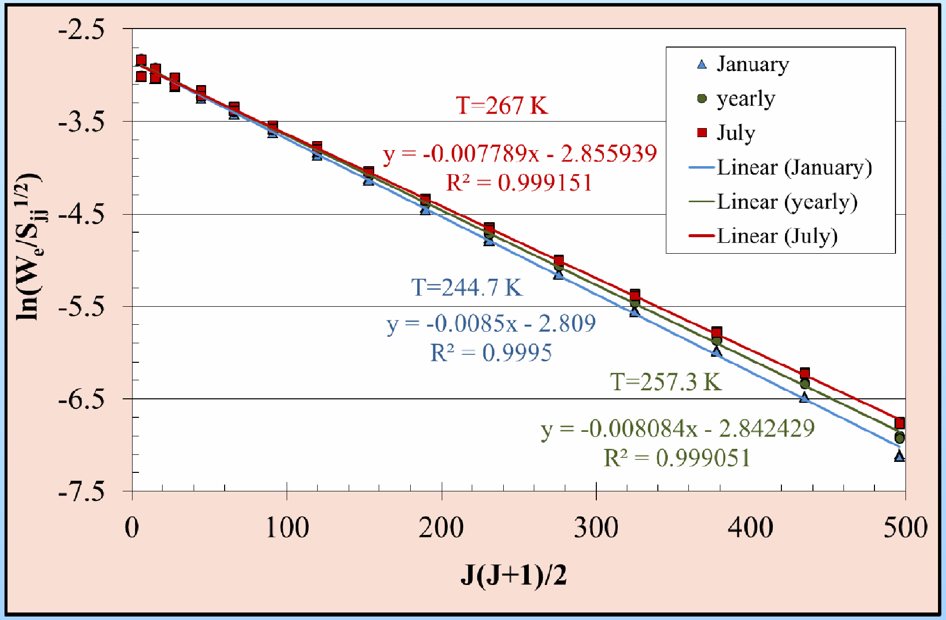
Baseline extraction

2) Polynomial fit
(second order)

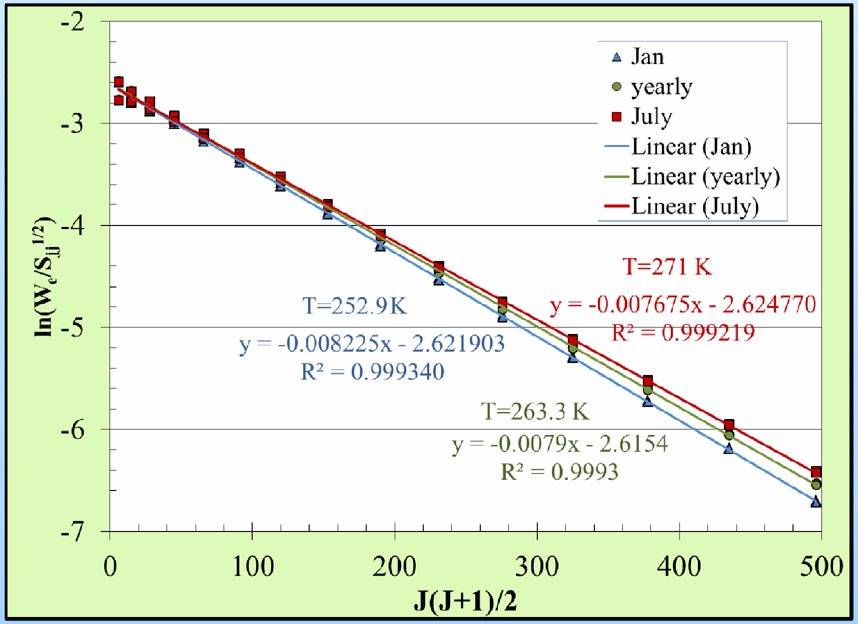


Equivalent widths and corresponding temperatures

ZA=30°, obs. angle=50°

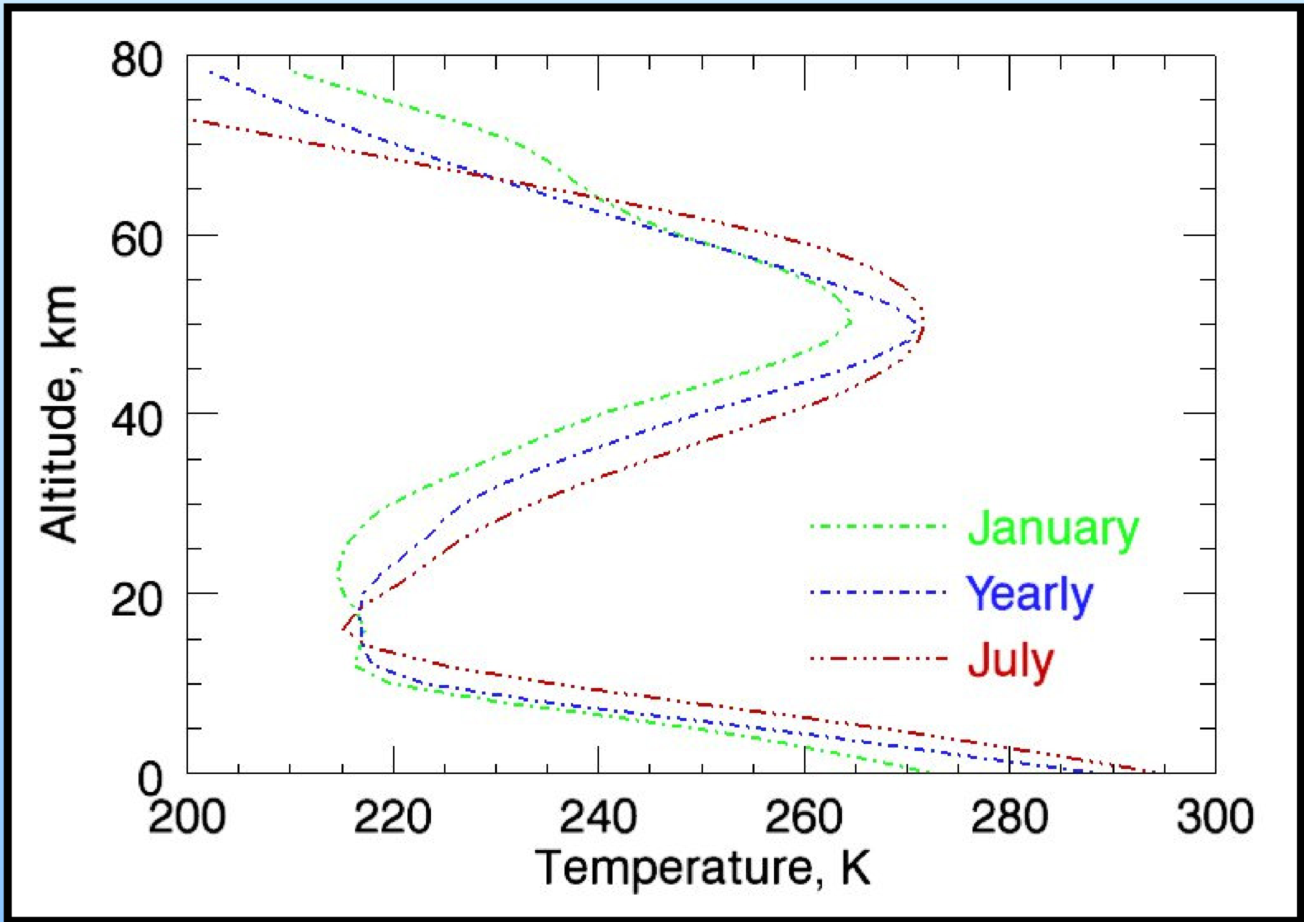


ZA=30°, obs. angle=15°



Computed dependencies of $\boldsymbol{ln(W_e/S_{jj}^{1/2})}$ on $\boldsymbol{J(J+1)/2}$ at different observation angles for 3 cases: yearly mean, January and July data from U.S. Standard atmosphere 1976. The corresponding temperatures are calculated. At smaller observation angles (towards horizon) higher corresponding temperatures are obtained.

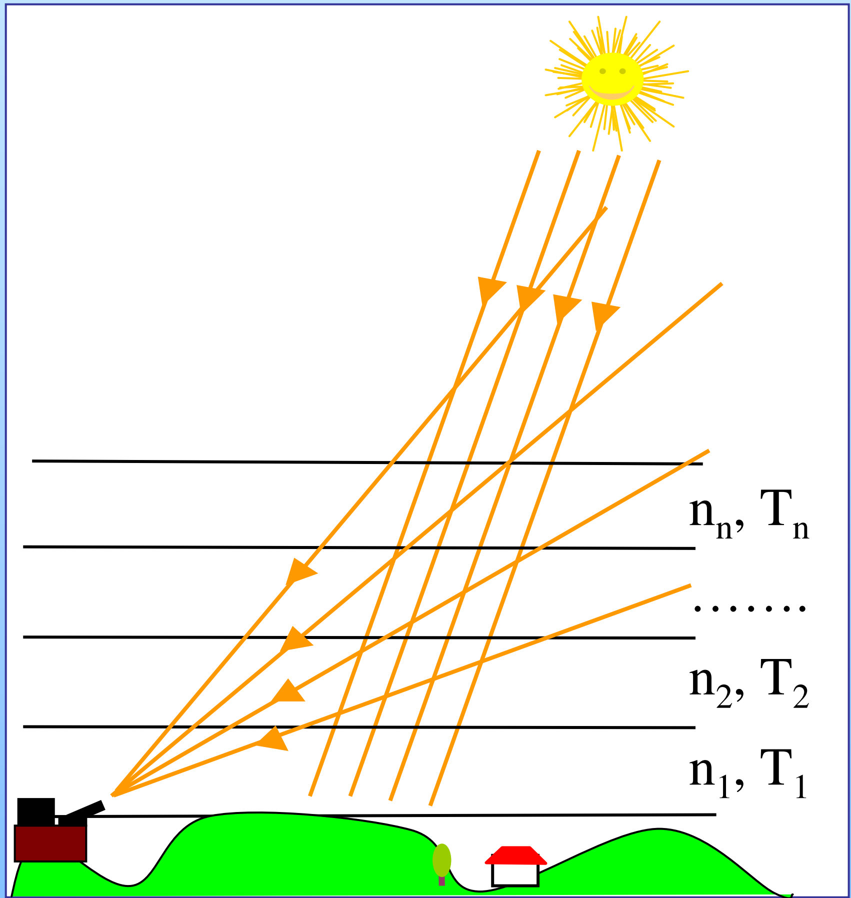
Model temperature profiles



Temperatures and corresponding standard atmosphere altitudes, obtained by the We dependencies

	Absorption, ZA=0°	Extinction, ZA=30°, OA=50°	Extinction, ZA=30°, OA=15°	
US Standard 1976	T H	T H	T H	T_{eff} H
January		244.7 K 6 km	252.9 K 4 km	243.93 K 6 km
Yearly mean	263.22 K 4 km	257.3 K 5 km	263.3 K 4 km	250.27 K 6 km
July		267.0 K 5 km	271.0 K 4.5 km	258.33 K 6 km

Geometry of the indirect observations



Measurement geometry (single scattering assumed) along different directions below the Sun current position. Thus the scattered light absorption under different angles towards horizon can be registered.

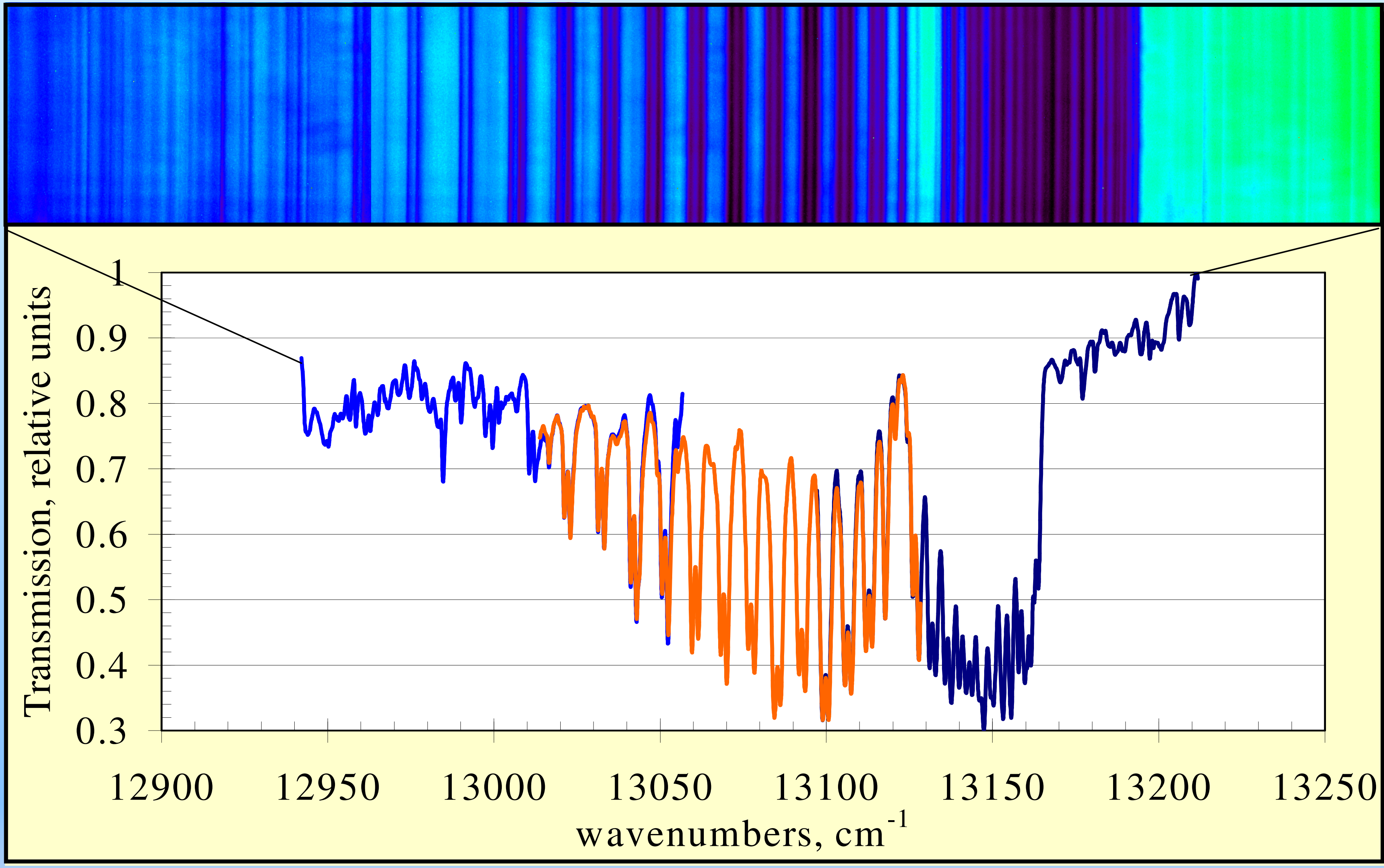
Measurements

Stara Zagora spectrometric system

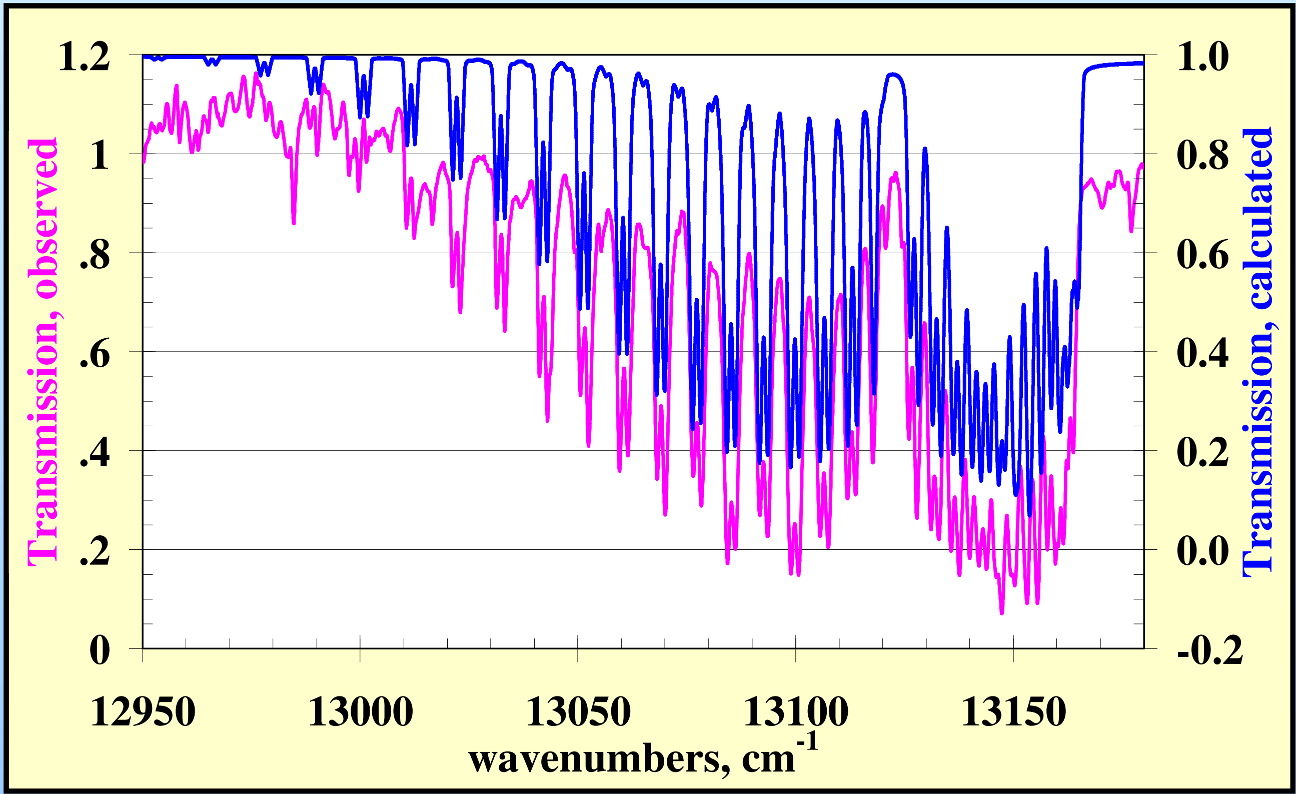
- 8" Mead LX90 telescope;
- Jobin-Yvon monochromator, HR640 type;
- CCD camera SXV-M7 of Starlight Xpress;
- PC.

Measurements

Registered images and the derived spectra on 24.06.2011 at observation angle 50°



Comparison between the computed and the observed spectra on 24.06.2011



Computations:

ZA=19.1°

obs. angle=50°

H_{atm}=60 km

dz=1km

June temperatures

normed to unity

Measurements:

- The influence of the CCD sensitivity is removed;
- The background is extracted;
- The spectrum is normed to unity.

Results

- A method to compute the extinction of the solar radiation from the bands of the atmospheric system of the molecular oxygen in the Earth atmosphere was developed;
- Absorption and single scattering are included in the computations;
- The optimal number of included transitions and the optimal values of the atmospheric layers thickness and of the atmospheric height were estimated.
- the radiation extinction at different angles of observation and using different atmosphere model parameters was computed. The obtained differences were examined.
- The profiles of the separate rotational lines were obtained and a way to calculate correctly the equivalent widths was found out.
- The dependences assuming strong absorption were built for different models and different observation angles. The corresponding temperatures and atmospheric heights were obtained.
- Based on the obtained results it can be concluded that using spectroscopic measurements the corresponding atmospheric temperature could be evaluated.

- Ground based measurements of O_2 extinction were processed by the use of theoretical spectra computed for the same conditions. The obtained measured and calculated spectra coincide very well.

Conclusions

Based on the obtained results it can be concluded that the computation of the extinction spectra and the equivalent widths is accurate.

The computed theoretical spectra can be used to model real measurement conditions.

Theoretical spectra are needed to process correctly the measurements.

By the use of theoretical estimates and spectroscopic measurements the corresponding atmospheric temperature could be evaluated.

Thanks for the attention