united nations educational, scientific and cultural organization

international atomic energy agency

the
abdus salam
international centre for theoretical physics

School on "Exploring the Atmosphere by Remote Sensing Techniques"
18 October - 5 November 1999

1151-23

"Infrared Methods & Techniques for Atmospheric Science"

Lecture 2: Radiative Transfer, Molecular Spectra,
Tropospheric Sounding

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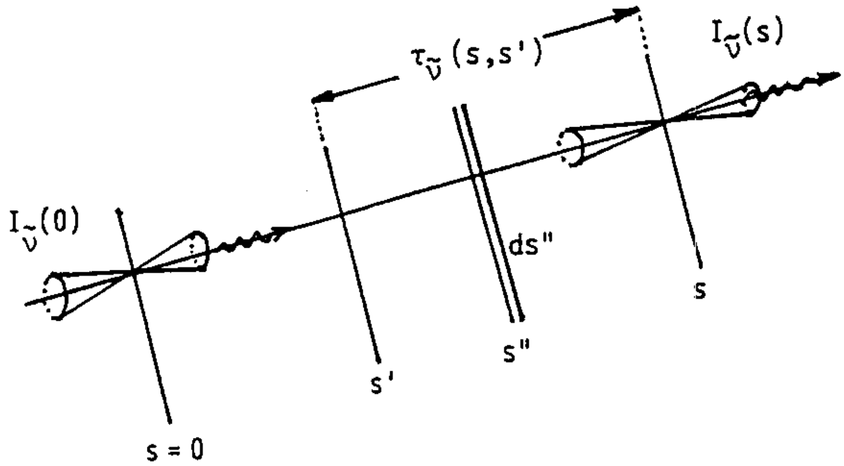
Infrared methods and techniques for atmospheric science



Géométrie pour l'équation du transfert radiatif

$I_{\tilde{\nu}}(s)$ = radiance $\quad W\,cm^{-2}\,sr^{-1}\,/\,cm^{-1}$

s = coordinate along the ray (or path)

Radiative transfer equation in the infrared

Integral form along a given ray:

$$I_{\tilde{\nu}}(s) = I_{\tilde{\nu}}(0)\exp\left[-\tau_{\tilde{\nu}}(s,0)\right] + \int_0^s J_{\tilde{\nu}}(s')\exp\left[-\tau_{\tilde{\nu}}(s,s')\right]\alpha_{\tilde{\nu}}(s')\,ds'$$

$I_{\tilde{\nu}}$ = spectral $\left\{ \begin{array}{l} \text{intensity} \\ \text{radiance} \end{array} \right.$ $\quad W\,cm^{-2}\,sr^{-1}/cm^{-1}$

Optical depth between s and s' along a ray

$$\tau_{\tilde{\nu}}(s,s') = \int_{s'}^{s} \alpha_{\tilde{\nu}}(s'')\,ds''$$

Transmission

$$T_{\tilde{\nu}}(s,s') = \exp\left[-\tau_{\tilde{\nu}}(s,s')\right]$$

Absorption coefficient

$\alpha_{\tilde{\nu}}(s'') \qquad \dfrac{1}{cm}$

Radiative transfer equation (MW and IR)

radiance $I_{\tilde{\nu}}$ $W\ cm^{-2}\ sr^{-1} / cm^{-1}$

wavenumber $\tilde{\nu}$ cm^{-1}

Local form:

$$\boxed{\frac{dI_{\tilde{\nu}}}{ds} = -\alpha_{\tilde{\nu}} \left(I_{\tilde{\nu}} - J_{\tilde{\nu}} \right)}$$

$J_{\tilde{\nu}}$ source function

$\alpha_{\tilde{\nu}}$ absorption coefficient $1/cm$

s coordinate along the ray (or path)

Exercise:

Check that the integral form:

$$I_{\tilde{\nu}}(s) = I_{\tilde{\nu}}(0) \exp\left[-\tau_{\tilde{\nu}}(s,0)\right] + \int_0^s J_{\tilde{\nu}}(s') \exp\left[-\tau_{\tilde{\nu}}(s,s')\right] \alpha_{\tilde{\nu}}(s') d$$

is a formal solution of the local equation with the definitions given before or below.

Radiative transfer equation
(useful relations with derivatives)

From:

$$T_{\tilde{\nu}}(s,s') = \exp\left[-\int_{s'}^{s} \alpha_{\tilde{\nu}}(s'')\,ds''\right]$$

one gets:

$$\frac{\partial T_{\tilde{\nu}}(s,s')}{\partial s} = -\,\alpha_{\tilde{\nu}}(s)\,T_{\tilde{\nu}}(s,s')$$

$$\frac{\partial T_{\tilde{\nu}}(s,s')}{\partial s'} = \alpha_{\tilde{\nu}}(s')\,T_{\tilde{\nu}}(s,s')$$

This helps to write:

New form of the radiative transfer equation

$$I_{\tilde{\nu}}(s) = I_{\tilde{\nu}}(0)\,T_{\tilde{\nu}}(s,0) + \int_{0}^{s} J_{\tilde{\nu}}(s')\,\frac{\partial T_{\tilde{\nu}}(s,s')}{\partial s'}\,ds'$$

$$K_{\tilde{\nu}}(s,s') = \frac{\partial T_{\tilde{\nu}}(s,s')}{\partial s'}$$

Weighting function in geometrical coordinate

$$K_{\tilde{\nu}}(p,p') = \frac{\partial T_{\tilde{\nu}}(p,p')}{\partial \ln p'}$$

weighting function in pressure coordinate (for vertical nadir retrieval)

black body

- The material medium is absorbing all the frequencies (wavelengths, wavenumbers) that it can emit
- The radiation field is isotropic
- The radiation field is homogeneous
- The spectral distribution depends only on the temperature of the medium

$I_{\tilde{\nu}}(s)$ is independent of s

limiting case $\alpha_{\tilde{\nu}} \to \infty$

In the local form of the radiative transfer equation:

$$\underbrace{\frac{dI_{\tilde{\nu}}}{ds}}_{=0} = - \underbrace{\alpha_{\tilde{\nu}}}_{\to\infty} \underbrace{\left(I_{\tilde{\nu}} - J_{\tilde{\nu}} \right)}_{\equiv 0}$$

$$\boxed{I_{\tilde{\nu}} = J_{\tilde{\nu}} \equiv B_{\tilde{\nu}}(T)}$$

The source function is equal to the Planck function

Emission only

At local thermodynamic equilibrium (LTE)

$$J_{\tilde{\nu}}(s') \equiv B_{\tilde{\nu}}(s') \qquad \text{Planck Function}$$

$$I_{\tilde{\nu}}(s) = \int_0^s B(\tilde{\nu}, T(s')) \frac{\partial T_{\tilde{\nu}}(s,s')}{\partial s'} ds'$$

For a homogeneous medium at uniform temperature

$$I_{\tilde{\nu}}(s) = B(\tilde{\nu}, T) \left[1 - T_{\tilde{\nu}}(s,0) \right]$$

$$T_{\tilde{\nu}}(s,0) = \exp\left[- \tau_{\tilde{\nu}}(s,0) \right]$$

$$\tau_{\tilde{\nu}}(s,0) = \int_0^s \alpha_{\tilde{\nu}}(s')ds' = \alpha_{\tilde{\nu}} L$$

$\tau_{\tilde{\nu}}(s,0) \ll 1$ optically thin $I_{\tilde{\nu}} = B(\tilde{\nu},T)\, \tau_{\tilde{\nu}}$

$\tau_{\tilde{\nu}}(s,0) \gg 1$ optically thick $I_{\tilde{\nu}} = B(\tilde{\nu},T)$

The material medium behaves like a black body

Line spectrum

$$\tau_{\tilde{\nu}}(s,0) = \sum_i \sum_j \int_0^s k_{\tilde{\nu}_j}^{N_i}(T(s))\, \phi(\tilde{\nu}-\tilde{\nu}_j, P(s), T(s))\, N_i(s)\, ds$$

N_i local concentration of species i molecule cm^{-3}

$k_{\tilde{\nu}_j}^{N_i}$ line intensity for line centred at wavenumber $\tilde{\nu}_j$ for species i

cm^{-1}/(molecule cm^{-2})

$\phi(\Delta\tilde{\nu}, P, T)$ spectral profile for the line (1/cm^{-1})
accounting for collisions, ...

$$\int_{-\infty}^{+\infty} \phi(\Delta\tilde{\nu}, P, T)\, d(\Delta\tilde{\nu}) = 1$$

normalised line profile

1/cm^{-1} cm^{-1}

Temperature dependence of the line intensity

$$k_{\tilde{\nu}}^{N}(T) = k_{\tilde{\nu}}^{N}(T_{ref}) \frac{Z(T_{ref})}{Z(T)} \exp\left[-\frac{hcE''}{kT}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right] \frac{1-\exp\left(-\frac{hc\tilde{\nu}}{kT}\right)}{1-\exp\left(-\frac{hc\tilde{\nu}}{kT_{ref}}\right)}$$

$Z(T)$ = total partition function at temperature T

T_{ref} = 296 K

$k_{\tilde{\nu}}^{N}(T_{ref})$ in cm^{-1}/(molecule cm^{-2}) and $\tilde{\nu}$, E'', ...
given in the spectroscopic databases for atmospheric molecule

HITRAN, GEISA, ATMOS, JPL, SAO, ...

Continuous spectra

$$\tau_{\tilde{\nu}}(s,0) = \sum_i \int_0^s \sigma_i(\tilde{\nu}, P(s), T(s))\, N_i(s)\, ds$$

N_i local concentration of species i molecule cm^{-3}

σ_i cross section for species i cm^2/molecule

For O_3 * in the UV $\sigma_i(\tilde{\nu}, T)$

* in the visible $\sigma_i(T)$

Hence if σ_i is depending on $\tilde{\nu}$ only

$$\tau_{\tilde{\nu}}(s,0) = \sum_i \sigma_i(\tilde{\nu})\, Q_i$$

$$Q_i = \int_0^s N_i(s)\, ds \qquad \text{molecule } cm^{-2}$$

column amount

For "heavy" molecules (N_2O_5, $ClONO_2$ ..) or CFCs the cross sections are tabulated as a function of:

- wavenumber
- temperature
- (in some cases) total pressure

See special directory in HITRAN or GEISA

TOVS = TIROS Operational Vertical Sounder

on NOAA - XX satellites X = 14, 15 ...

Caractéristiques du sondeur TOVS

(suite)

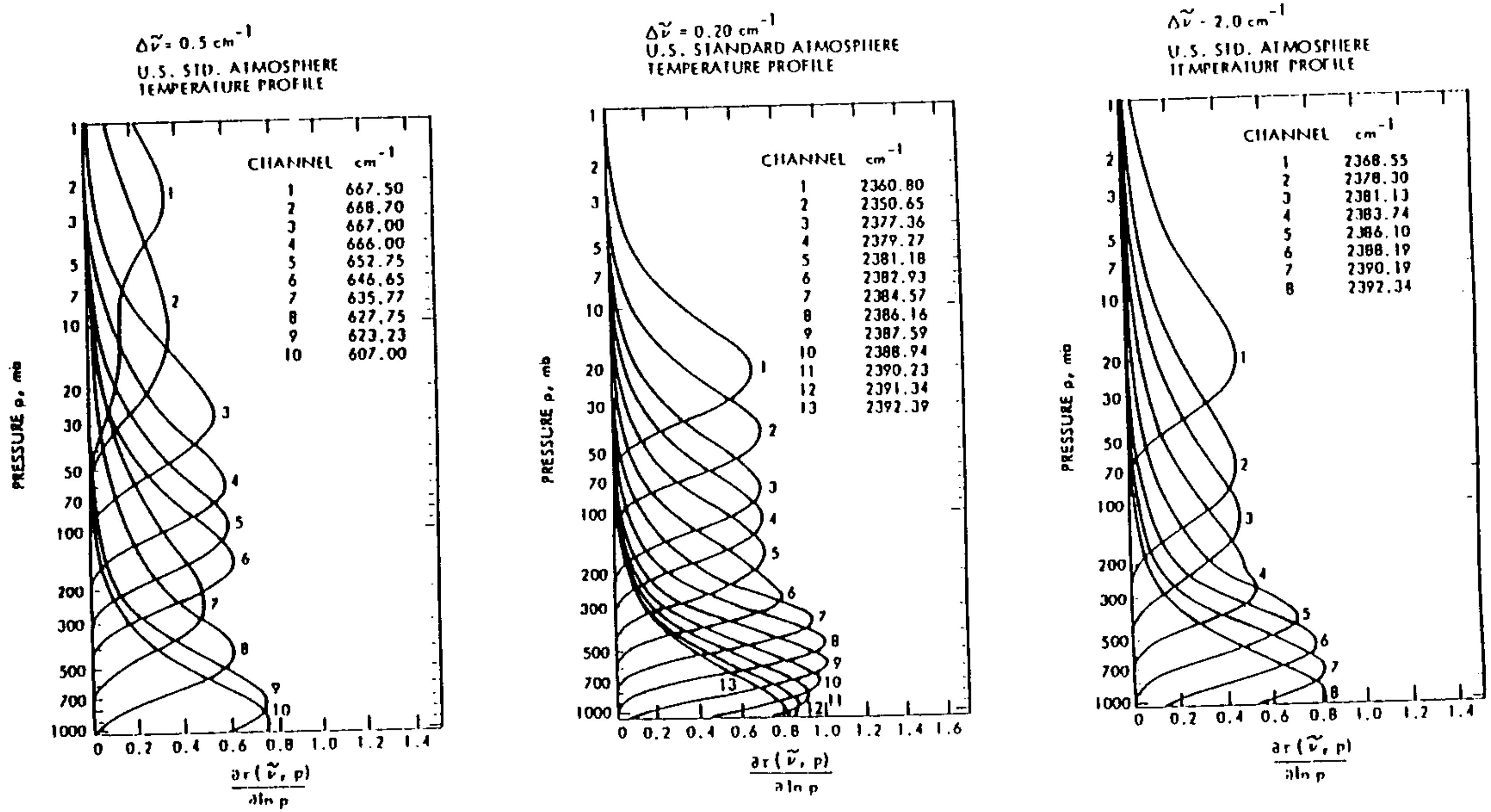
Sondeur HIRS

(High resolution Infrared Radiation Sounder)

k	$\tilde{\nu}_k$ (cm^{-1})	$\Delta\tilde{\nu}_k$ (cm^{-1})	P_k	Quantité mesurée
1	668	3	30 mb	Profil vertical de température
2	679	10	60 mb	
3	691	12	100 mb	
4	704	16	400 mb	
5	716	16	600 mb	
6	732	16	800 mb	
7	748	16	900 mb	
8	898	35	Surface	
9	1028	25	25 mb	colonne d'ozone
10	1217	60	900 mb	Profil vertical de vapeur d'eau
11	1364	40	700 mb	
12	1484	80	500 mb	
13	2190	23	1000 mb	Profil vertical de température
14	2213	23	950 mb	
15	2240	23	700 mb	
16	2276	23	400 mb	
17	2361	23	5 mb	
18	2513	35	Surface	
19	2671	100	Surface	
20	14367	900	Nuages/Surface	Albédo

Radiomètre infrarouge multicanal non - cryogénique

1 scène HIRS = 56 x 40 visées



WEIGHTING FUNCTIONS FOR NADIR VIEWING

(Kaplan et al. Appl. Opt. 16, 322-325, 1977)

OZONE COLUMN FROM TOVS (zeroth order)

$I_{\tilde{\nu}}$: measured radiance in the O_3 channel centered at $\tilde{\nu} = 1028\ cm^{-1}$ ($\lambda = 9.7\,\mu m$) with $\Delta\tilde{\nu} = 25\ cm^{-1}$

$$I_{\tilde{\nu}} = \varepsilon_e\, B(\tilde{\nu}, T_e)\, \tau_{\tilde{\nu}} + (1 - \tau_{\tilde{\nu}})\, B(\tilde{\nu}, T_{O_3})$$

ε_e = emissivity of the lower boundary (surface or clouds)

T_e = corresponding temperature

T_{O_3} = effective temperature of the emitting ozone layer (slow variation of T in the stratosphere)

$\tau_{\tilde{\nu}}$ = average transmission in the O_3 channel

OZONE COLUMN FROM TOVS (zeroth order) (continued)

One gets the average transmission:

$$\tau_{\tilde{\nu}} = \frac{I_{\tilde{\nu}} - B(\tilde{\nu}, T_{O_3})}{\varepsilon_e B(\tilde{\nu}, T_e) - B(\tilde{\nu}, T_{O_3})}$$

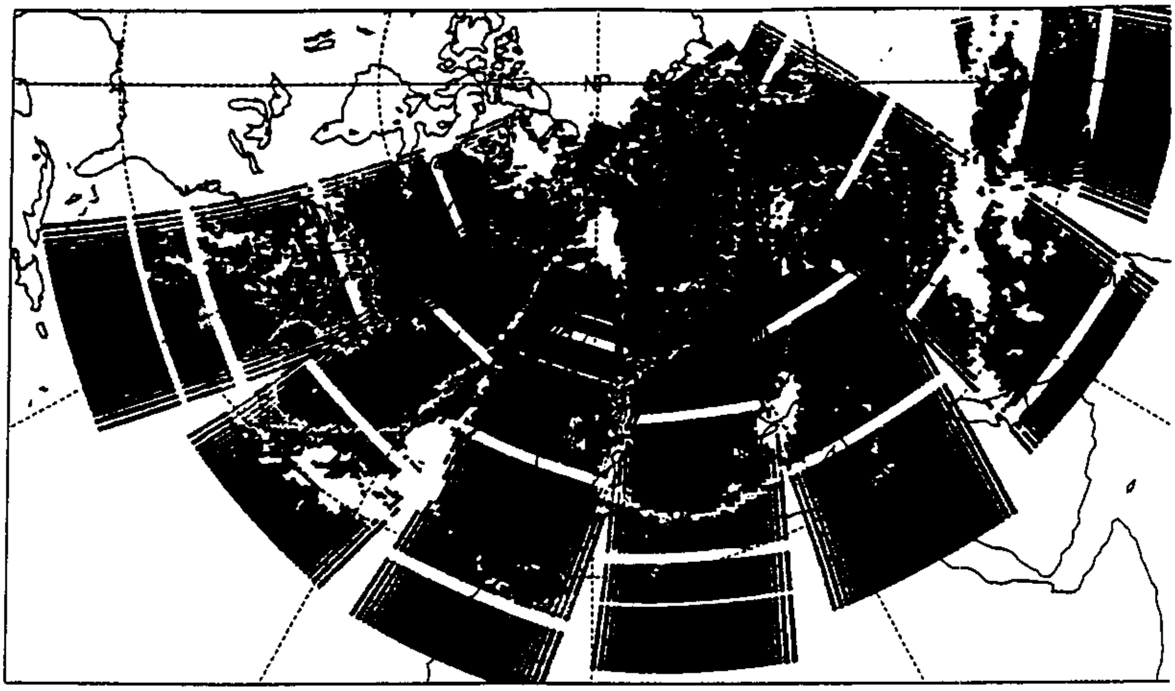
hence $\int_{P_{inf}}^{P_{sup}} N_{O_3} \, dz$ = vertical column between appropriate levels

$P_{eff} \simeq 25\,mb$ maximum of the weighting function

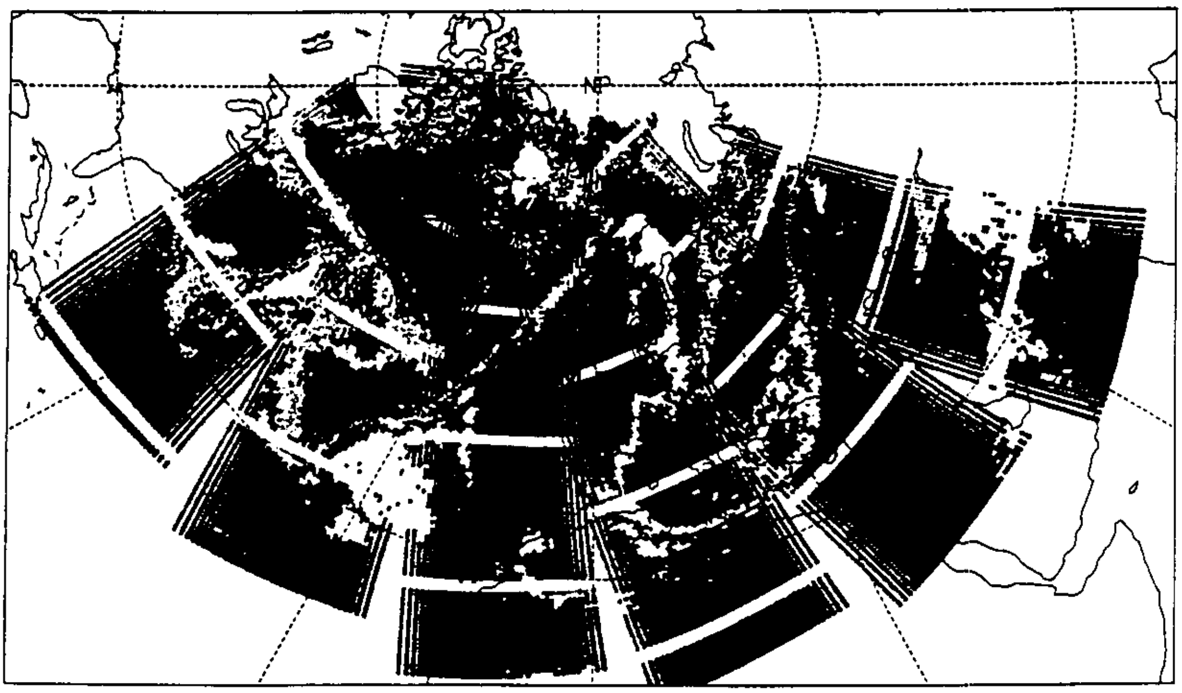
Ancillary parameters needed:

ε_e, T_e, T_{O_3} deduced from other channels or from climatology

TOVS/HIRS2 03 M95081

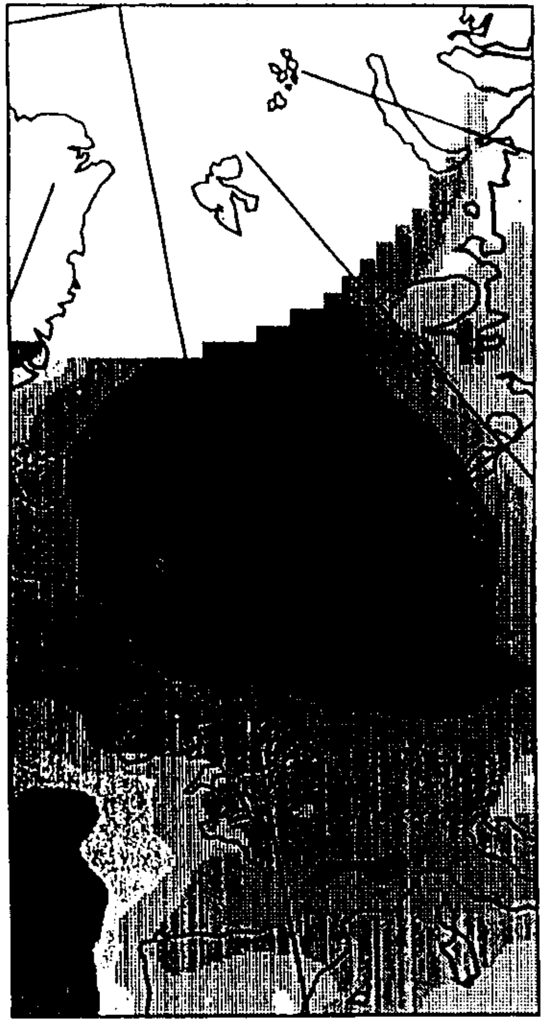


TOVS/HIRS2 03 S95081

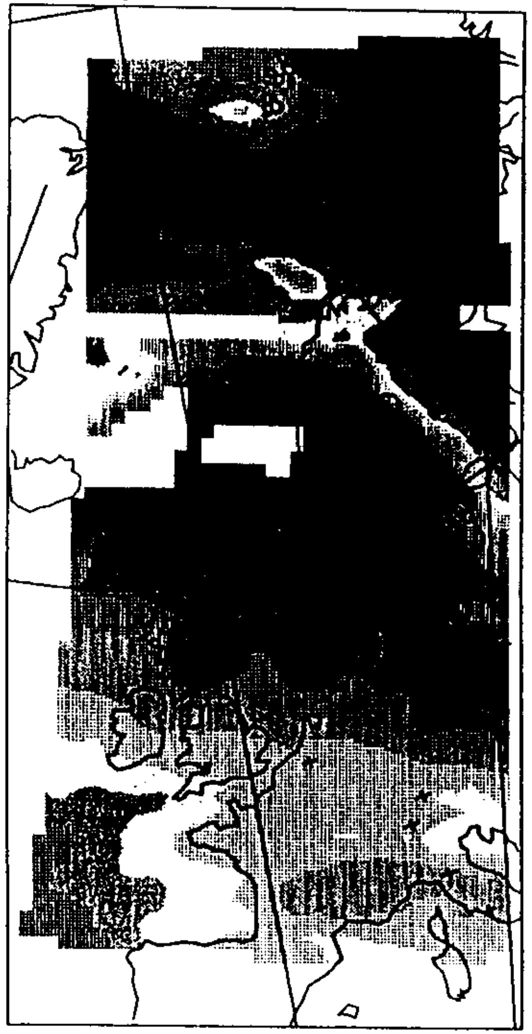


METEO FRANCE CNRM

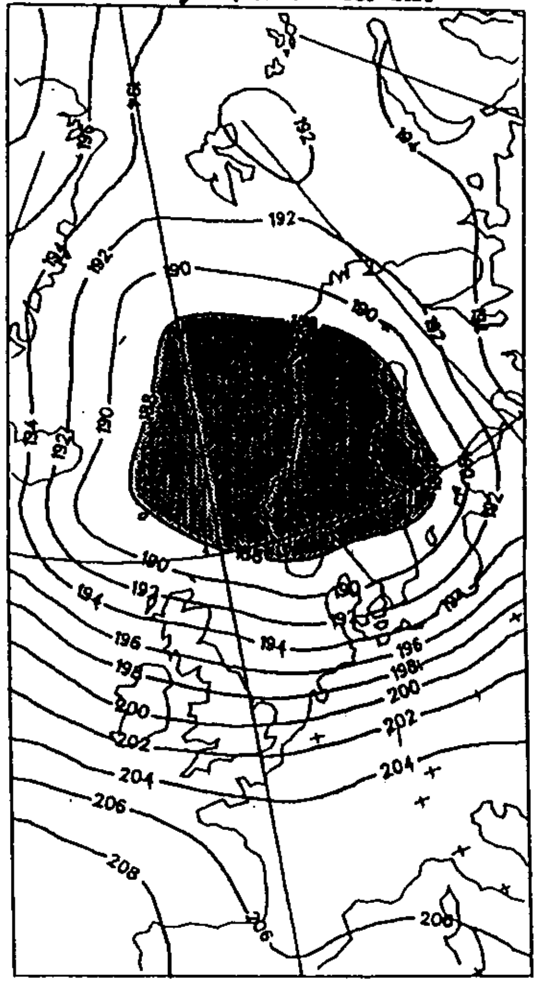
TOTAL OZONE TOMS
January 31, 1989



TOTAL OZONE TOVS/HIRS2
January 31, 1989 8H30 GMT



TEMPERATURE 50hPa
January 31, 1989 6H GMT



Tropospheric trace species and their main signatures in the mid-infrared

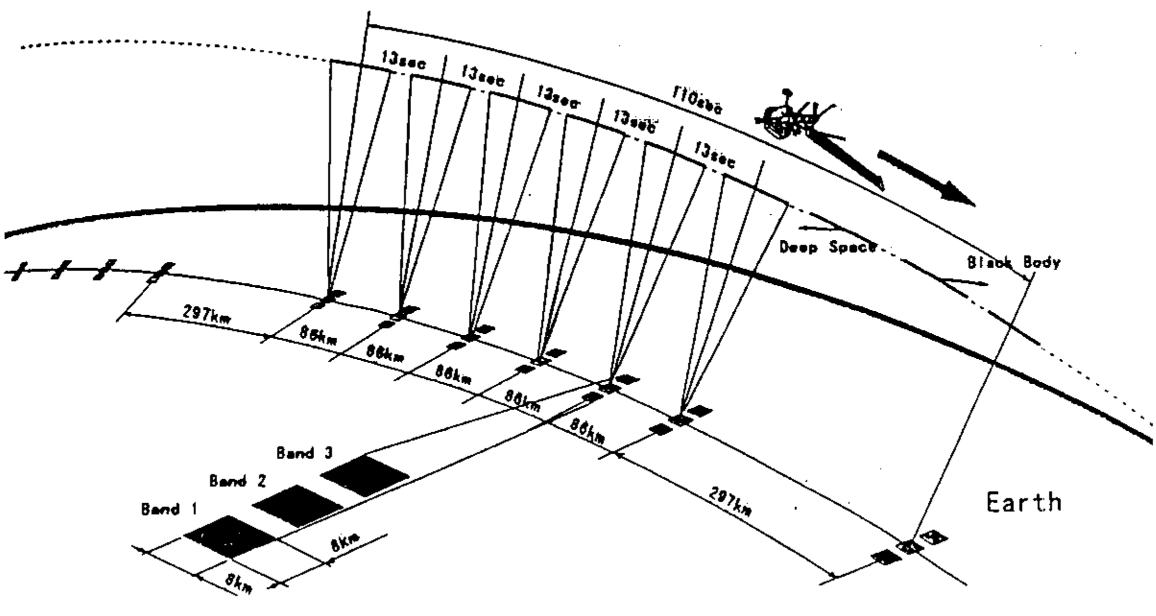
Species	*Spectral range* *(cm^{-1})*	*Transition*	*Mixing ratio*	*Lifetime*
CO_2	590- 750 (667.4) 2230-2400 (2349.1)	ν_2 ν_3	3.6×10^{-4} 360 ppmv	–
H_2O	780-2900 (1594.7)	ν_2	10^{-2}-10^{-4}	–
CO	1910-2290 (2143.3)	1-0	2×10^{-7} 200 ppbv	50 days
CH_4	990-1770 (1310.8) 2810-3210 (3019.5)	ν_4 ν_3	1.7×10^{-6} 1.7 ppmv	10 years
O_3	920-1240 (1042.1) 940-1270 (1103.1) 1910-2320 (2110.8)	ν_3 ν_1 $\nu_1+\nu_3$	2×10^{-8} 20 ppbv	90 days
NO_2	1210-1340 (1284.9) 2120-2270 (2223.8)	ν_1 ν_3	3×10^{-7} 300 ppbv	100 days
SO_2	1310-1400 (1362.1)	ν_3	10^{-9} 1 ppbv	~ 1-2 days
HNO_3	840- 920 (879.1) 850- 920 (896.4)	ν_5 $2\nu_9$	10^{-9} 1 ppbv	~ 15 days
CFC-11 $CFCl_3$	800- 885 (846.5) 1045-1120 (1085.0)		2×10^{-7} 200 pptv	65 days
CFC-12 CF_2Cl_2	850- 950 (922.2) 1070-1190 (1161.0)	ν_8 ν_6	4×10^{-10} 400 pptv	130 years
HCFC-22 CHF_2Cl	820- 840 (829.0)	$2\nu_6$	1.5 150 pptv	15 years

IMG = Interferometric Monitor for Greenhouse gases

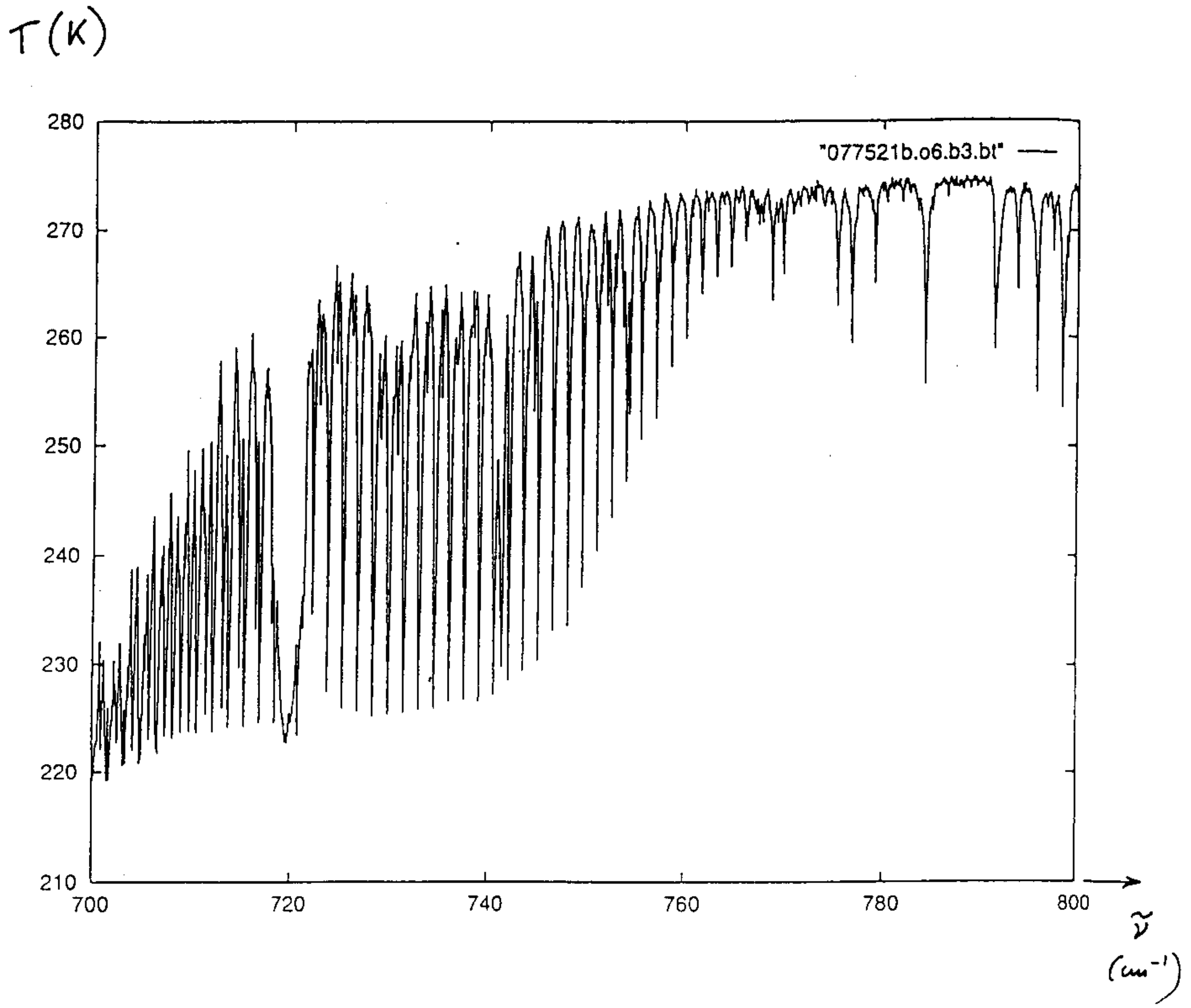
IMG Sensor

Principal characteristics	
Spectral range	714～3030cm − 1 (14 − 3.3 μ m)
Number of band	3
Band 1	2325～3030cm − 1 (4.3 − 3.3 μ m)
Band 2	2000～2500cm − 1 (5.0 − 4.0 μ m)
Band 3	714～2000cm − 1 (14 − 5.0 μ m)
Number of sampling	band 1: approx. 16 × 10 4 band 2: approx. 10 × 10 4 band 3: approx. 10 × 10 4
Spectral resolution	≦ 0.1cm − 1 (apodized)
Stability of measurement	≦ 0.38K(1 σ)
Data rate	882kbps
Weight	129.7kg(except IRU's)
Power consumption	149W
Dimension	1150 × 930 × 650mm

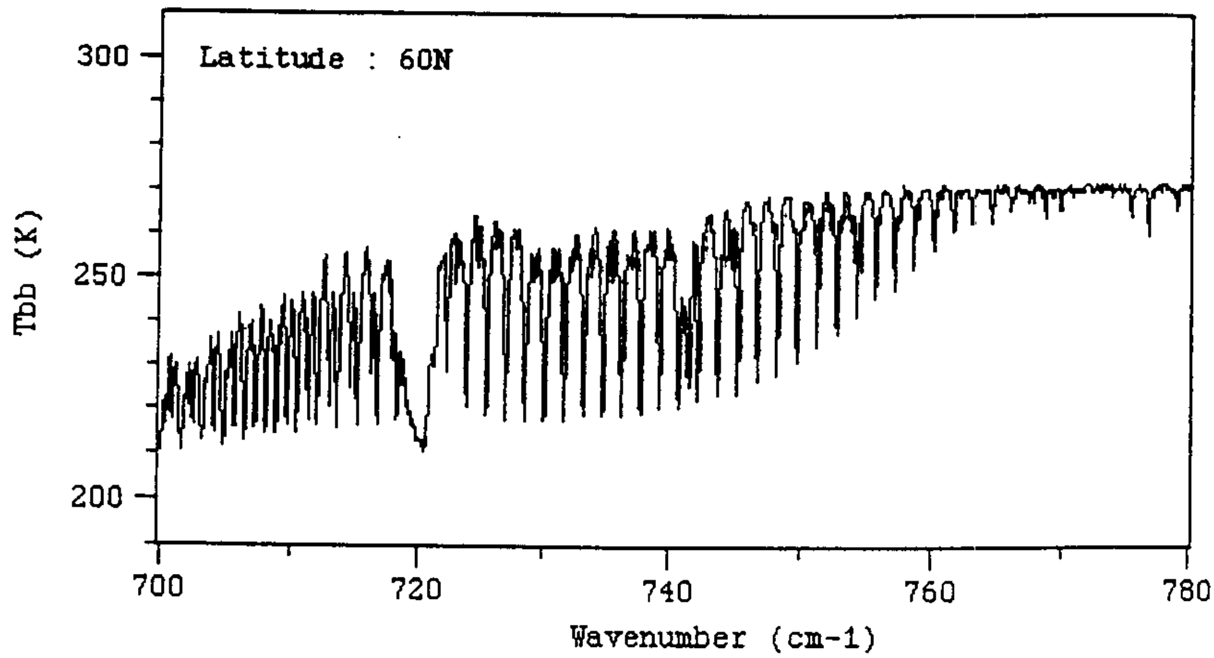
(18)

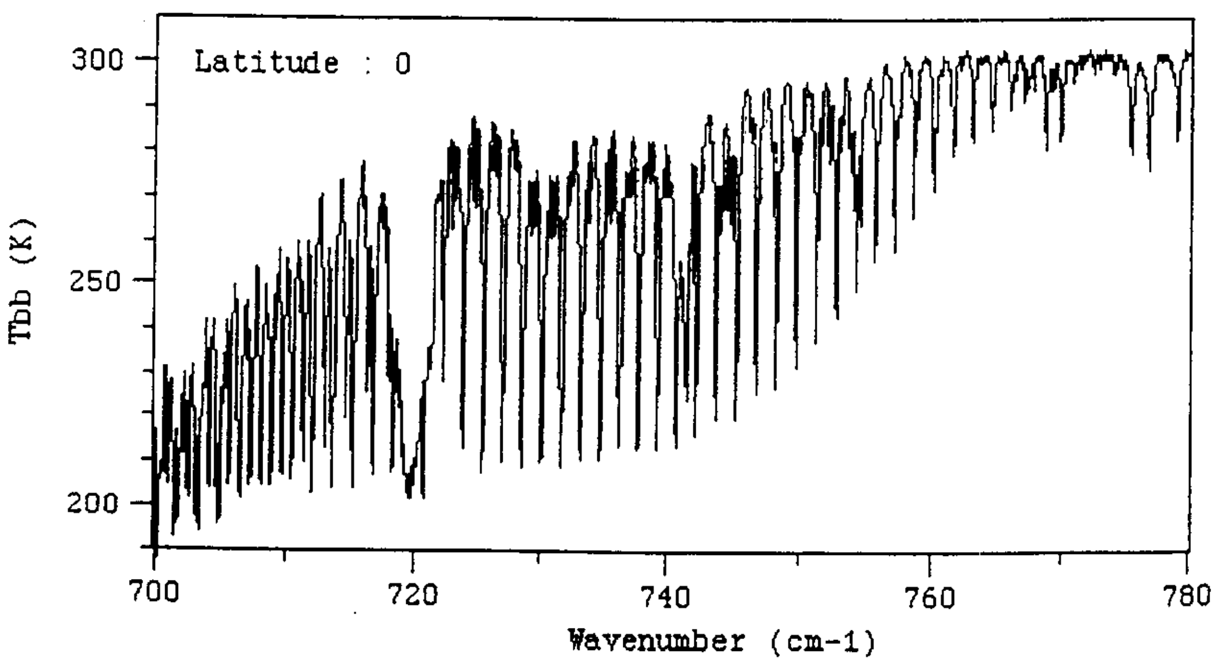


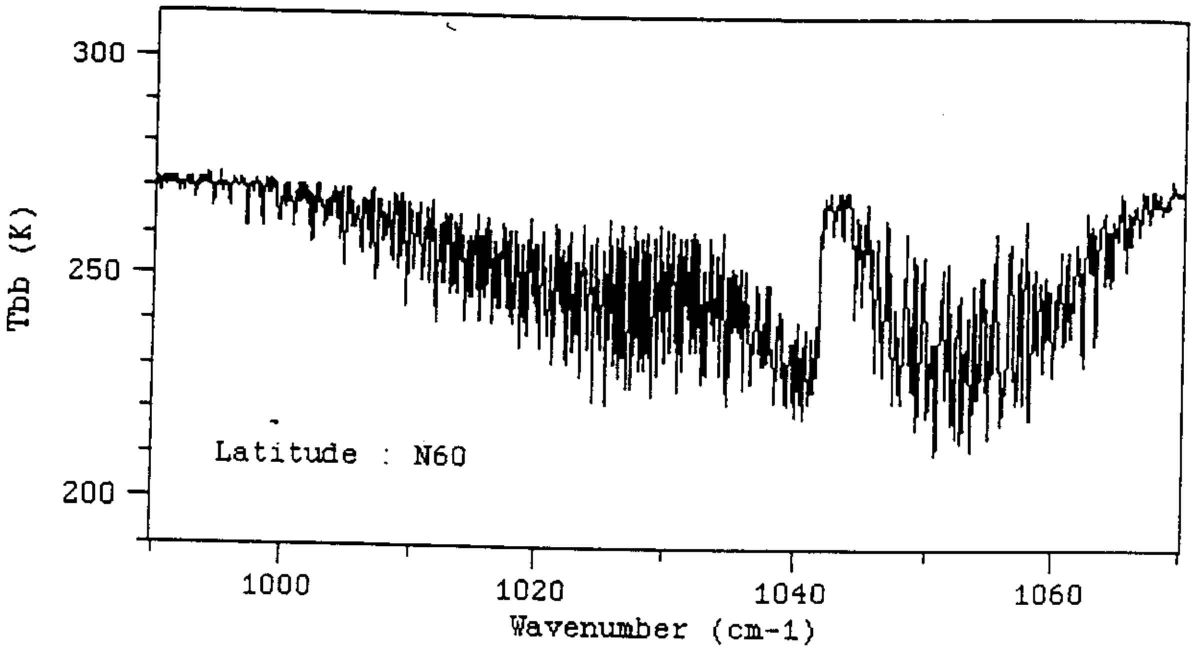
IMG Observation Pattern/Foot Print

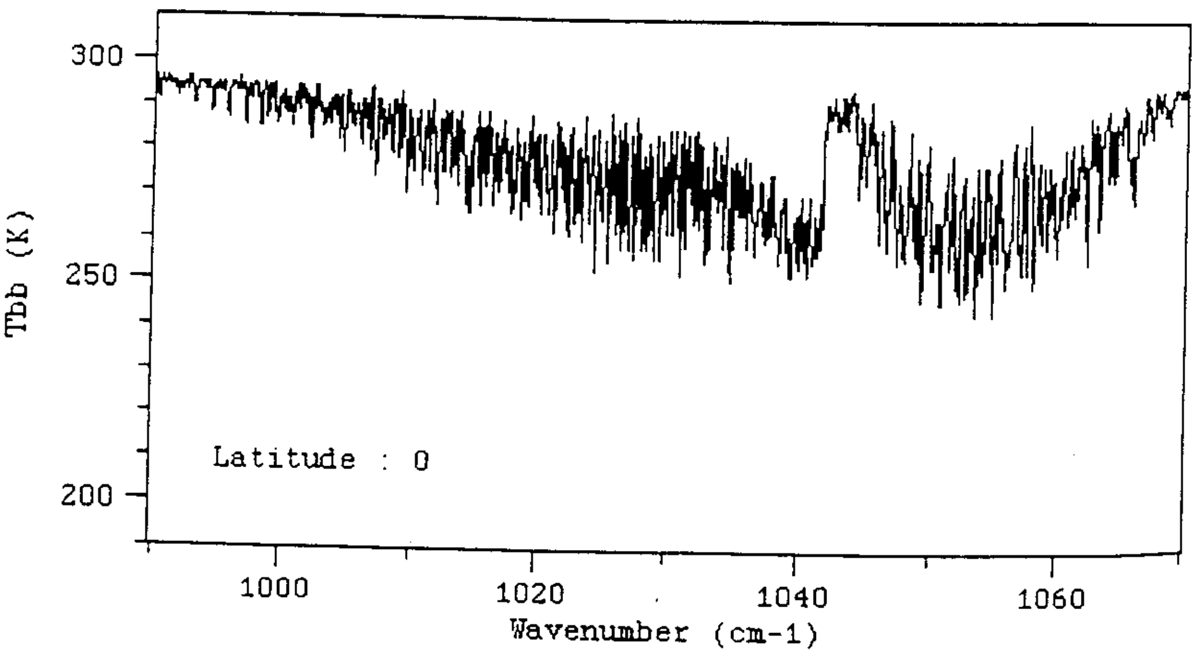

T(K)
280
270
260
250
240
230
220
210
700
720
740
760
780
800
"077521b.o6.b3.bt"
$\tilde{\nu}$ (cm^{-1})

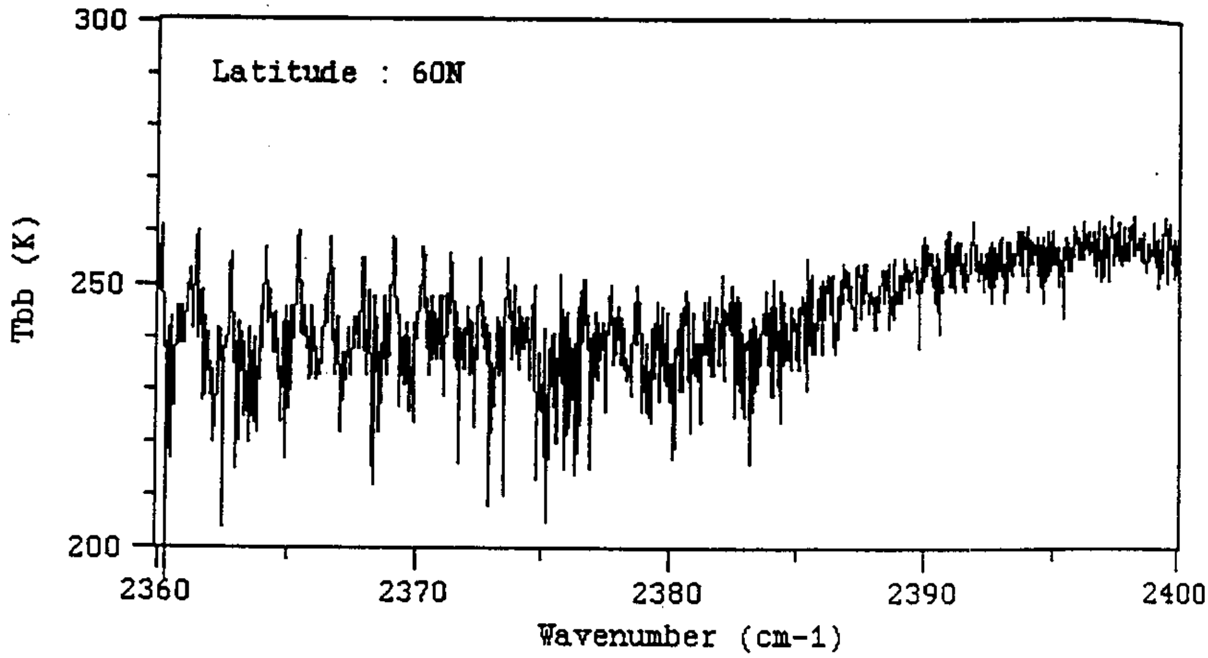
IMG

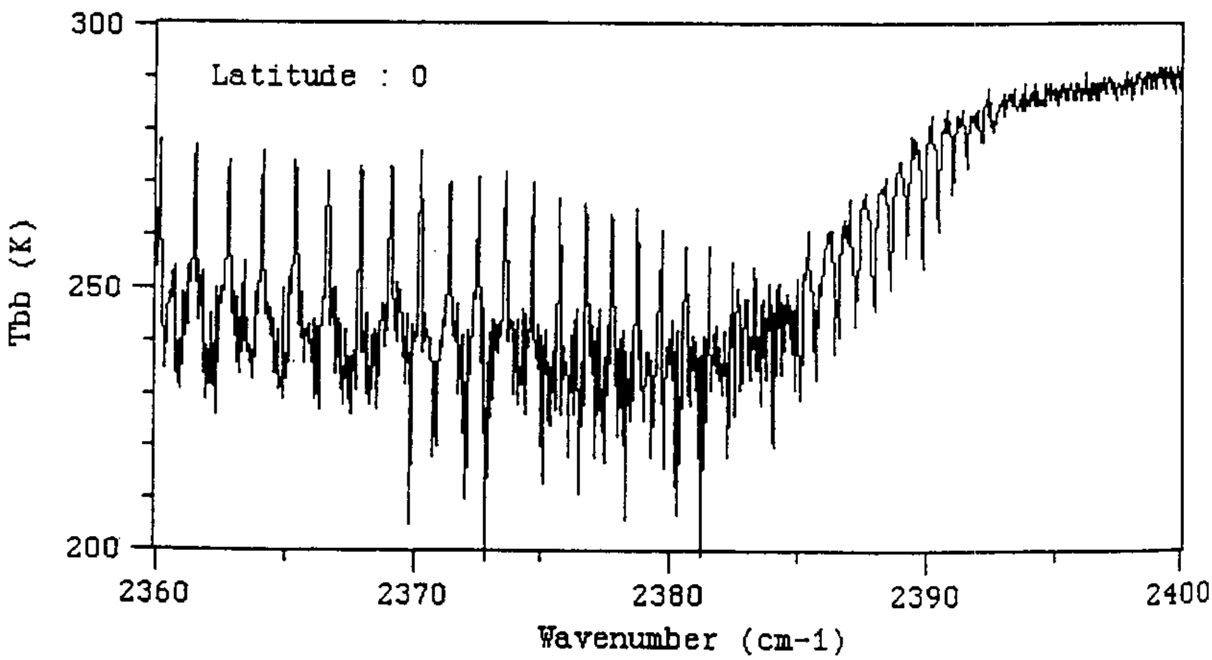

Latitude : 60N
Tbb (K)
300
250
200
700
720
740
760
780
Wavenumber (cm-1)


Latitude : 0
Tbb (K)
300
250
200
700
720
740
760
780
Wavenumber (cm-1)

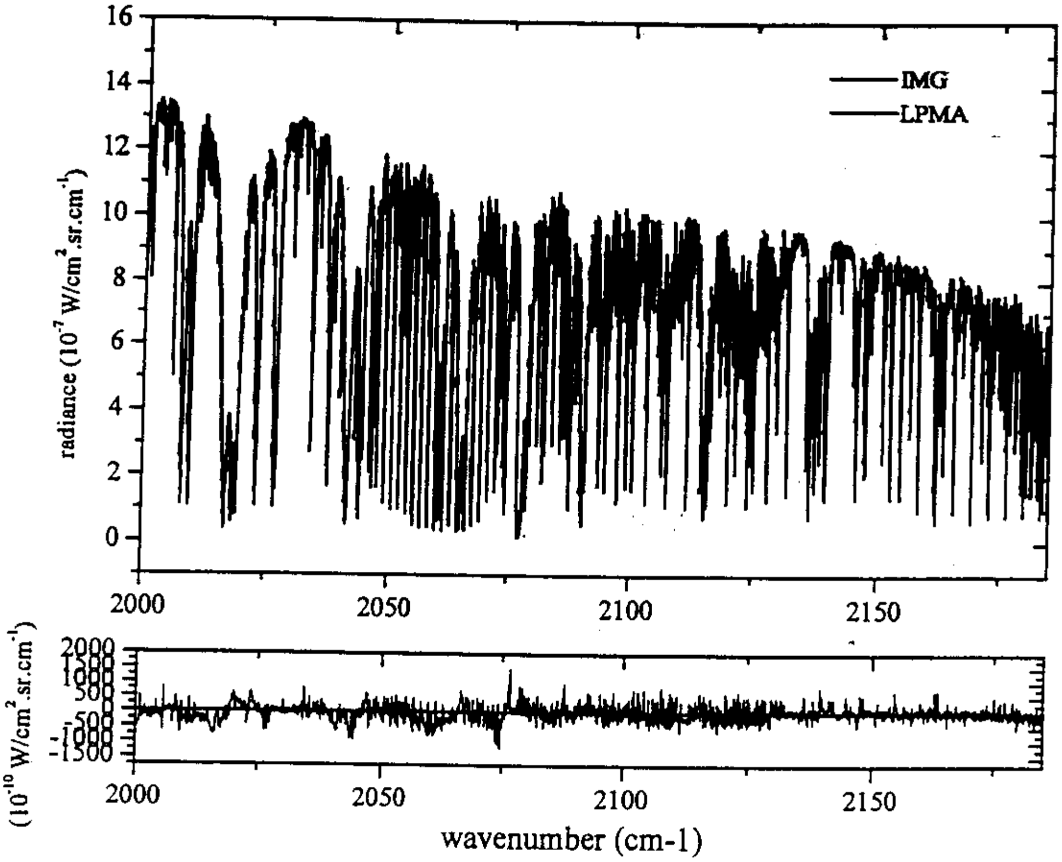

300
250
200
Tbb (K)
Latitude : N60
1000
1020
1040
1060
Wavenumber (cm-1)


300
250
200
Tbb (K)
Latitude : 0
1000
1020
1040
1060
Wavenumber (cm-1)


300
250
200
Tbb (K)
Latitude : 60N
2360
2370
2380
2390
2400
Wavenumber (cm-1)

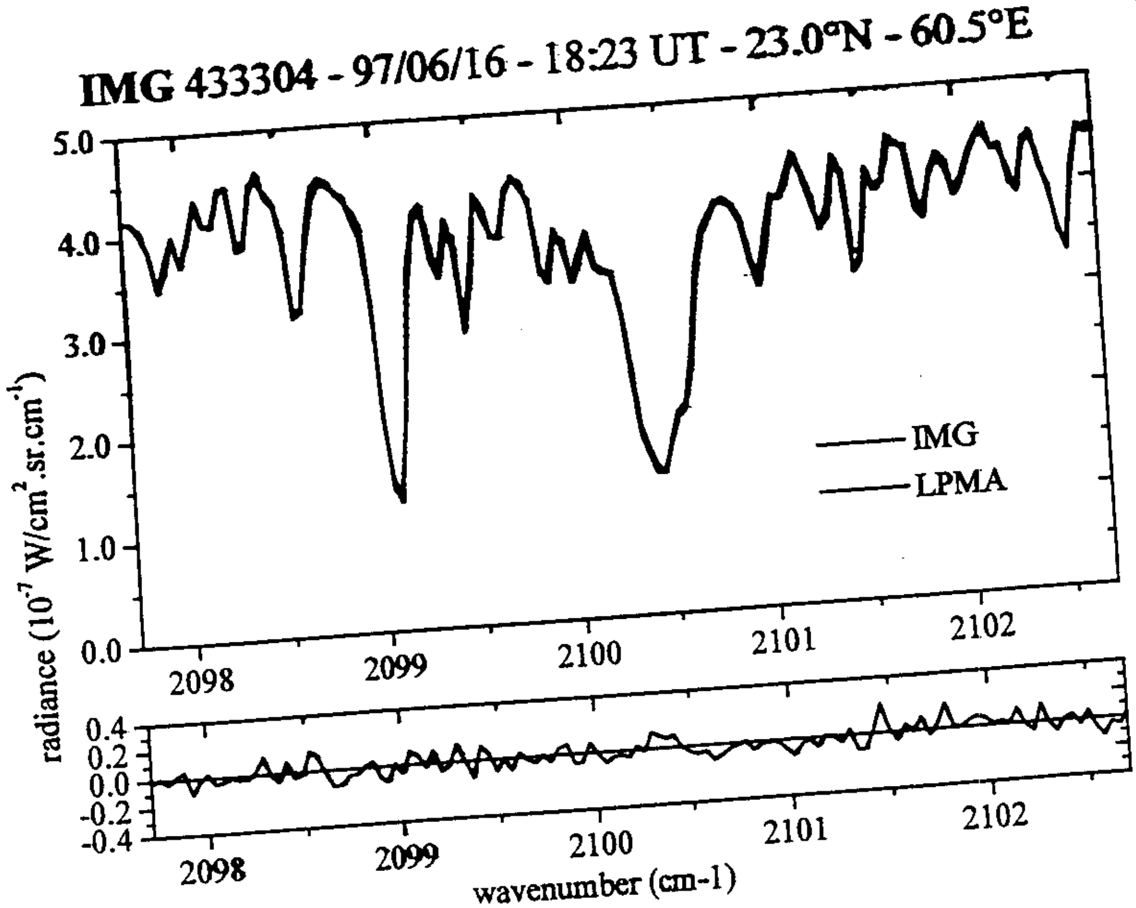

300
250
200
Tbb (K)
Latitude : 0
2360
2370
2380
2390
2400
Wavenumber (cm-1)

IMG - Band 2 - 97/06/16 - 22.8°N - 4.6°E

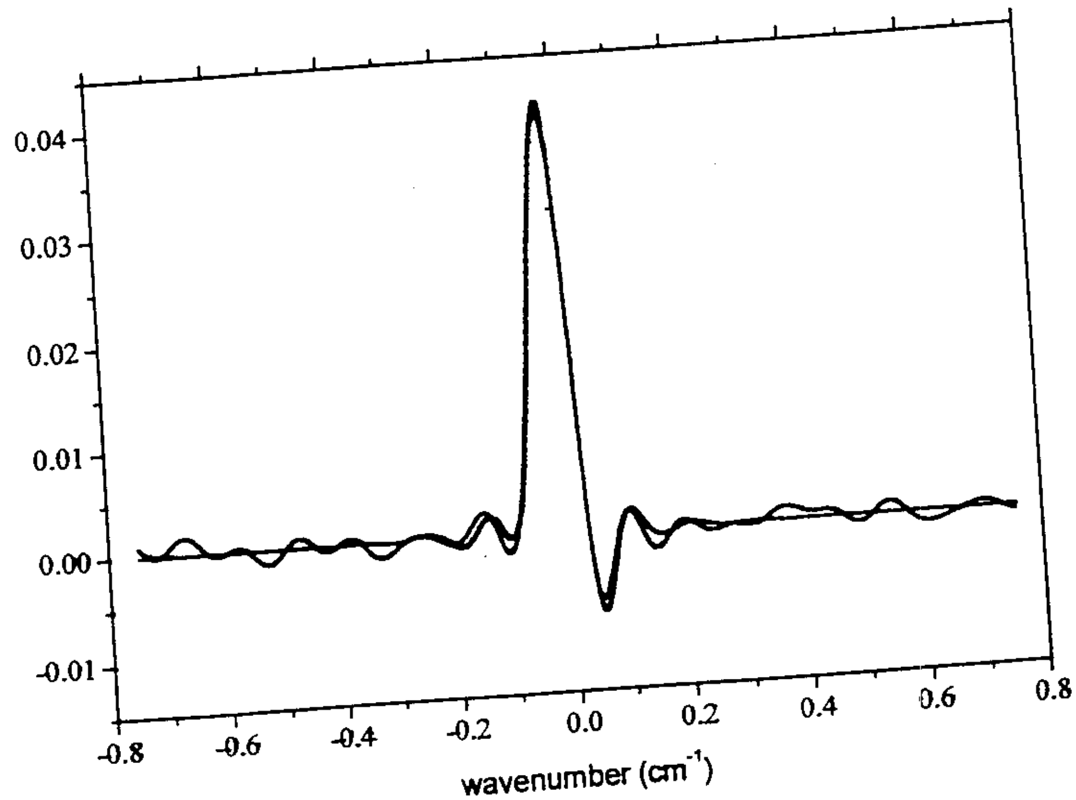


Global fit of an IMG spectrum

S. Payan & C. Camy-Peyret (LPMA)

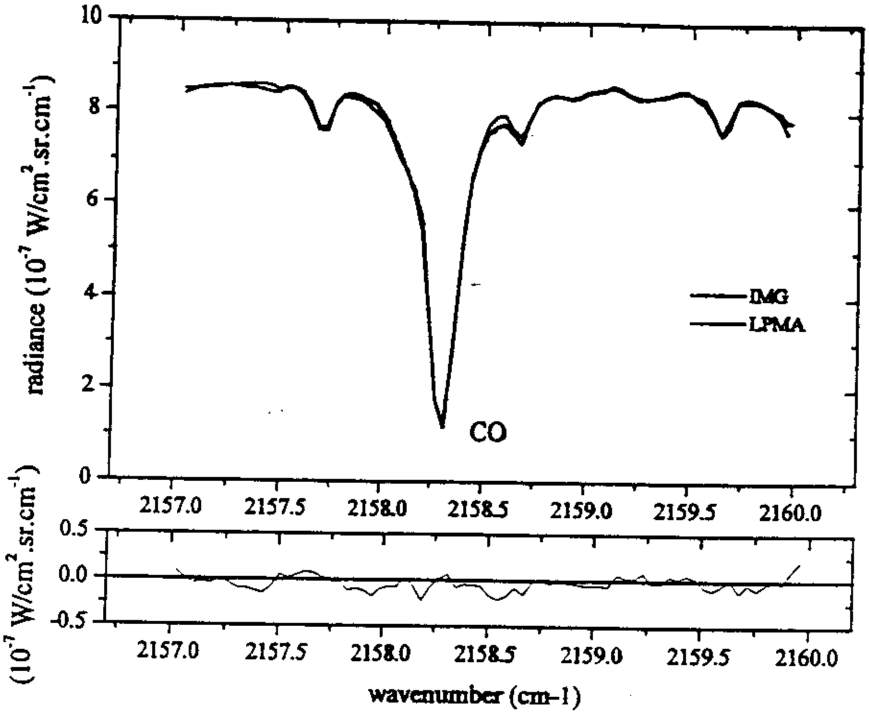


IMS instrument spectral response function (ISRF)



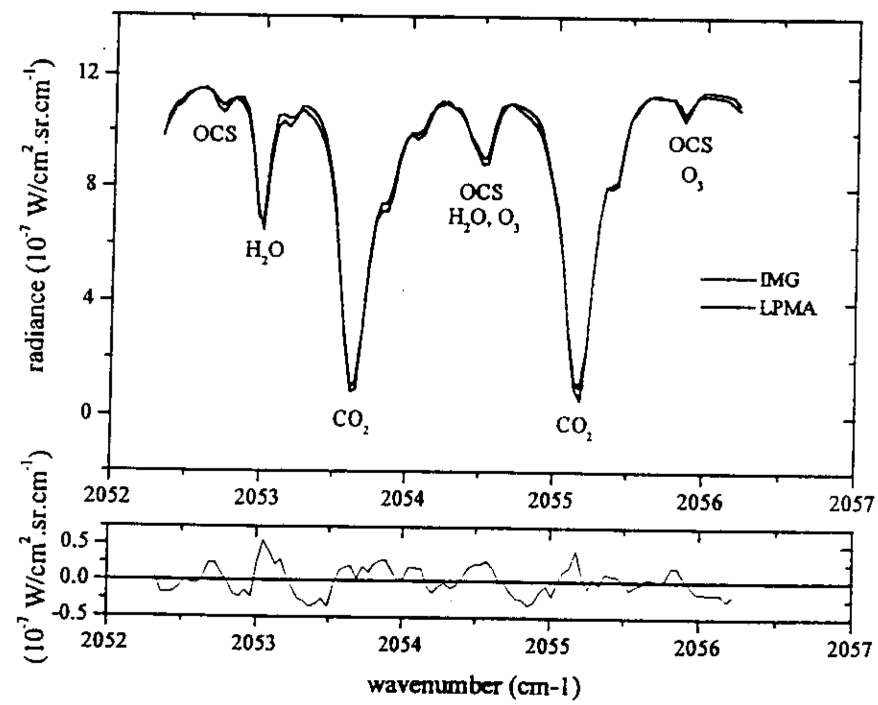
S. Payan & C. Camy-Peyret (LPMA)

Tropospheric CO micro-window (CO + OH → CO_2 + H)



CO column = (1.36 ± 0.02) 10^{18} molecule/cm^2
CO vmr at ground = 104 ± 15 ppbv

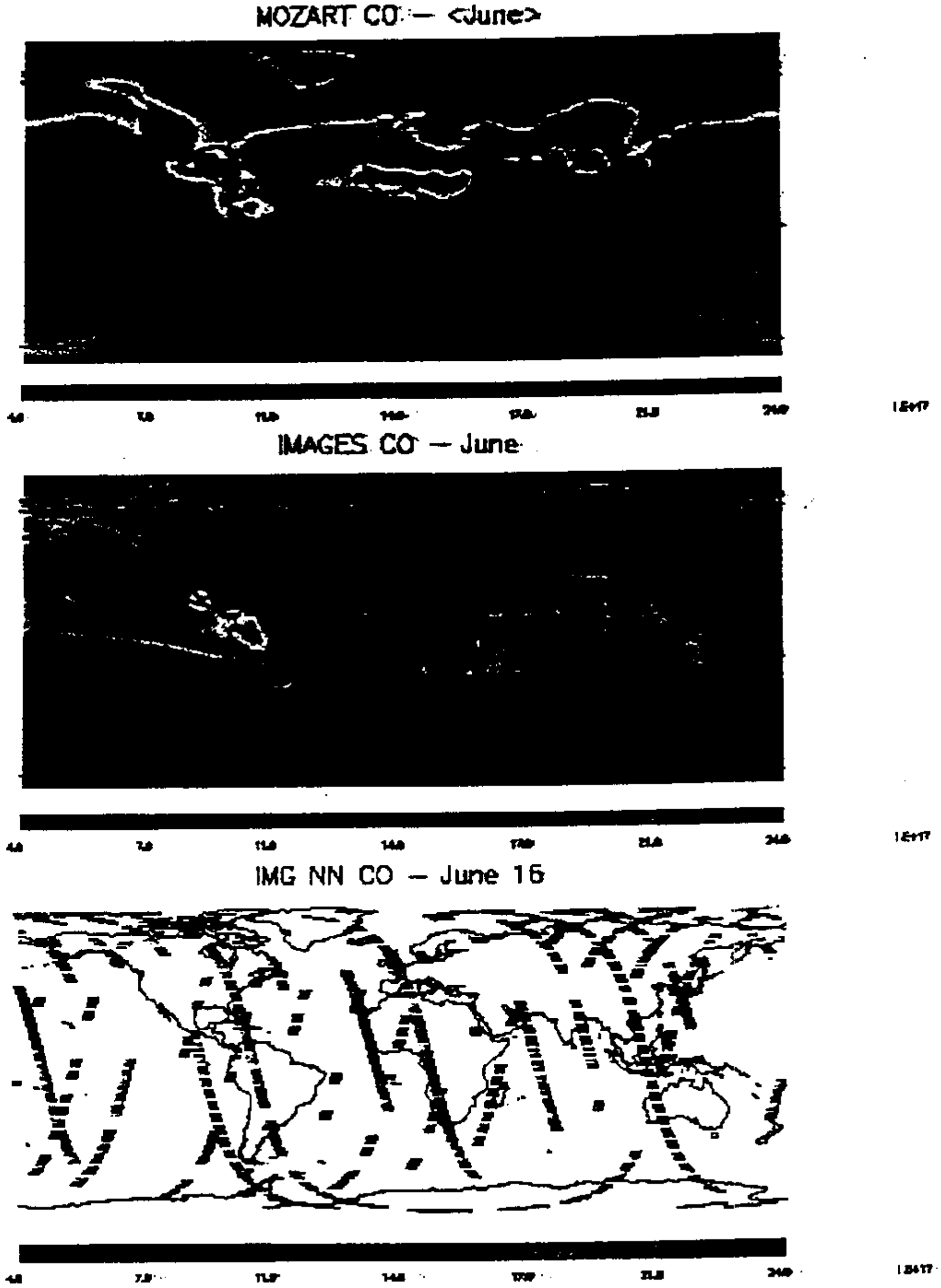
Tropospheric OCS micro-window (OCS + hν → CO + S)



OCS column = (1.32 ± 0.12) 10^{16} molecule/cm^2
OCS vmr at ground = 0.7 ± 0.1 ppbv

S. Payan and C. Camy-Peyret (LPMA)

From C. Clerbaux Service d'Aéronomie (SA), Paris, France

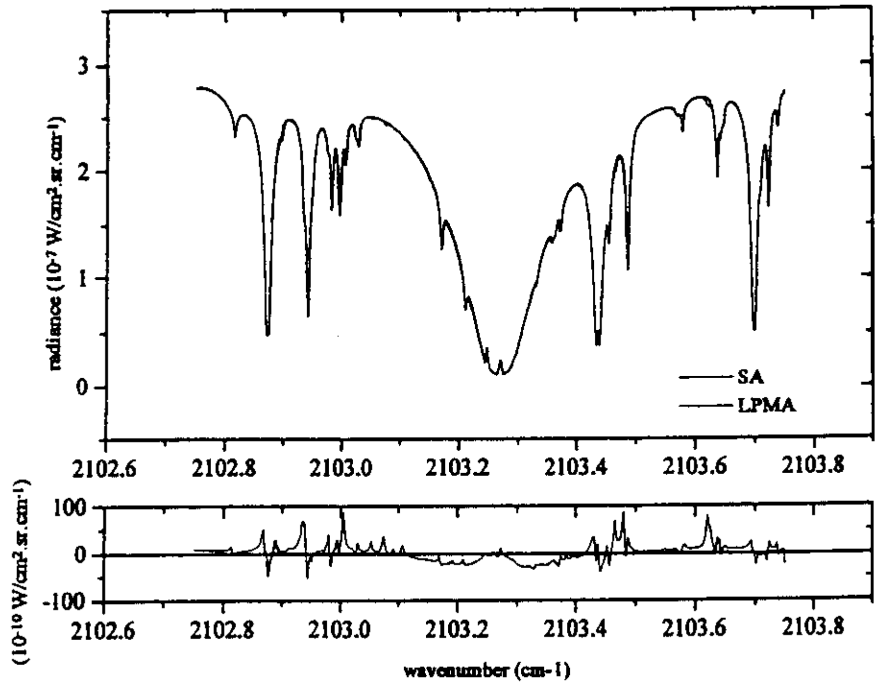


IMG NN CO : Inversion de CO à partir des spectres IMG avec un réseau de neurones (Cathy Clerbaux, Service d'Aéronomie)

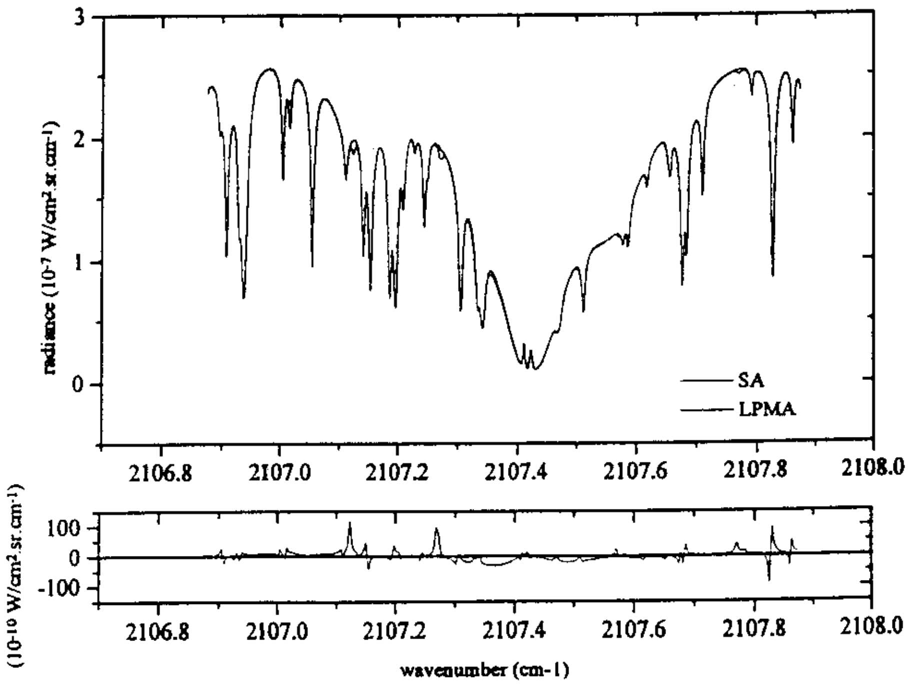
MOZART CO : CTM-3D (NCAR, USA)

IMAGES CO : CTM-3D (NCAR USA)

Max 1

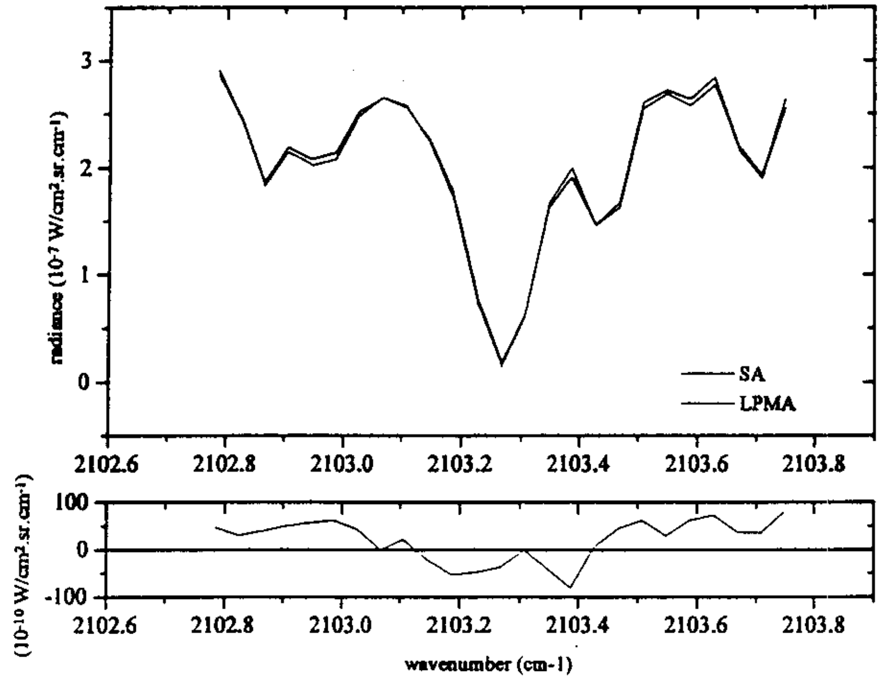


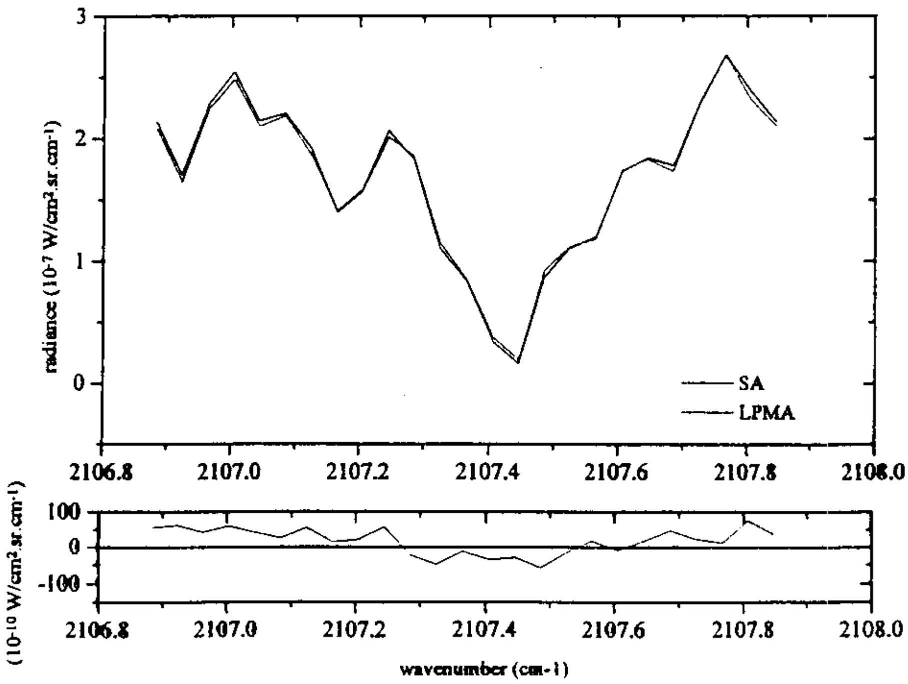
Max 2



Comparison of "infinite resolution" spectra
calculated by SA and LPMA
around 2 lines of CO

blind test C - IMG spectra





retrieval of IMG simulated spectra
after convolution of the "infinite resolution" spectra
+ noise added around 2 lines of CO

IASI

EUMETSAT – CNES
on METOP

Infrared Atmospheric Sounding Interferometer

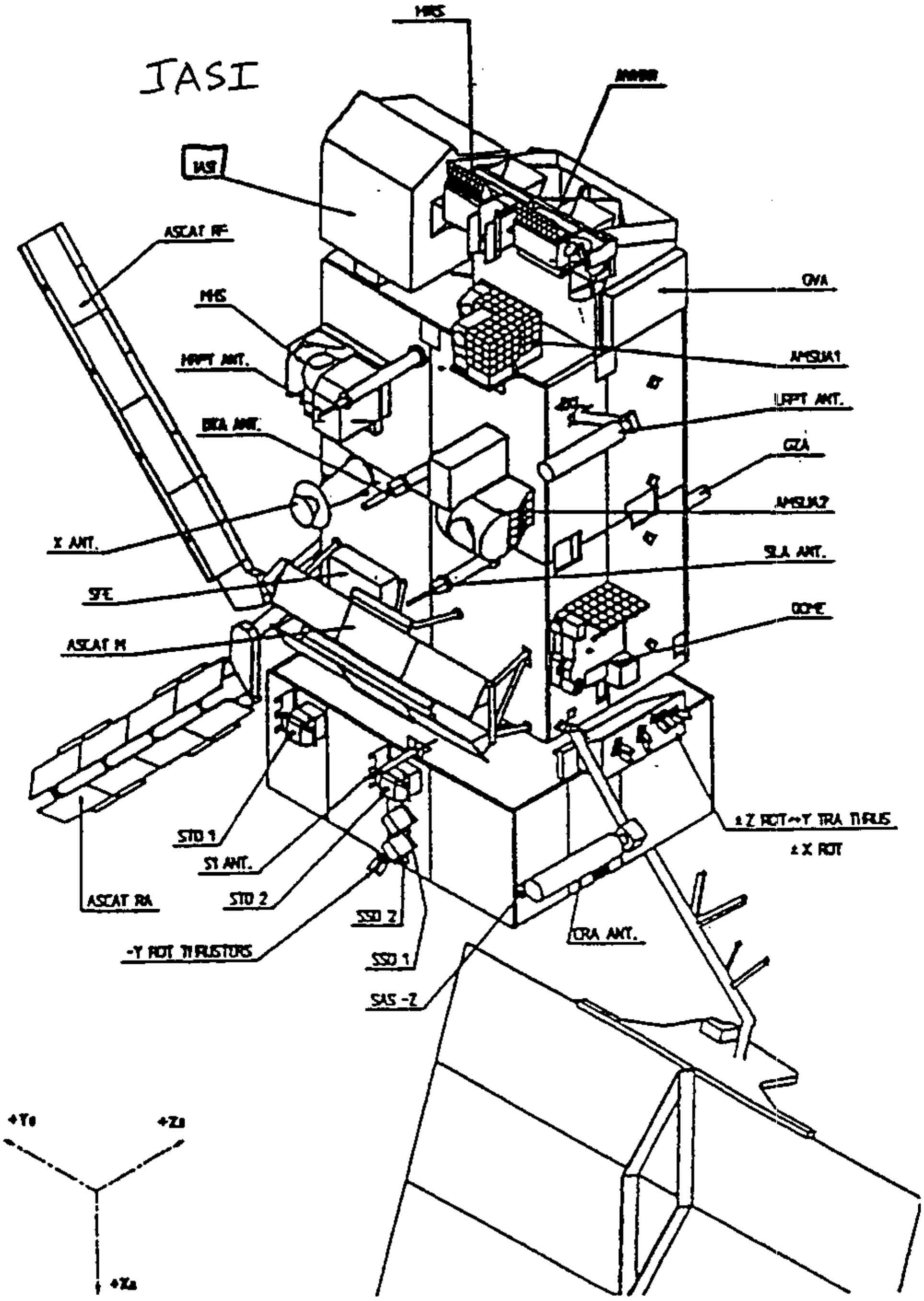
Band	Interval	Resolution
1	$645 - 1210\ cm^{-1}$	$\lesssim 0.5\ cm^{-1}$
2	$1210 - 2000\ cm^{-1}$	
3	$2000 - 2760\ cm^{-1}$	

Expected performances for operational meteorology

		TOVS
<u>Temperature profile</u>		
precision	1K	2K
vertical resolution	1 km	4 km
horizontal resolution	30 km	
<u>Humidity profile</u>		
precision	10%	25%
vertical resolution	1 km → 2 km (tropopause)	thick layers

Information on the <u>ozone distribution</u>
3 pieces of information

<u>Trace species in the troposphere</u>
columns of CO, CH_4, N_2O ...



METOP satellite overall configuration

OTHER INSTRUMENTS ON METOP

AVHRR (Advanced Very High Resolution Radiometer)

HIRS (High Resolution Infrared Radiation Sounder)

MHS (Microwave Humidity Sounder)

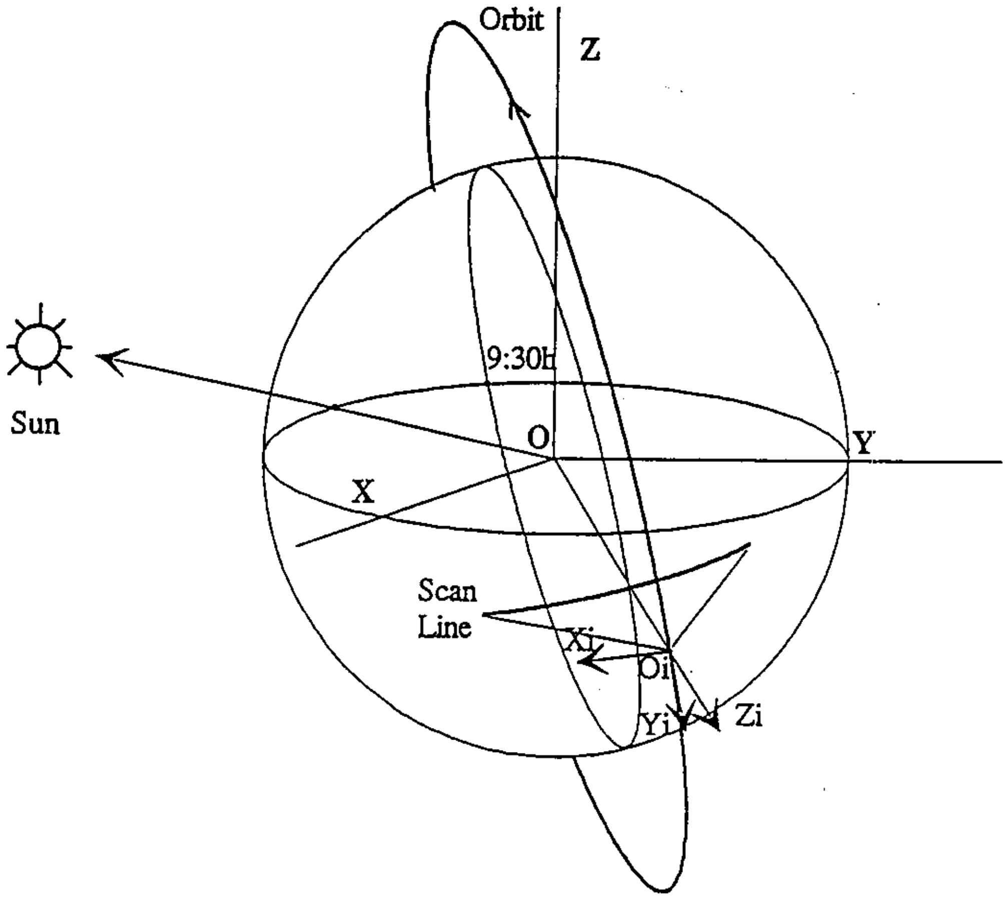
GOME-2 (Global Ozone Monitoring Experiment)

GRAS (GNSS Receiver for Atmospheric Sounding)

ASCAT (Advanced wind SCATterometer)

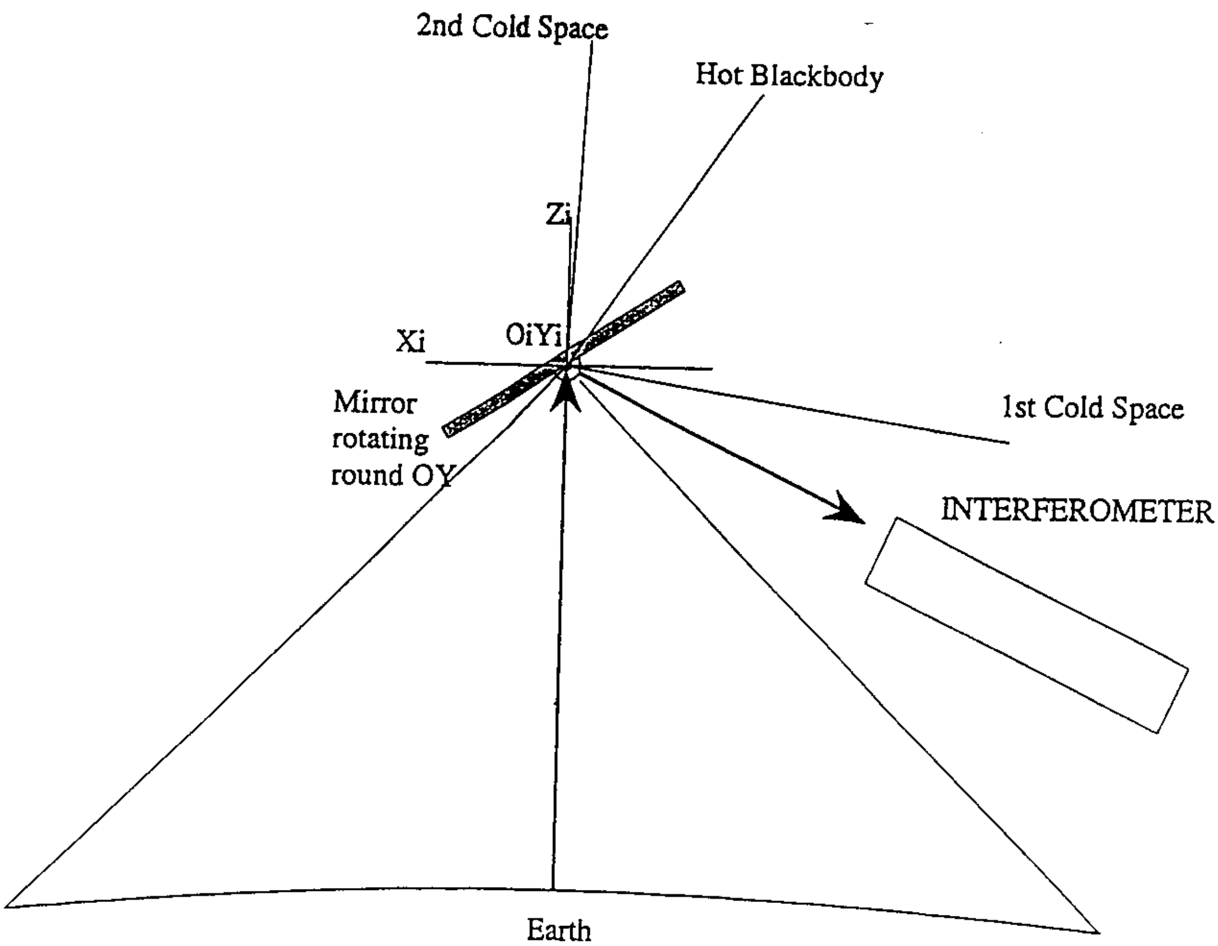
+ ...

Expected launch date of Metop: end 2003

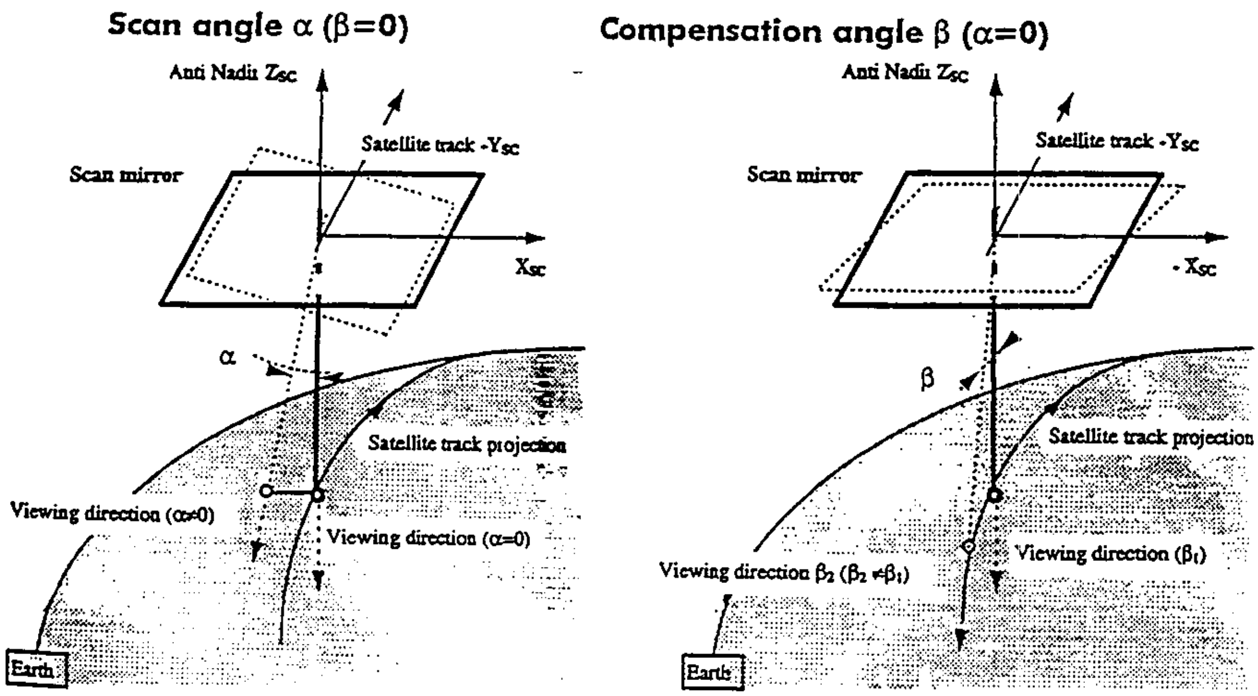


IASI scan pattern axis definition

METOP (in the morning orbit) will complement (or replace) the NOAA-xx satellites.

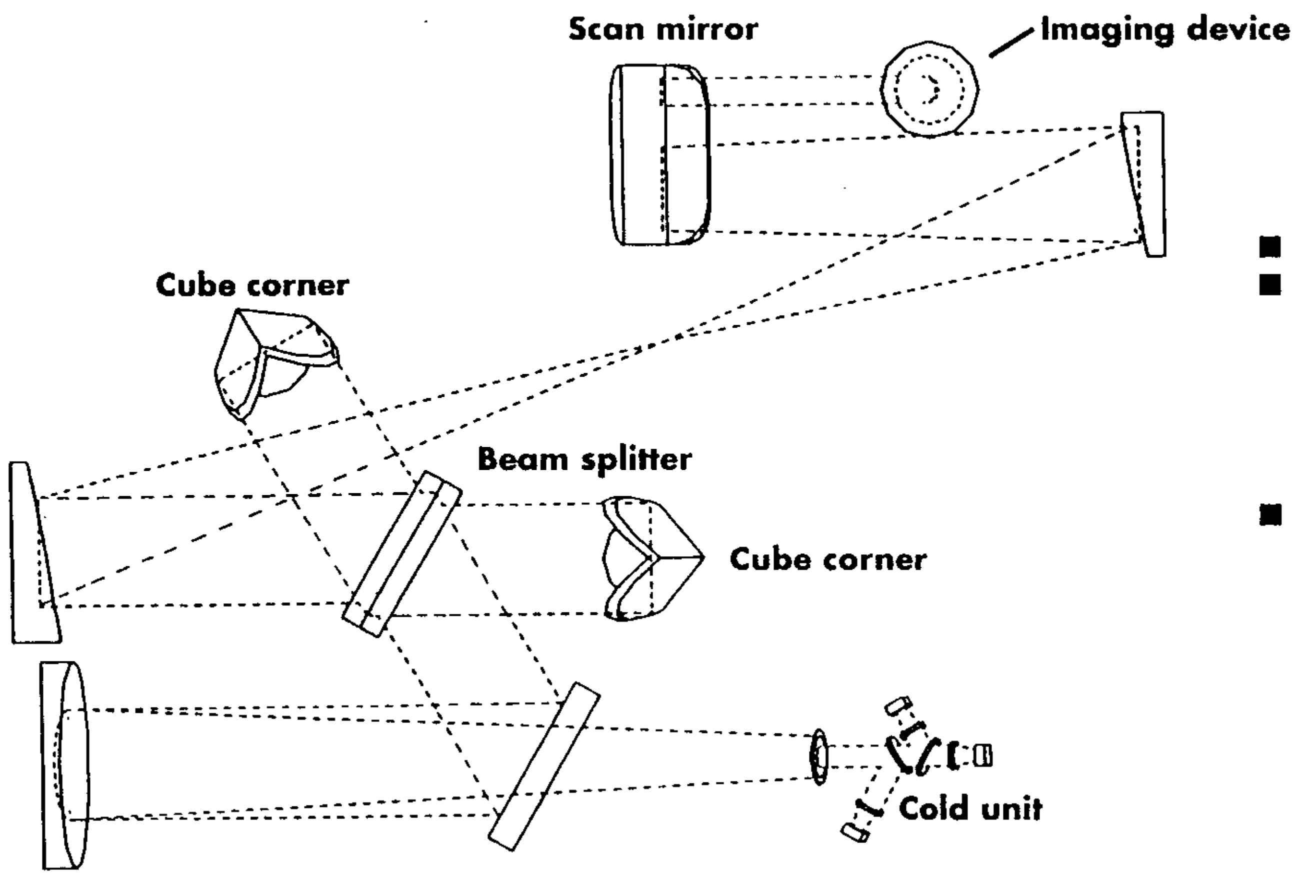


Scan subsystem of IASI


Scan angle α (β=0)
Anti Nadir Zsc
Satellite track -Ysc
Scan mirror
Xsc
α
Satellite track projection
Viewing direction (α≠0)
Viewing direction (α=0)
Earth
Compensation angle β (α=0)
Anti Nadir Zsc
Satellite track -Ysc
Scan mirror
- Xsc
β
Satellite track projection
Viewing direction β2 (β2 ≠β1)
Viewing direction (β1)
Earth

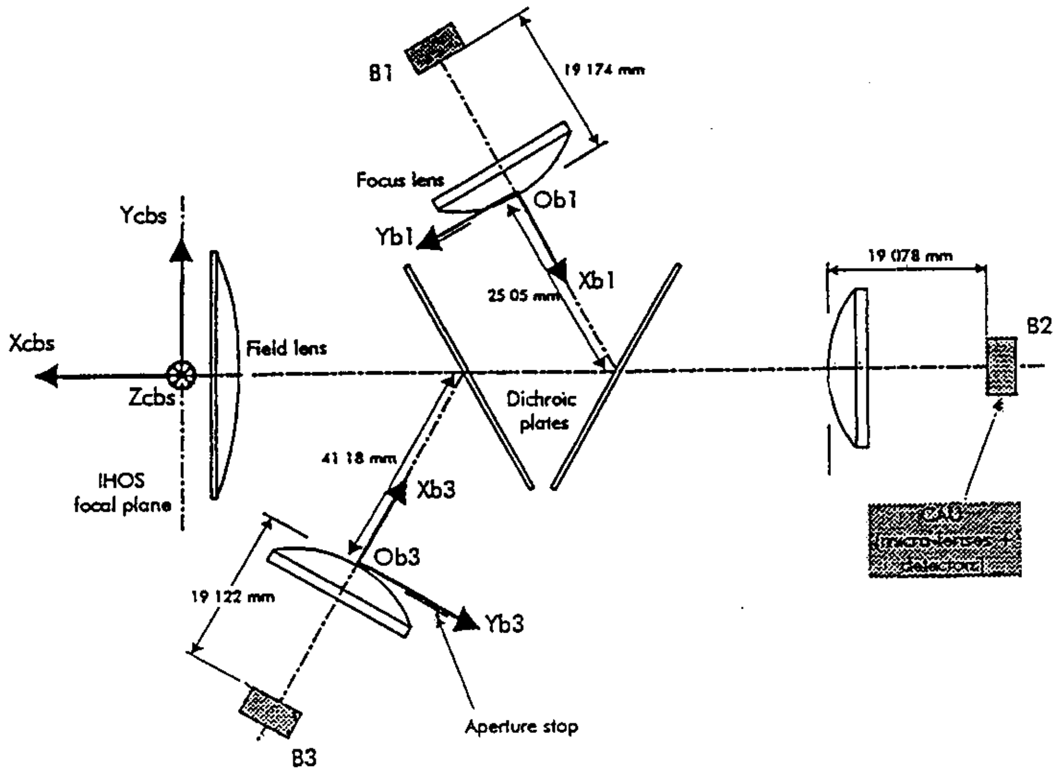
IASI

OPTICAL LAYOUT

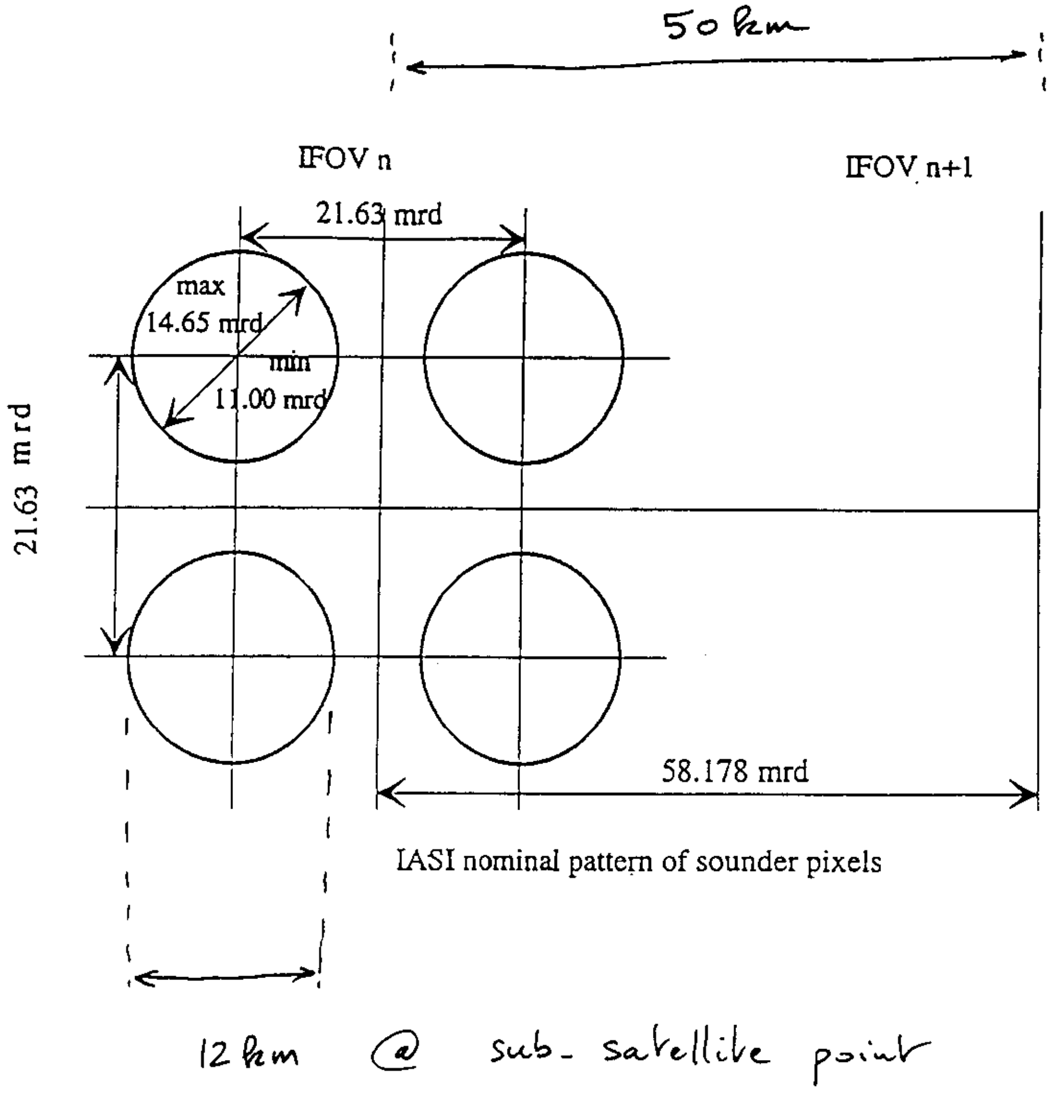


- APERTURE: 6cm
- APERTURE STOP ON:
  - scan mirror
  - cube corners
  - cold optics
  - detectors

- EARTH IMAGING ON ENTRANCE APERTURE OF COLD UNIT.



CBS OPTICAL LAY-OUT



IASI nominal pattern of sounder pixels

INSTRUMENT SUMMARY

cnes

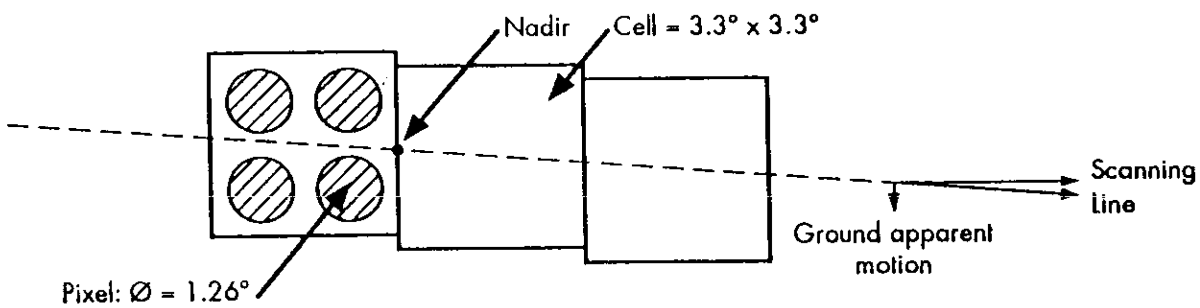
Spectral Band: 645 cm^{-1} (15.5 μm) to 2940 cm^{-1} (3.4 μm)
Spectral Resolution: 0.25 cm^{-1} without apodisation
Spectral Calibration: $\Delta\nu < 0.01$ cm^{-1}

Radiometric Resolution:

Band	Spectral Band cm^{-1}	Spectral Resolution cm^{-1}	Radiometric Resolution NeΔT	at
1	645 - 1100	0.5	< 0.2 K	250 K
2	1100 - 2000	0.5	< 0.2 K	250 K
3	2000 - 2500	0.5	< 0.2 K	280 K

Radiometric Calibration: NeΔT < 0.5K for T = 280 K

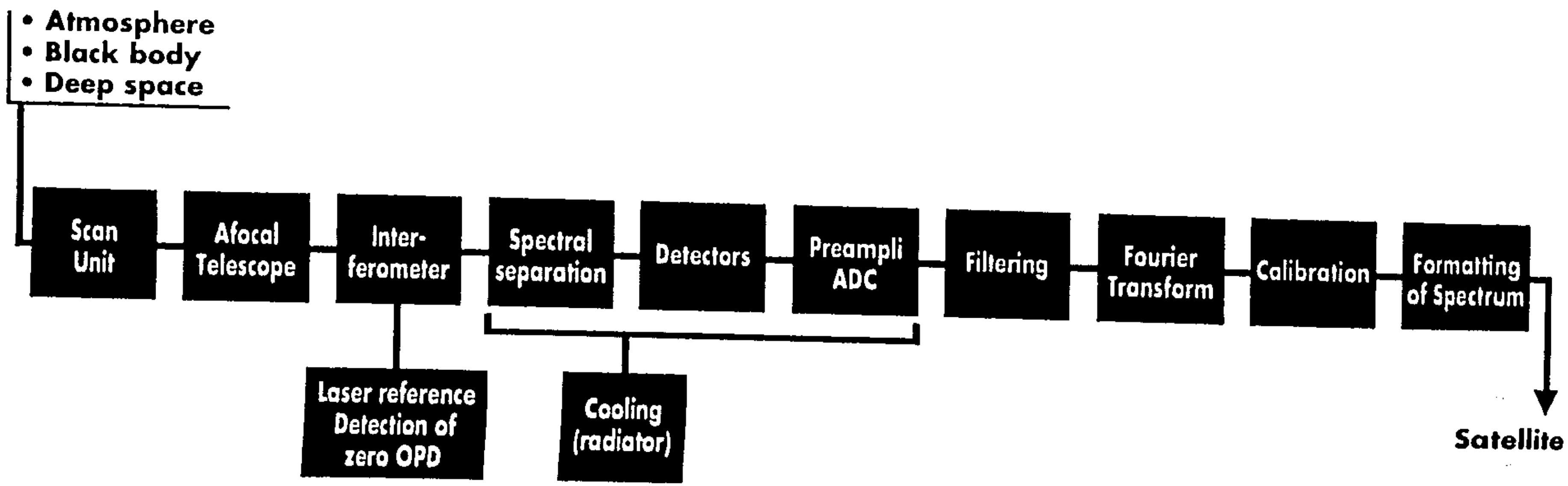
Spatial Sampling



Number of dwell cells in the line: 30 (±15)
Global Coverage
Lifetime 5 years

INSTRUMENT FUNCTIONAL UNITS

cnes



Instrument Budget

Two Parts	Optical Sensor	Ancillary	Total
Mass (Kg)	55	21	76
Power (W)	64	79	153
Bit Rate (Mbits/s)			1.5

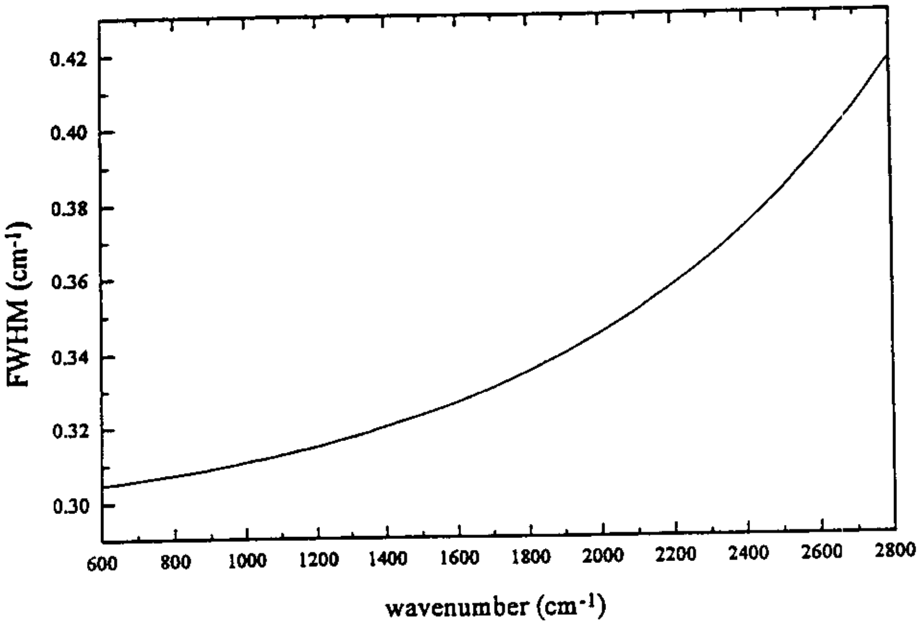


Figure 3.a
Variation of the resolution $\delta\tilde{\nu}_{FWHM}$ (FOV = 12 km).

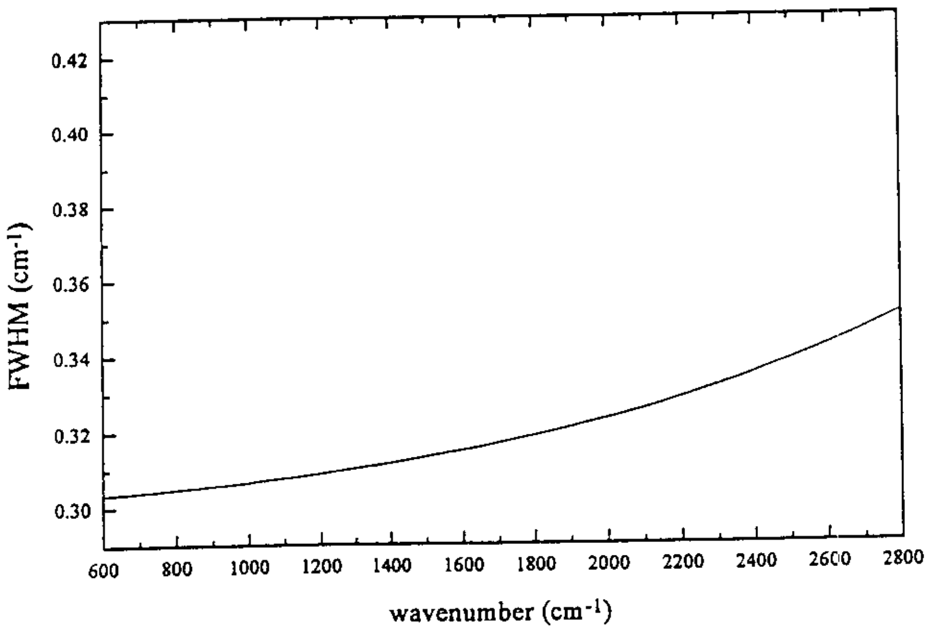


Figure 3.b
Variation of the resolution $\delta\tilde{\nu}_{FWHM}$ (FOV = 9 km).

Spectral resolution of IASI. Off-axis pixels

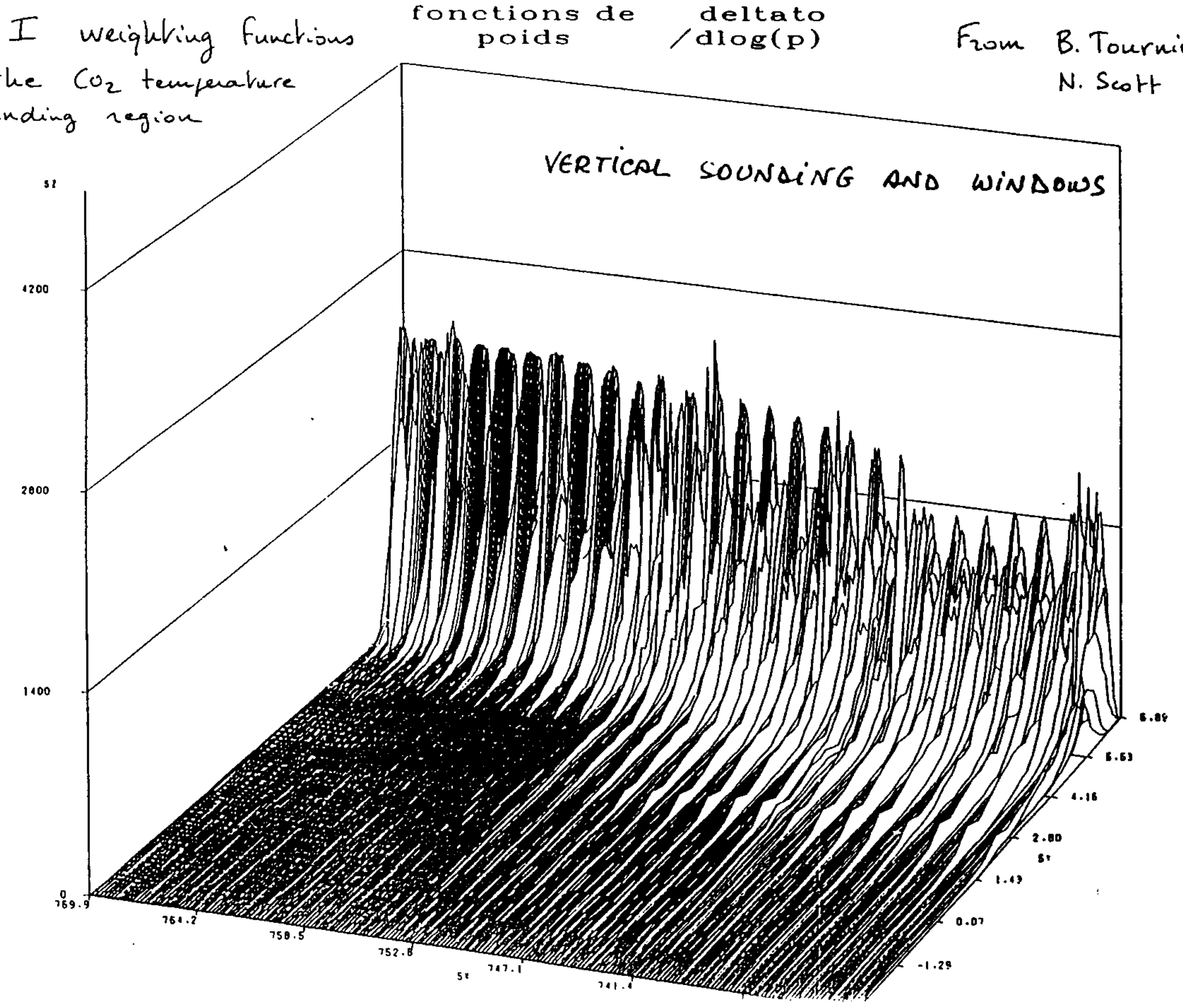
→ self-apodised or auto-apodised spectrum

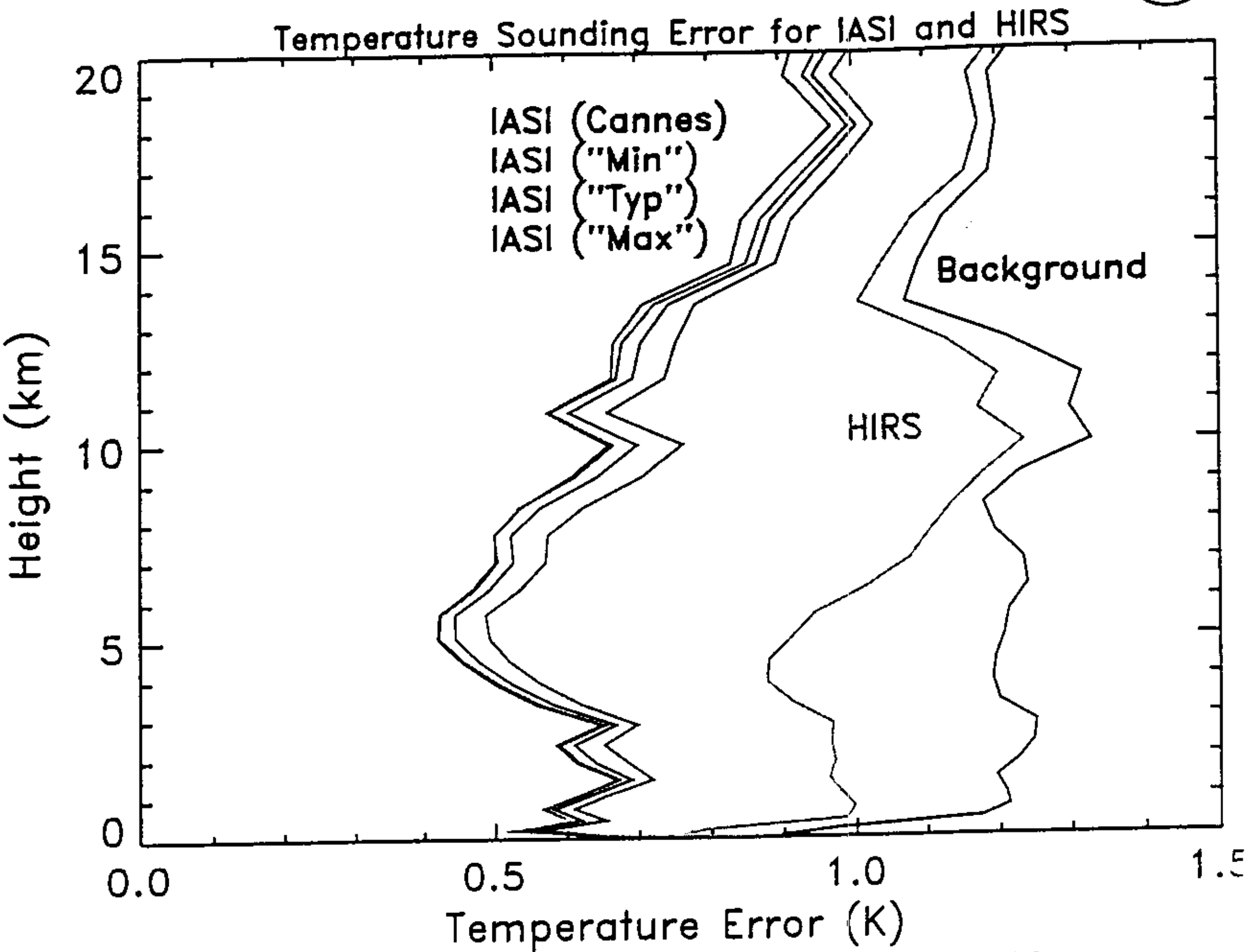
variable resolution, slight asymmetry

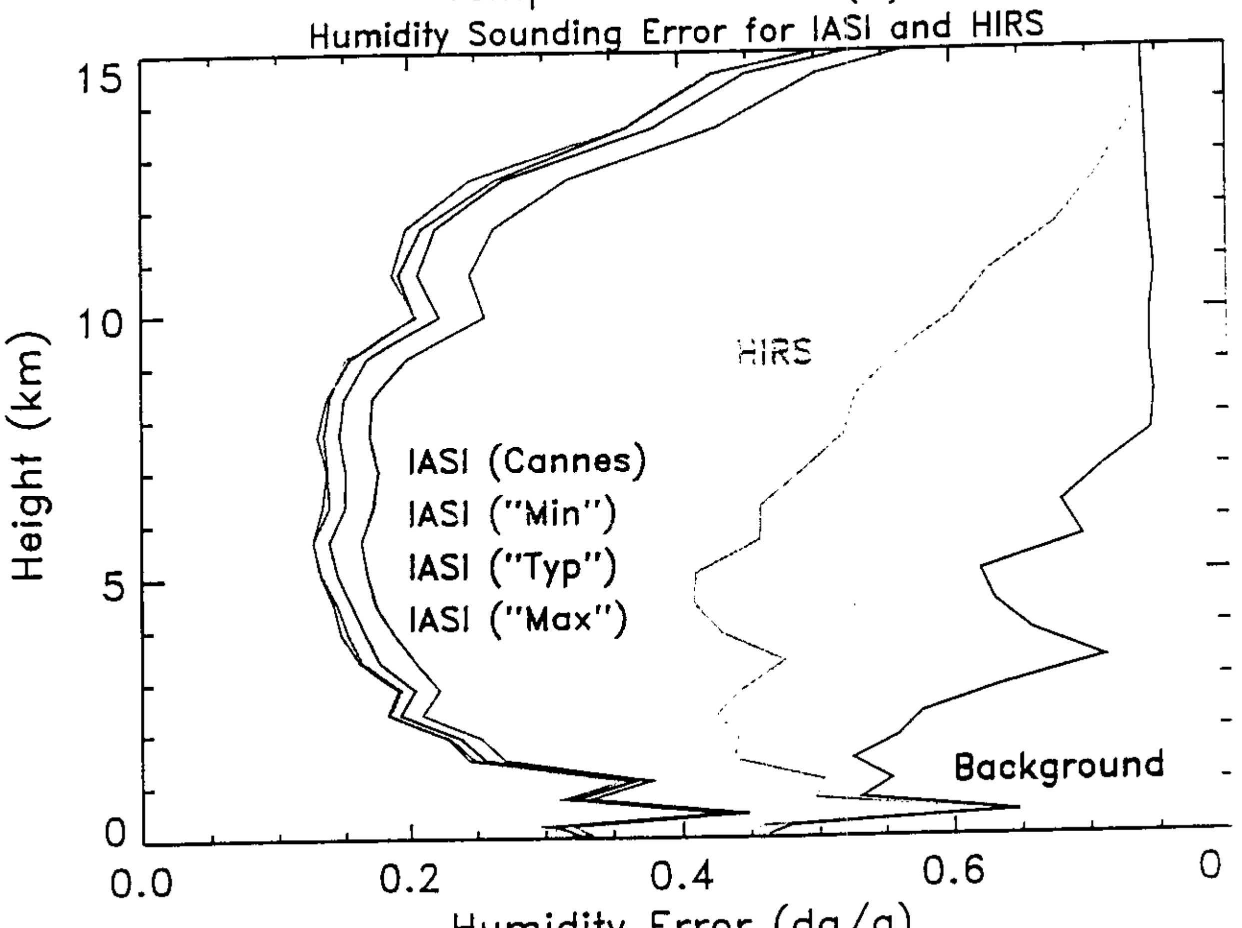
S. Payan & C. Camy-Peyret, IASI report on Instrument Spectral Response Function (ISRF)

IASI weighting functions in the CO_2 temperature sounding region

From B. Tournier (CNES)
N. Scott (LMD)



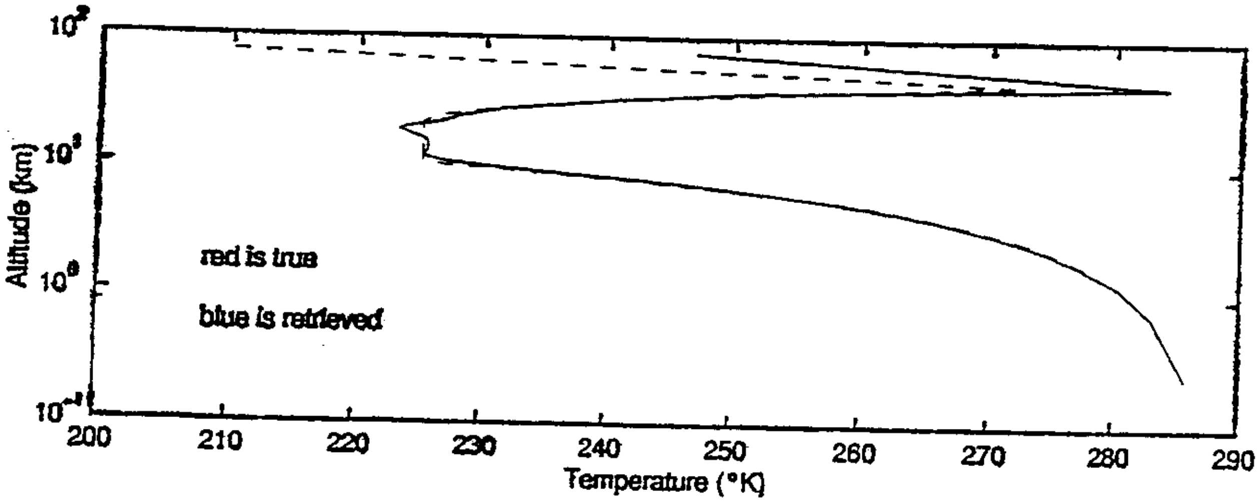


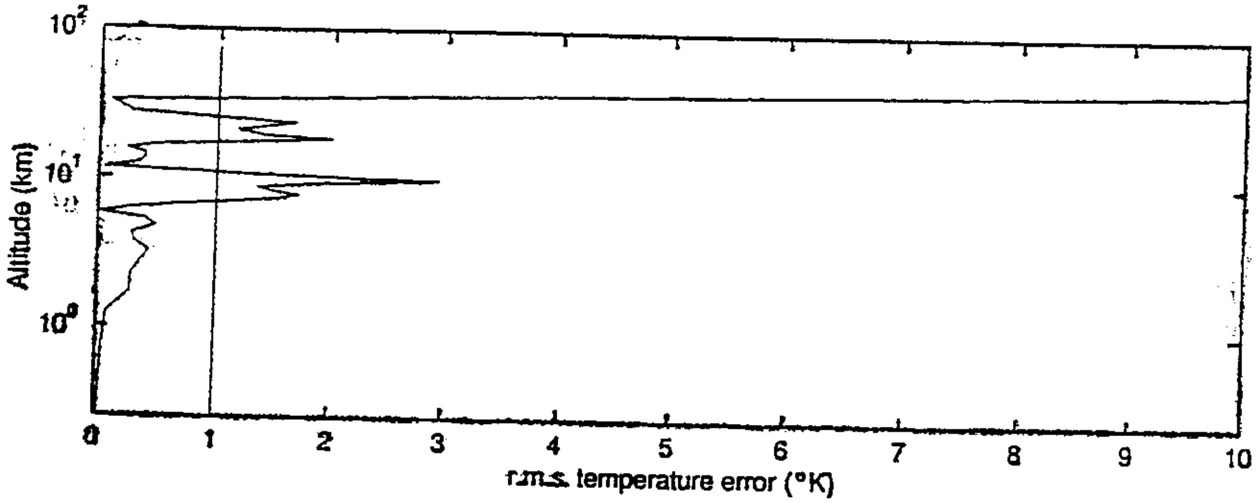


From J. Eyre (UKMo)

(43)

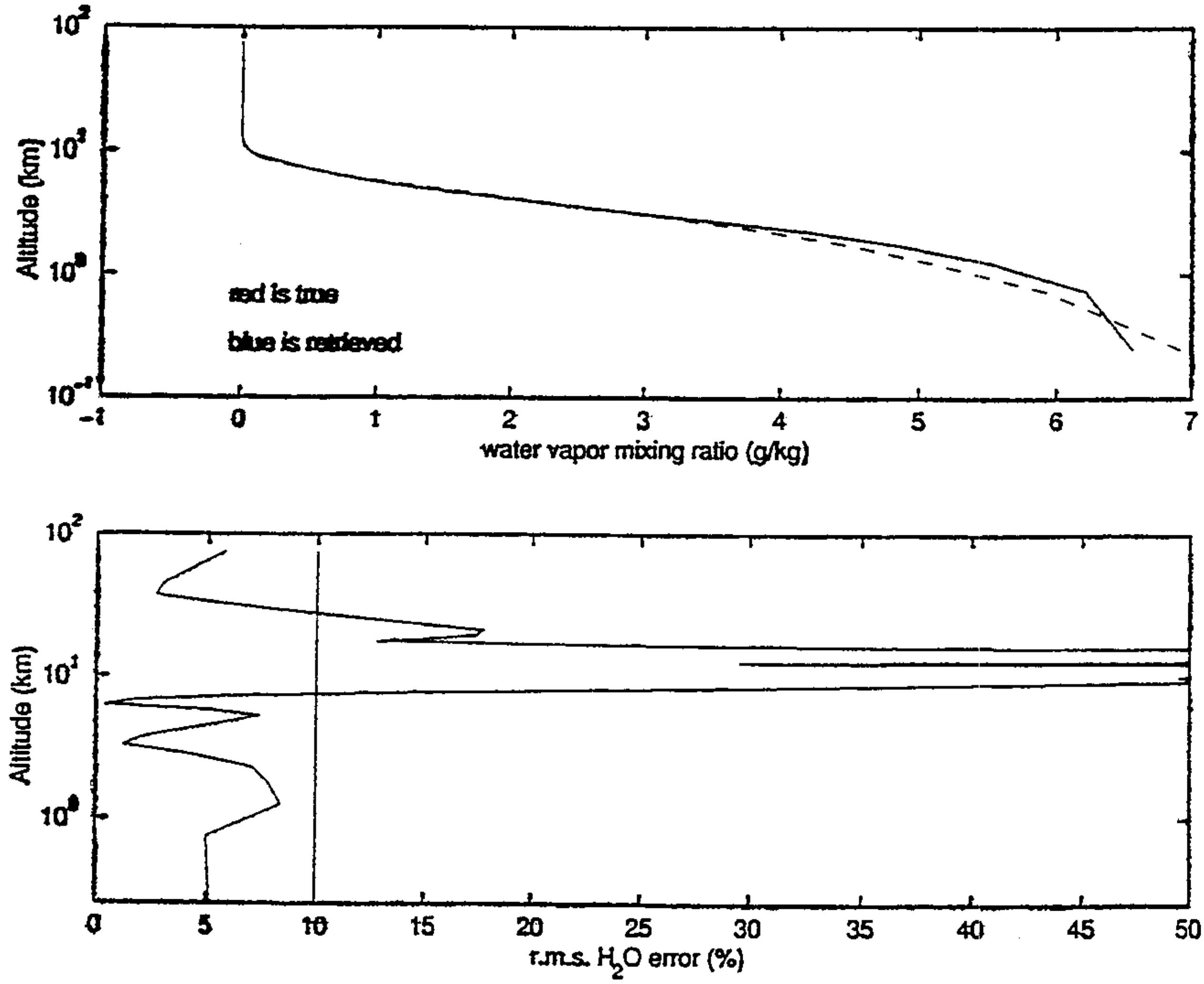
Simulated retrieval of T(z) for IASI





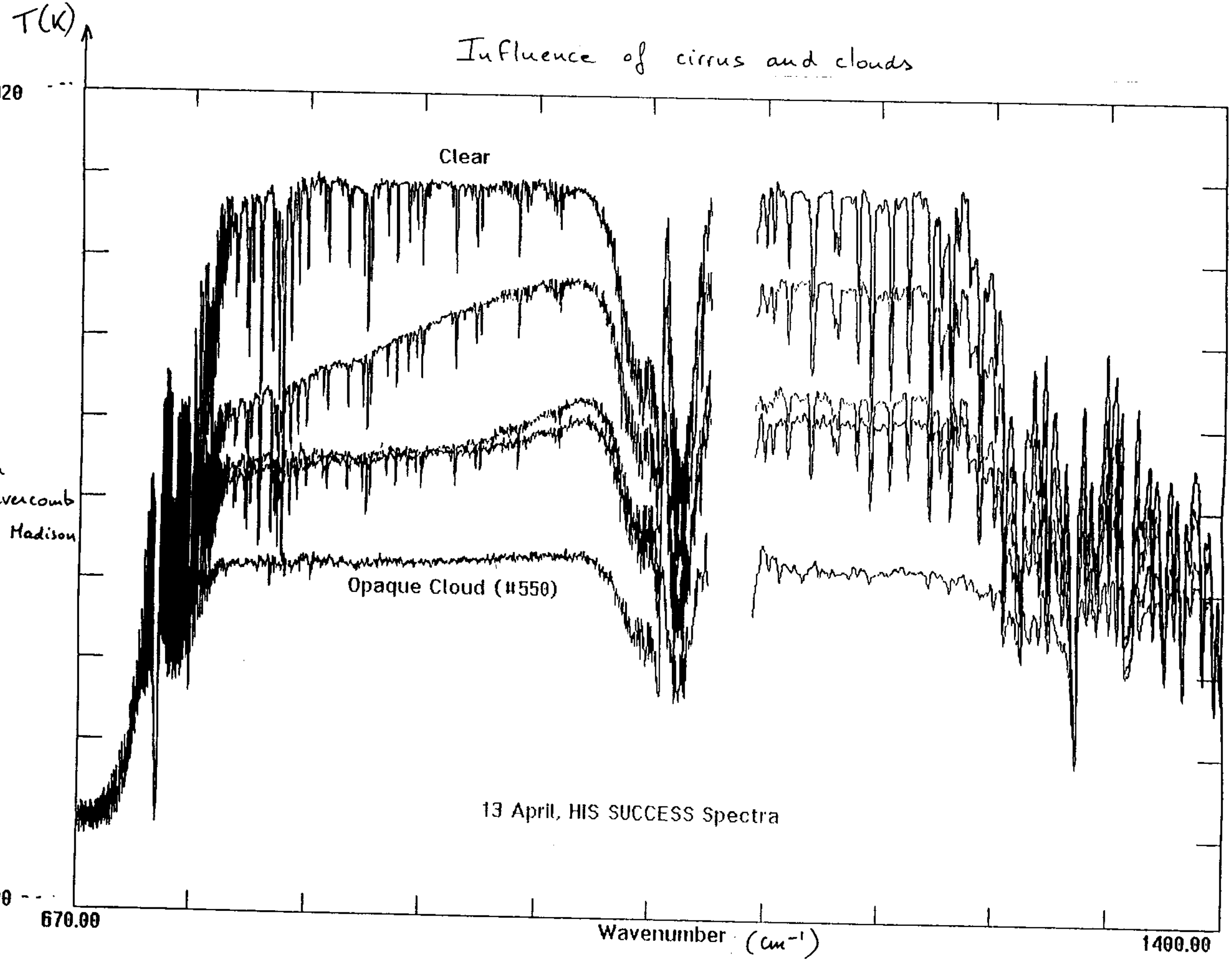
From C. Serio Univ. Basilicata

Simulated retrieval of $H_2O(z)$ for IASI



From C. Serio Univ. Basilicata

Influence of cirrus and clouds



From H. Revercomb Univ. Madison