→ ADVANCED ATMOSPHERIC TRAINING COURSE 2014

MID-IR Nadir/Limb Retrieval

Michael Höpfner

Karlsruhe Institute of Technology

IMK-ASF

27–31 October 2014 | Forschungszentrum Jülich | Germany

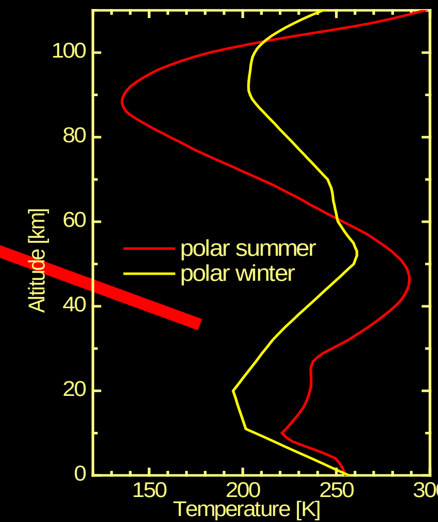
Thank’s to:

- André Butz
- Frank Hase
- Thomas v. Clarmann

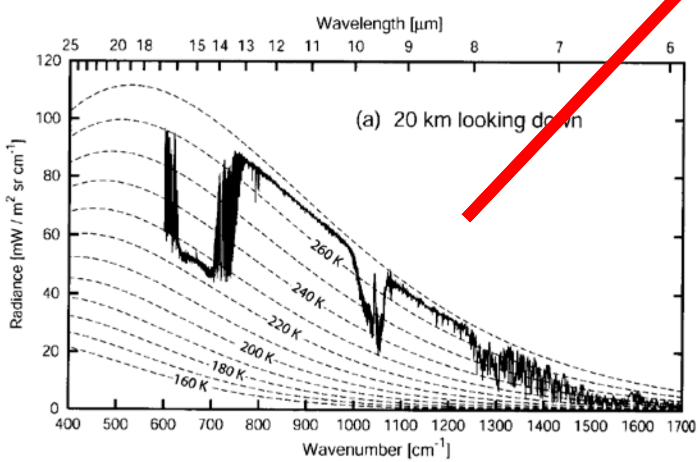
Inversion of remote sensing observations

Forward:

$$\hat{y} = \hat{F}(\hat{x})$$



Signal (e.g. nadir spectrum)



Radiative transfer

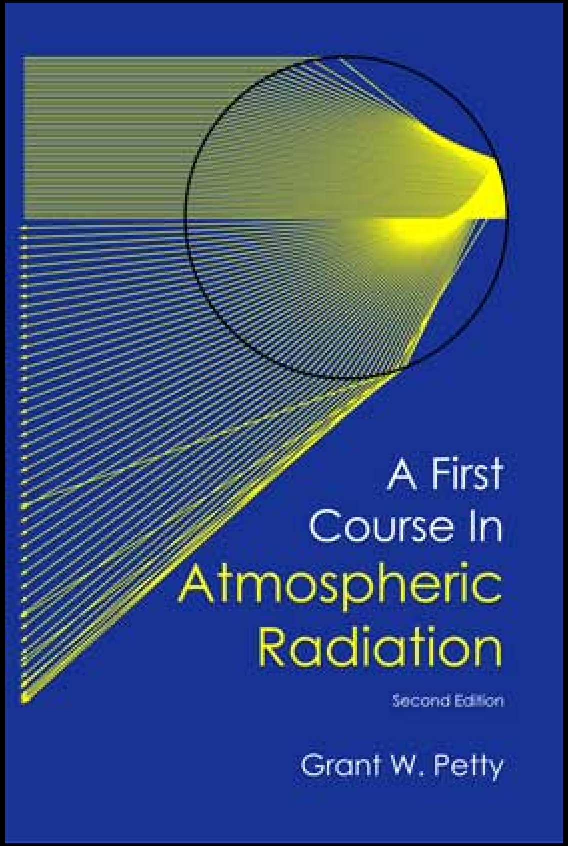
$$L_\lambda^{\uparrow}(\tau_\lambda,\mu,\varphi) = L_\lambda^{\uparrow}(\tau_{\lambda,Boden},\mu,\varphi)\, e^{-\frac{\tau_{\lambda,Boden}-\tau_\lambda}{\mu}} + \int_{\tau_\lambda}^{\tau_{\lambda,Boden}} J_\lambda(\tau'_\lambda,\mu,\varphi)\, e^{-\frac{\tau'_\lambda-\tau_\lambda}{\mu}} \frac{1}{\mu}\, d\tau'_\lambda$$

Inverse:

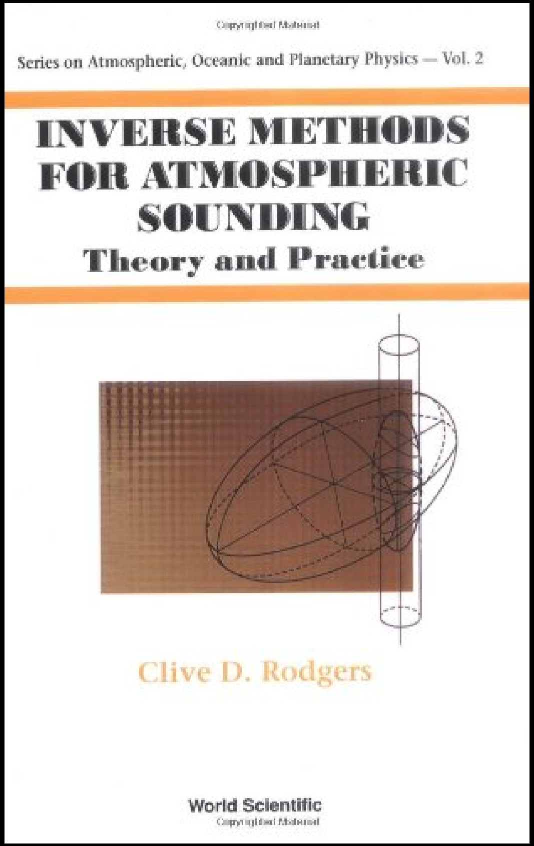
$$\hat{x} = \hat{F}^{-1}(\hat{y})$$

???

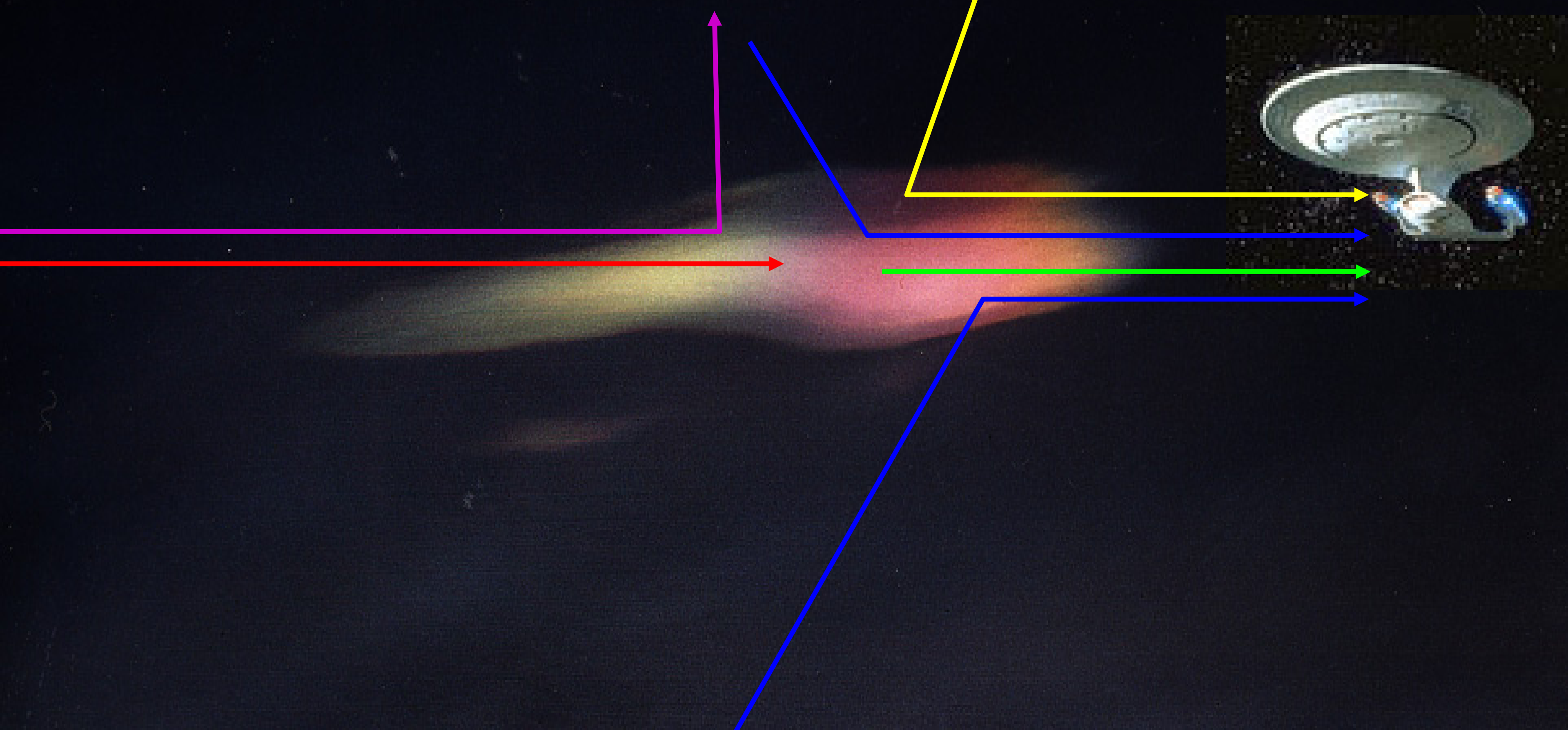
$$\hat{y} = \hat{F}(\hat{x})$$



$$\hat{x} = \hat{F}^{-1}(\hat{y})$$



$$
\begin{aligned}
dL_\lambda / ds = \; & - \beta_{a,\lambda} L_\lambda \; - \beta_{s,\lambda} L_\lambda \\
& + \beta_{a,\lambda} B_\lambda \\
& + \beta_{s,\lambda} (4\pi)^{-1} \int P(\boldsymbol{\Omega}', \boldsymbol{\Omega}) \, L_{diff}(\boldsymbol{\Omega}') \, d\boldsymbol{\Omega}' \\
& + \beta_{s,\lambda} (4\pi)\text{-}1 \; P(\boldsymbol{\Omega}, \boldsymbol{\Omega}_{sol}) \, F_{sol}
\end{aligned}
$$



Emission and Absorption

- **Only emission and absorption of radiation, no scattering**
  → most important for radiative transfer in MW and IR

- **Local thermodynamic equilibrium**
  → Planckfunction as source function
  → Kirchhoff's law: emission = absorption

$$dL_\lambda = L_\lambda(s+ds) - L_\lambda(s)$$
$$= dL_{\lambda,abs} + dL_{\lambda,emi}$$
$$= -\beta_{a,\lambda}(s) L_\lambda(s) ds + \beta_{a,\lambda}(s) B_\lambda(s) ds$$

Absorption coefficient: $\beta_{a,\lambda} = \sigma_{a,\lambda} N$

Absorption cross-section: $\sigma_{a,\lambda}$

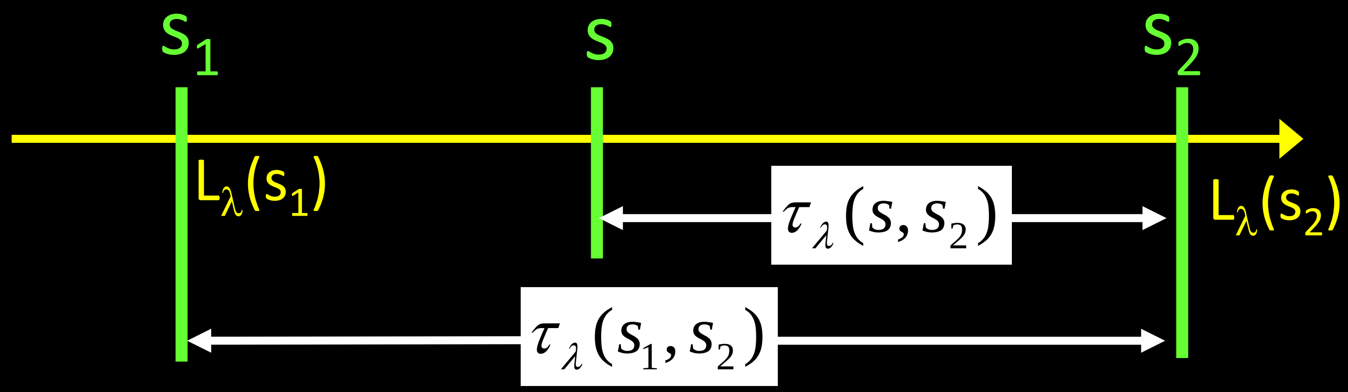
Number density: N

Planck function: $B_\lambda(s)$

Schwarzschild-equation:

$$\frac{dL_\lambda}{ds} = \beta_{a,\lambda}(s)\left(B_\lambda(s) - L_\lambda(s)\right)$$

Solution of Schwarzschild's equation



Optical depth:

$$\tau_\lambda(s_1, s_2) = \int_{s_1}^{s_2} \beta_{a,\lambda}(s)\,ds$$

$$L_\lambda(s_2) = L_\lambda(s_1)e^{-\tau_\lambda(s_1,s_2)} + \int_{s_1}^{s_2} \beta_{a,\lambda}(s)B_\lambda(s)e^{-\tau_\lambda(s,s_2)}\,ds$$

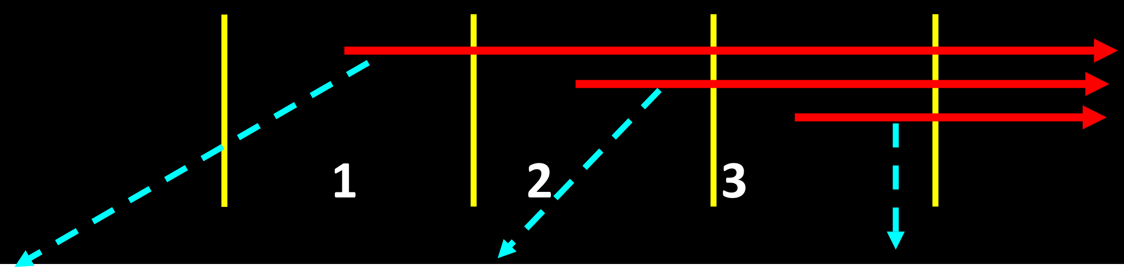
Emission of a layer with constant T

$$L_\lambda(s_2) = \int_0^{\tau_\lambda(s_1,s_2)} B_\lambda(s) e^{-\tau_\lambda(s,s_2)} d\tau_\lambda(s,s_2)$$

$$B_\lambda(s) = const = B_\lambda \longrightarrow$$

$$L_\lambda(s_2) = B_\lambda \int_0^{\tau_\lambda(s_1,s_2)} e^{-\tau_\lambda(s,s_2)} d\tau_\lambda(s,s_2) = B_\lambda(1-e^{-\tau_\lambda(s_1,s_2)}) = B_\lambda \underbrace{(1- \overbrace{t_\lambda(s_1,s_2)}^{\text{Transmission of the layer}})}_{\text{Emissivity of the layer}}$$

For three layers:



$$L_\lambda = B_{\lambda,1}(1-t_{\lambda,1})t_{\lambda,2}t_{\lambda,3} + B_{\lambda,2}(1-t_{\lambda,2})t_{\lambda,3} + B_{\lambda,3}(1-t_{\lambda,3})$$
$$= B_{\lambda,1}(t_{\lambda,2}t_{\lambda,3} - t_{\lambda,1}t_{\lambda,2}t_{\lambda,3}) + B_{\lambda,2}(t_{\lambda,3} - t_{\lambda,2}t_{\lambda,3}) + B_{\lambda,3}(1-t_{\lambda,3})$$

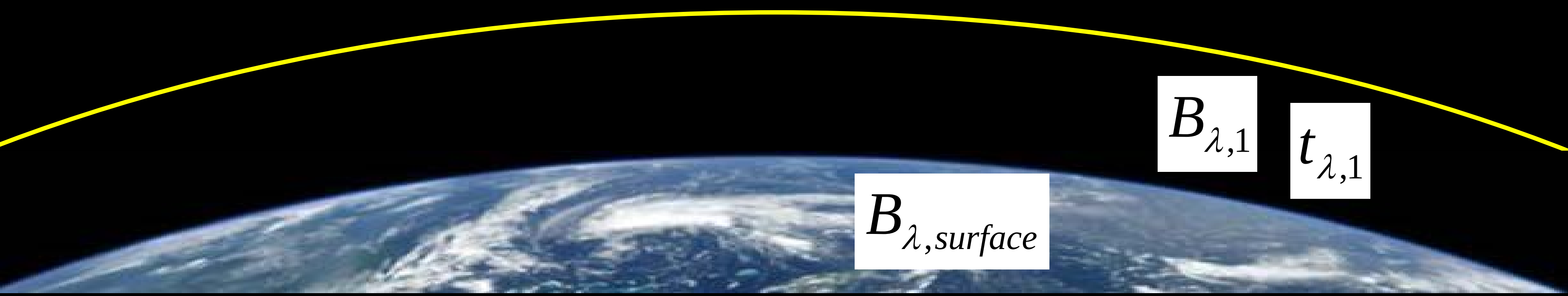
Thermal contrast in nadir sounding: the lowest layer

$$L_\lambda = B_{\lambda,surface} t_{\lambda,1} + B_{\lambda,1}(1 - t_{\lambda,1})$$

$B_{\lambda,surface} = B_{\lambda,1}$ → $L_\lambda = B_{\lambda,1}$

→ No information about transmission of lowest layer

$B_{\lambda,surface} \neq B_{\lambda,1}$ → $t_{\lambda,1} = \dfrac{L_\lambda - B_{\lambda,1}}{B_{\lambda,surface} - B_{\lambda,1}}$



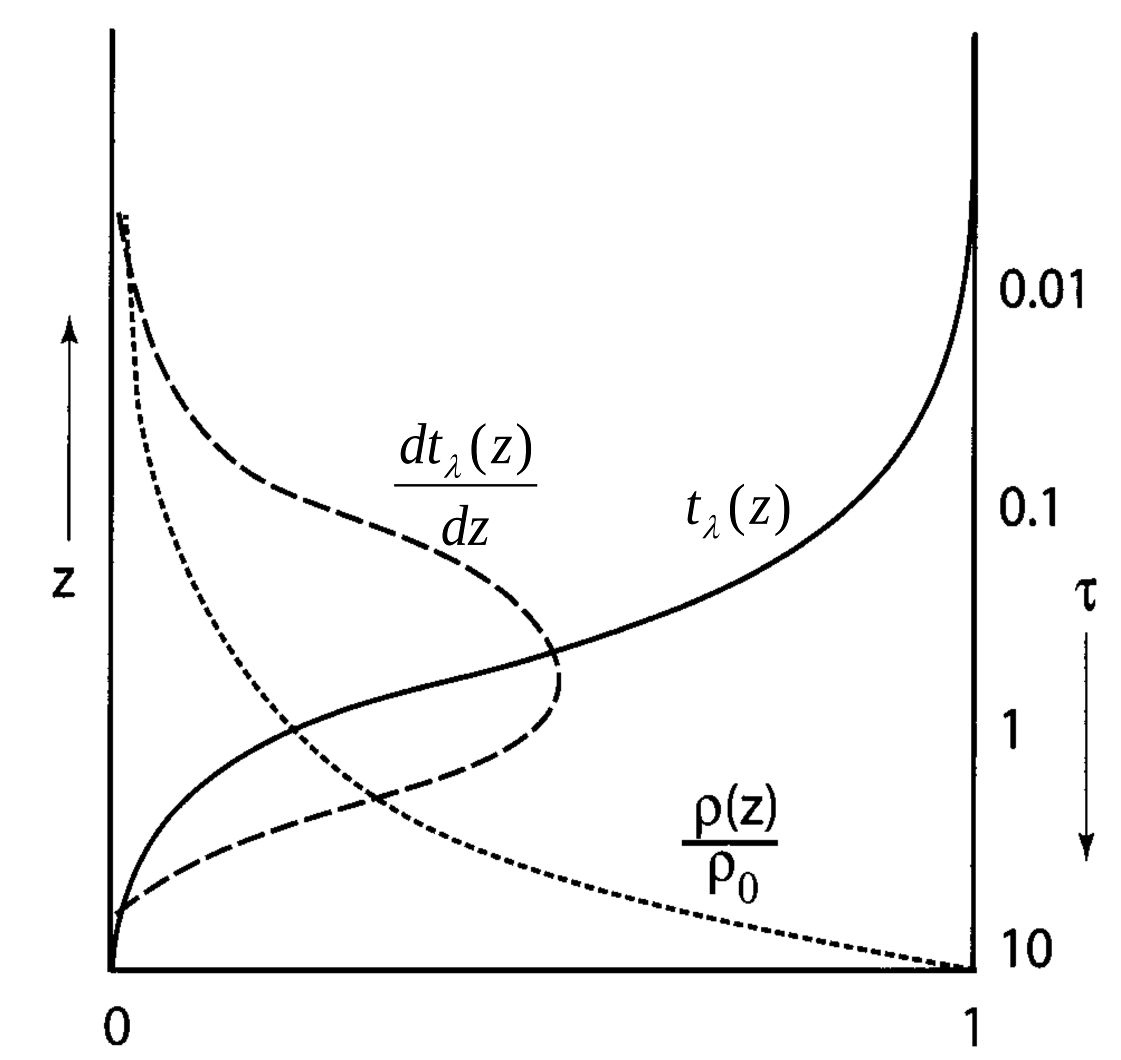
Schwarzschild's equation as function of transmission and weighting function

$$L_\lambda(s_2) = L_\lambda(s_1)e^{-\tau_\lambda(s_1,s_2)} + \int_{s_1}^{s_2} \beta_{a,\lambda}(s)B_\lambda(s)e^{-\tau_\lambda(s,s_2)}ds$$

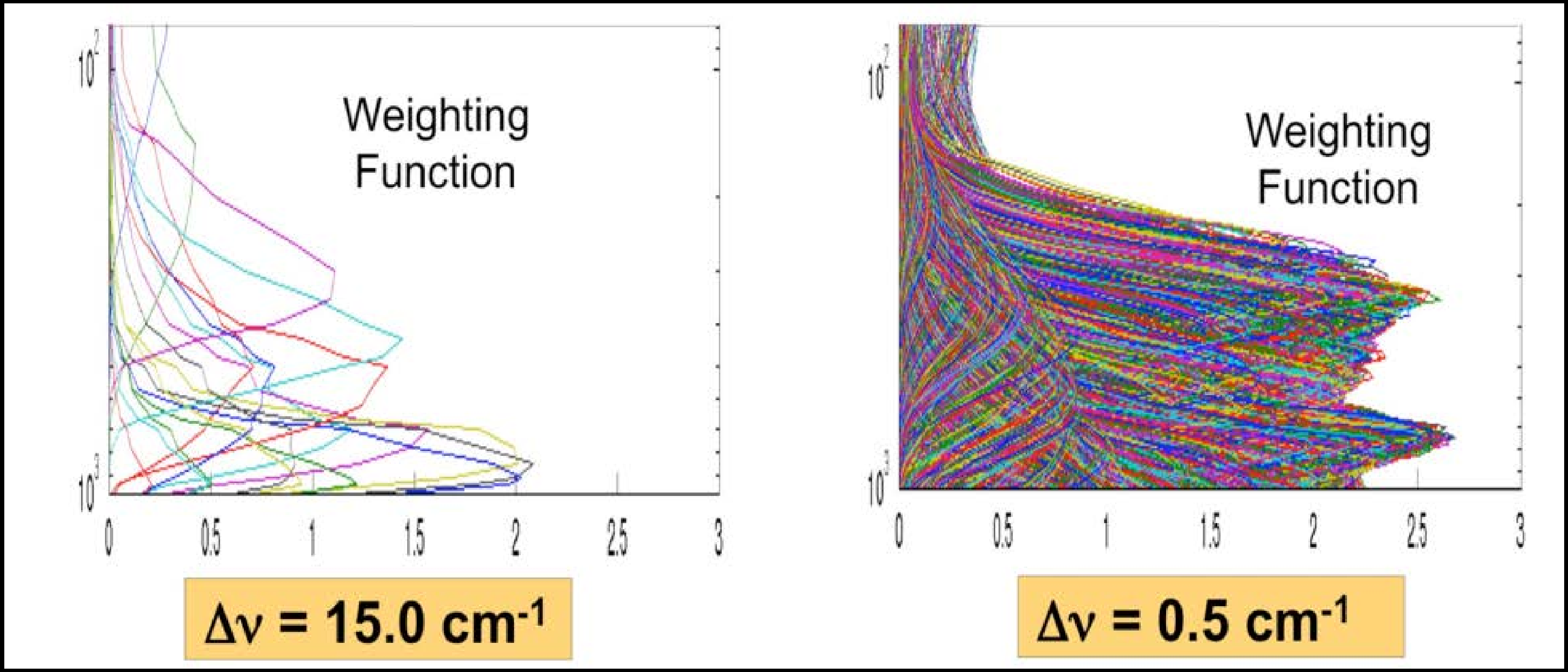
$$L_\lambda(s_2) = L_\lambda(s_1)t_\lambda(s_1,s_2) + \int_{s_1}^{s_2} B_\lambda(s)W_\lambda(s)ds$$

Transmission: $t_\lambda(s_1,s_2) = \exp[-\tau_\lambda(s_1,s_2)]$

Weighting function: $W_\lambda(s) = \frac{dt_\lambda(s,s_2)}{ds}$

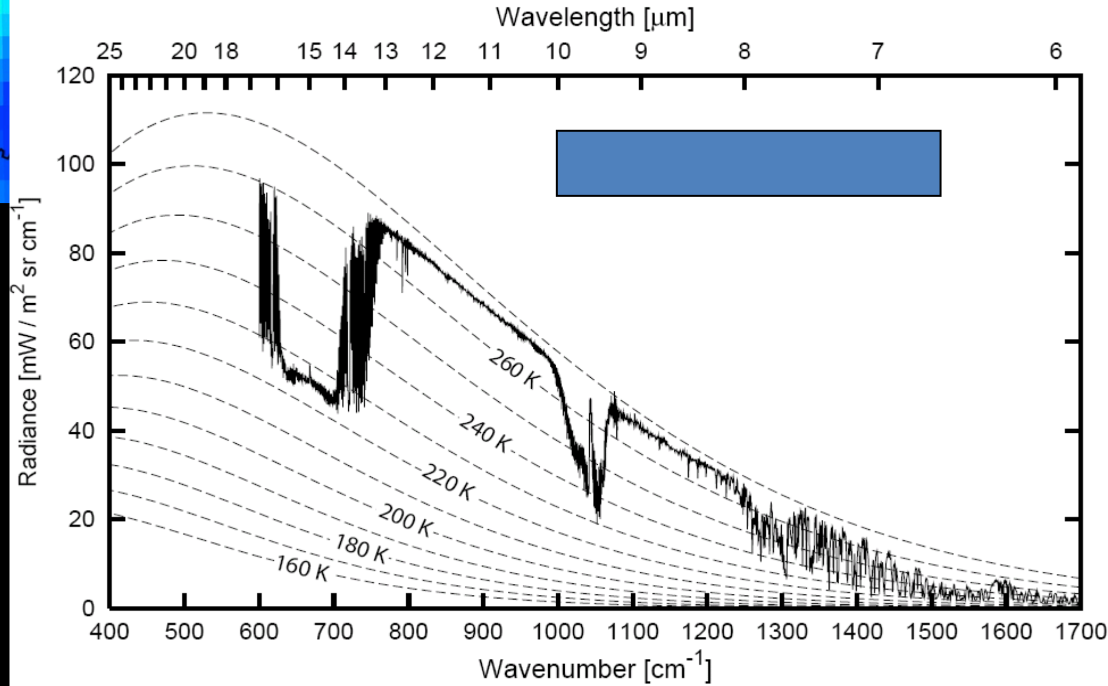

z
$\frac{dt_\lambda(z)}{dz}$
$t_\lambda(z)$
$\frac{\rho(z)}{\rho_0}$
0.01
0.1
τ
1
10
0
1

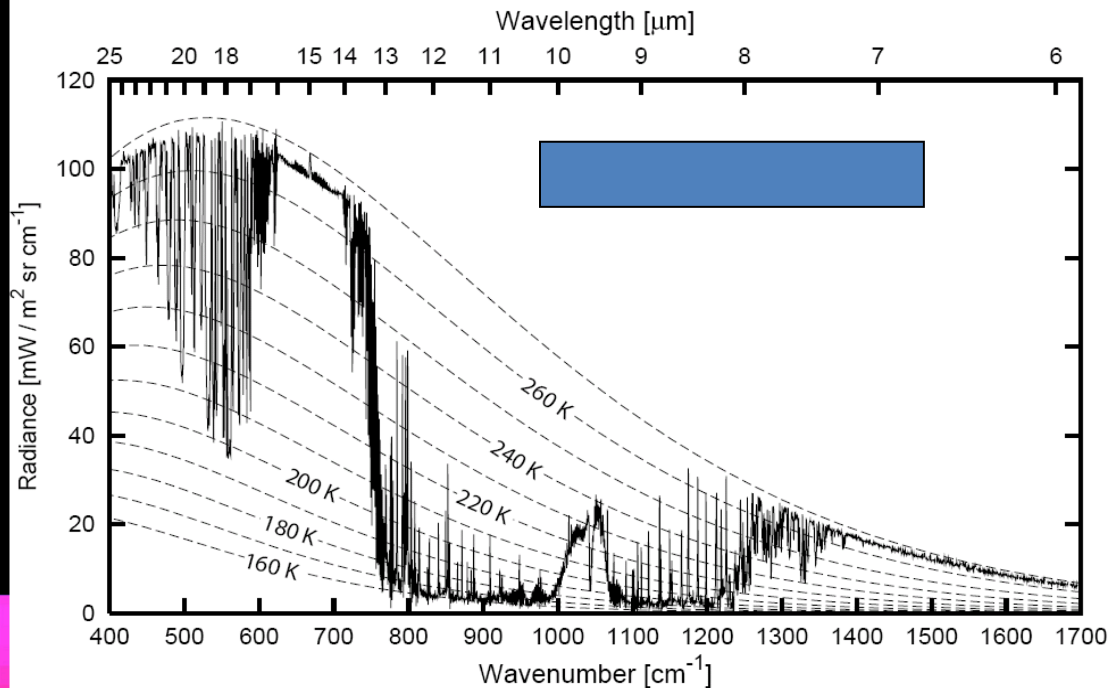
Nadir sounding weighting functions



Smith et al., 2009

Looking up or down?





Looking up: where?

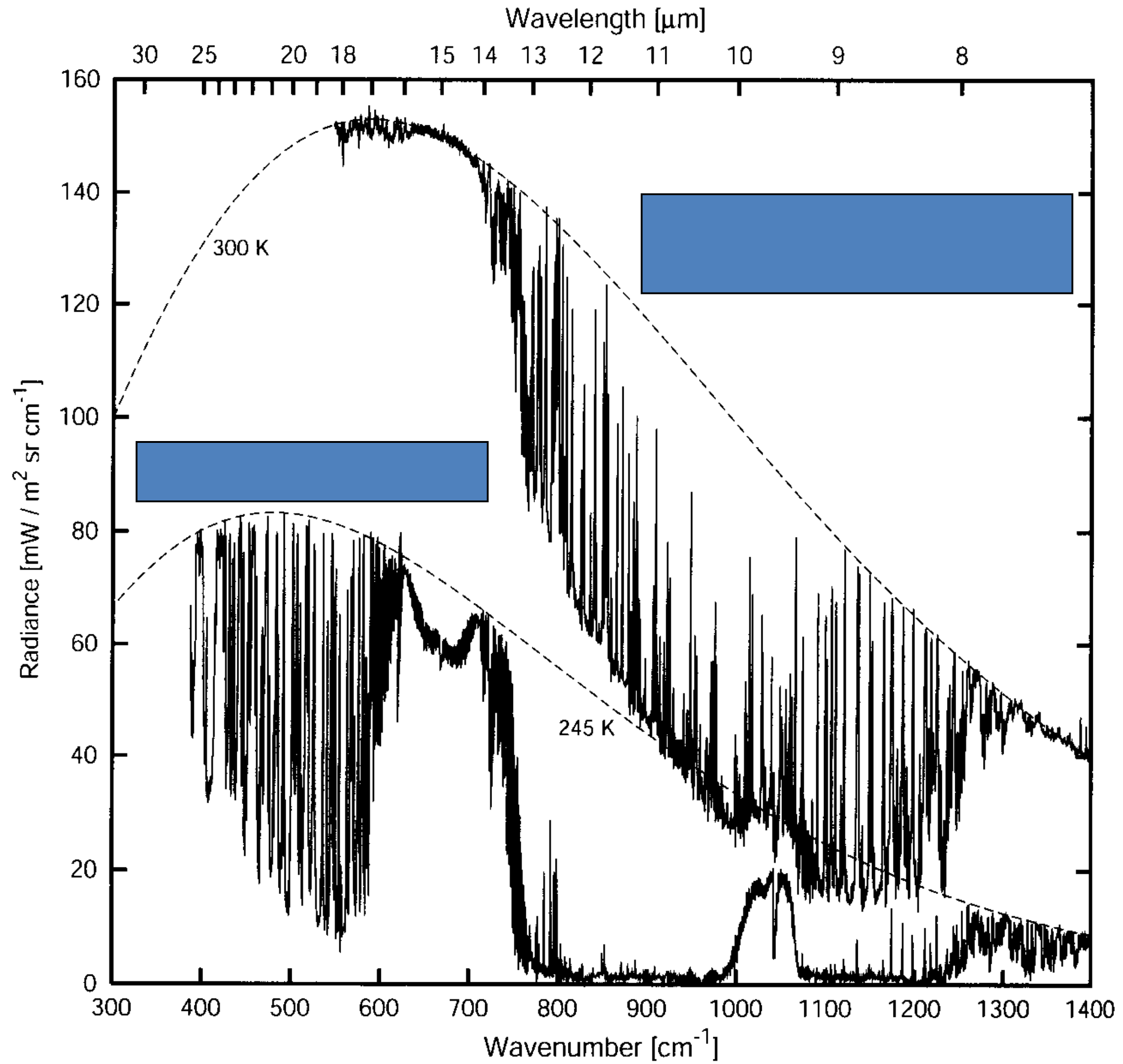
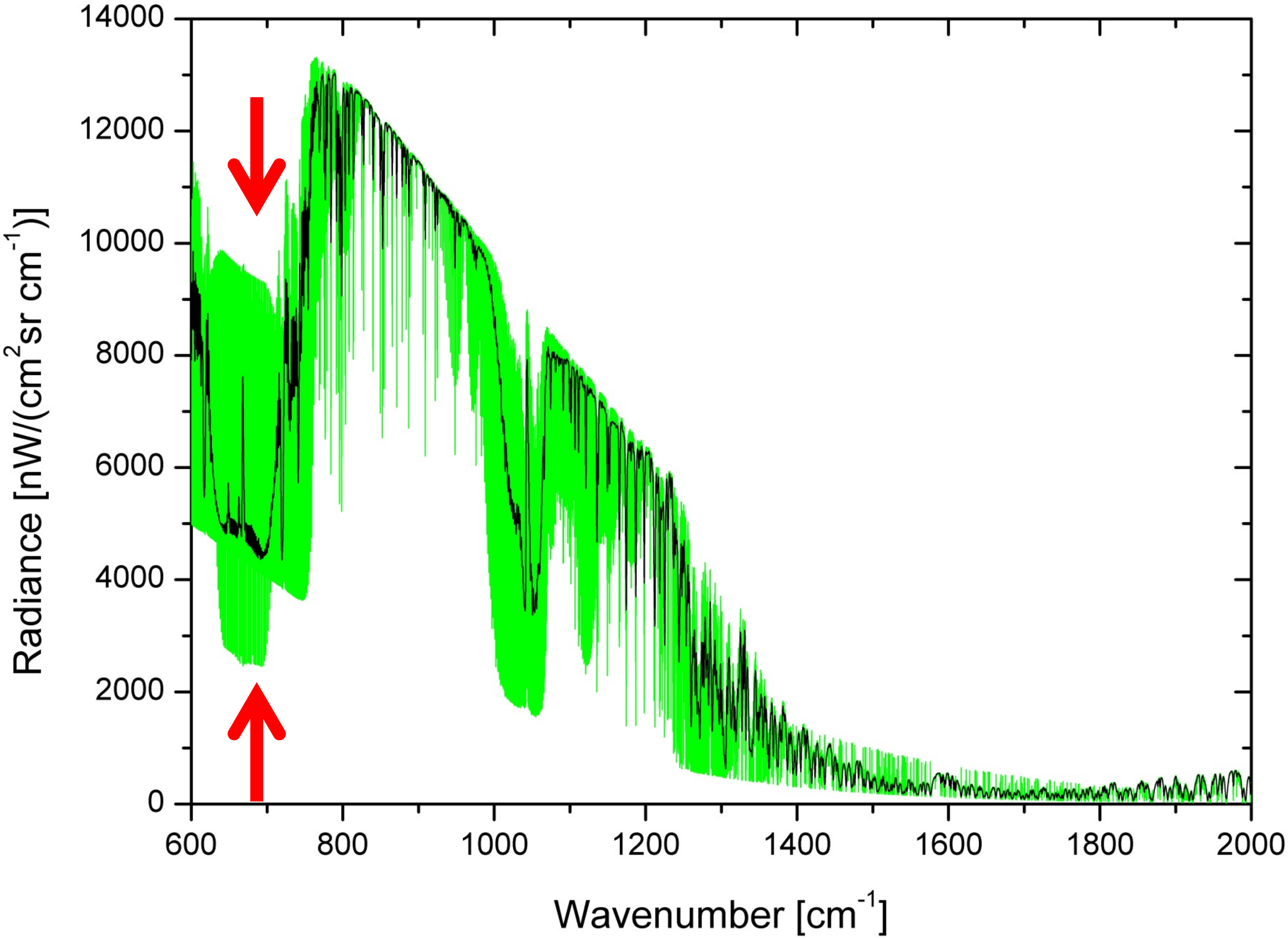
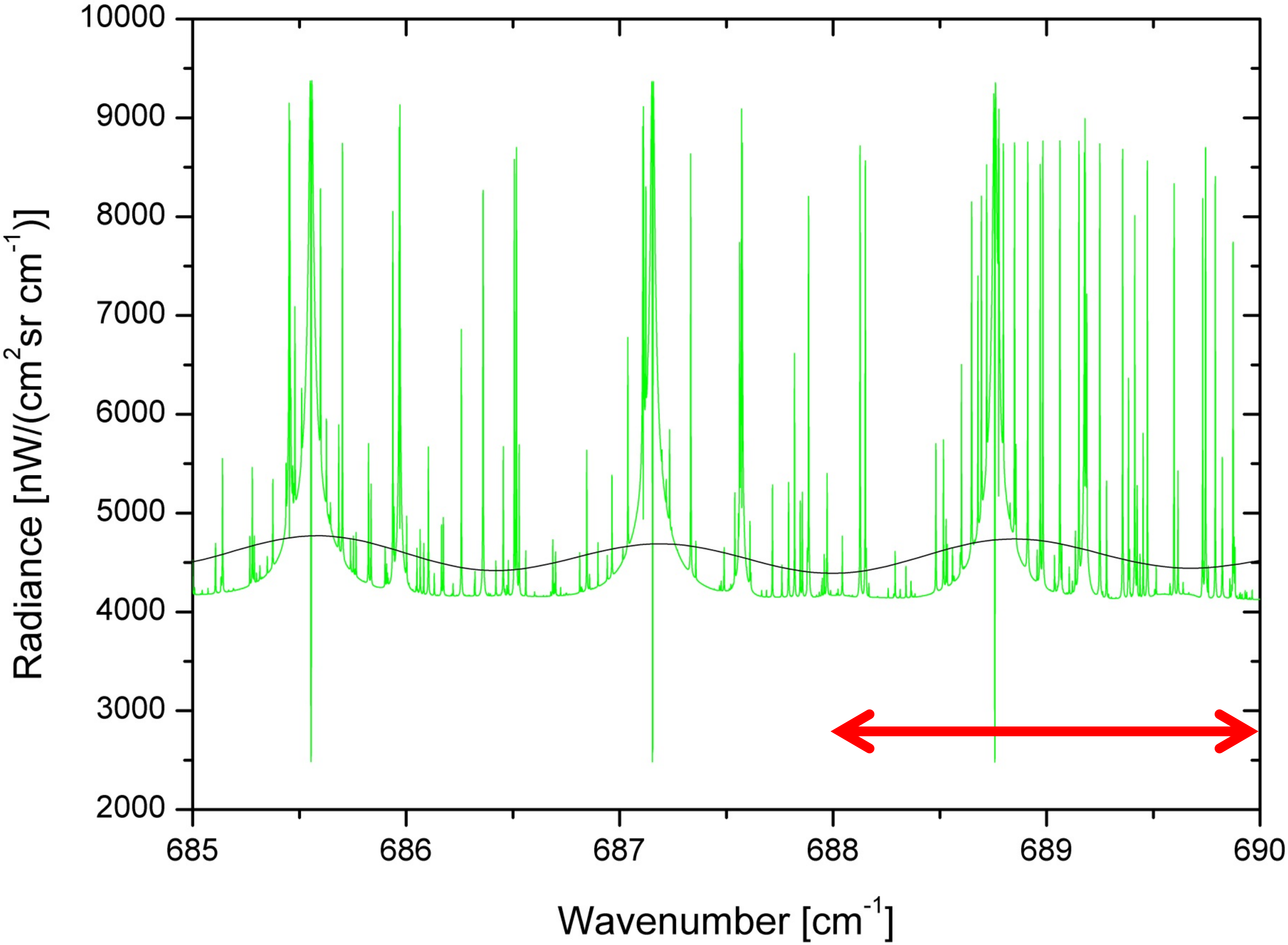


Fig. 8.1: Two examples of measured atmospheric emission spectra as seen from ground level looking up. Planck function curves corresponding to the approximate surface temperature in each case are superimposed (dashed lines). *(Data courtesy of Robert Knuteson, Space Science and Engineering Center, University of Wisconsin-Madison.)*

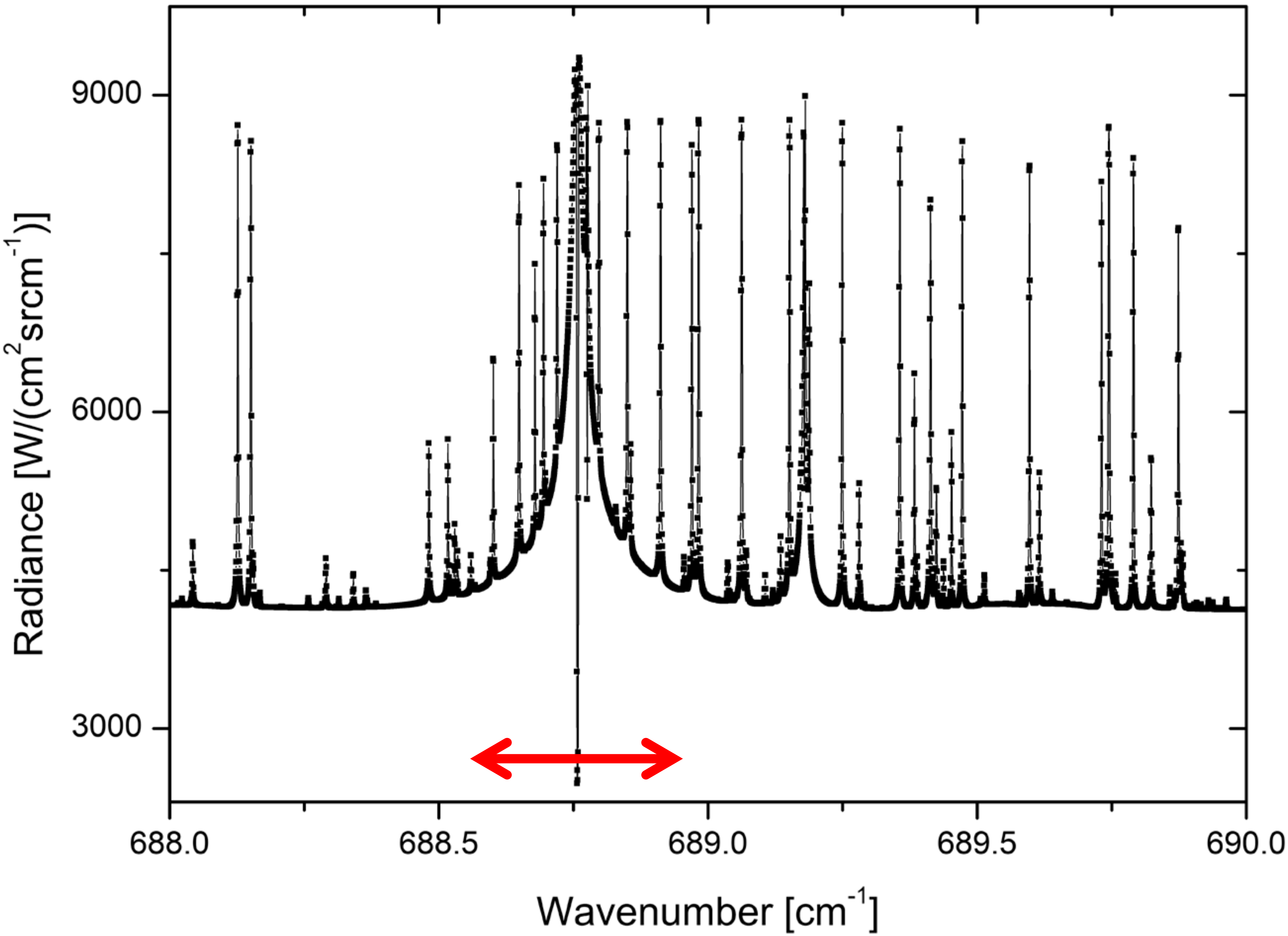
Petty216

‘IASI’ and ‘monochromatic’ spectrum

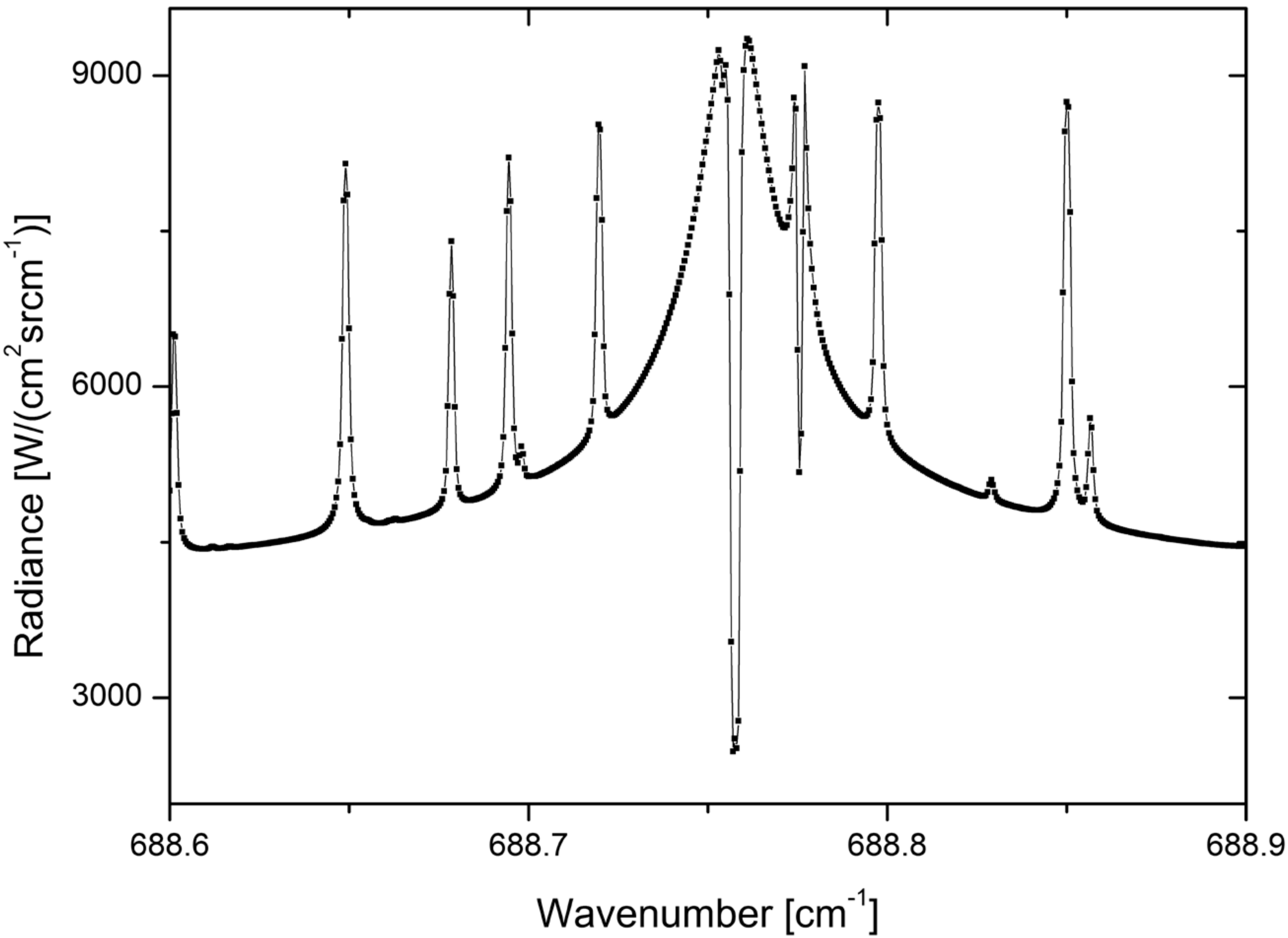




Radiance [nW/(cm²sr cm⁻¹)]
10000
9000
8000
7000
6000
5000
4000
3000
2000
685
686
687
688
689
690
Wavenumber [cm⁻¹]

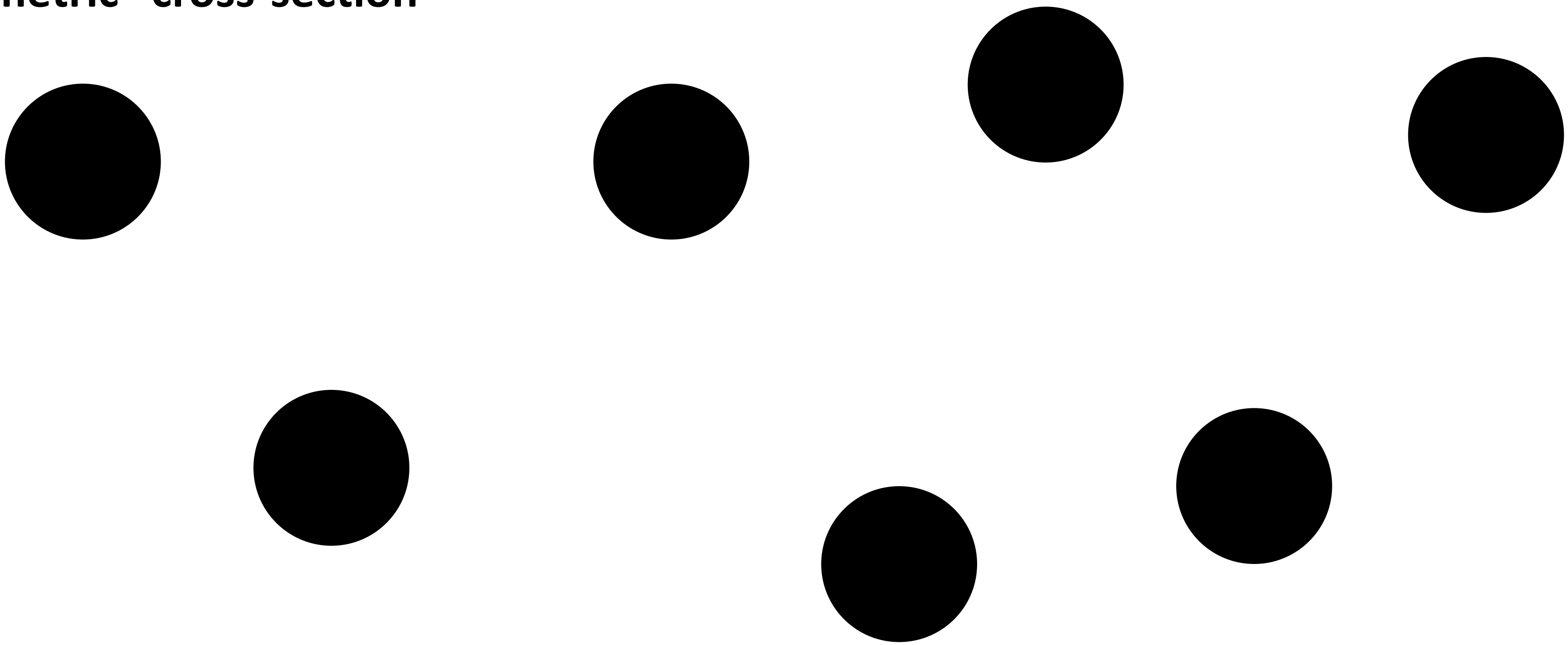


9000
6000
3000
688.0
688.5
689.0
689.5
690.0
Radiance [W/(cm²srcm⁻¹)]
Wavenumber [cm⁻¹]



9000
6000
3000
688.6
688.7
688.8
688.9
Radiance [W/(cm2srcm-1)]
Wavenumber [cm-1]

“Geometric” cross-section

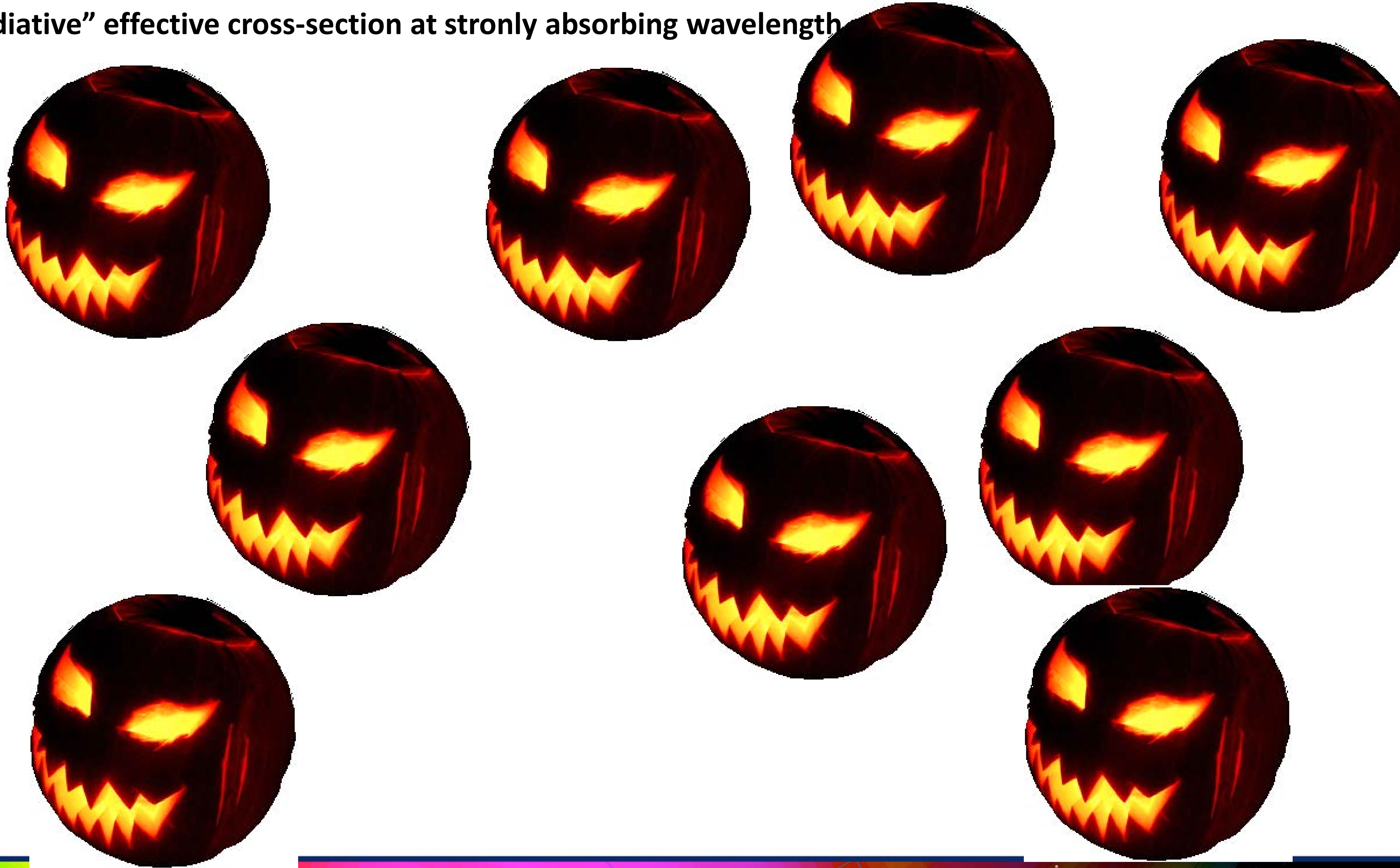


Absorption coefficient: $\beta_{a,\lambda} = \sigma_{a,\lambda} N$

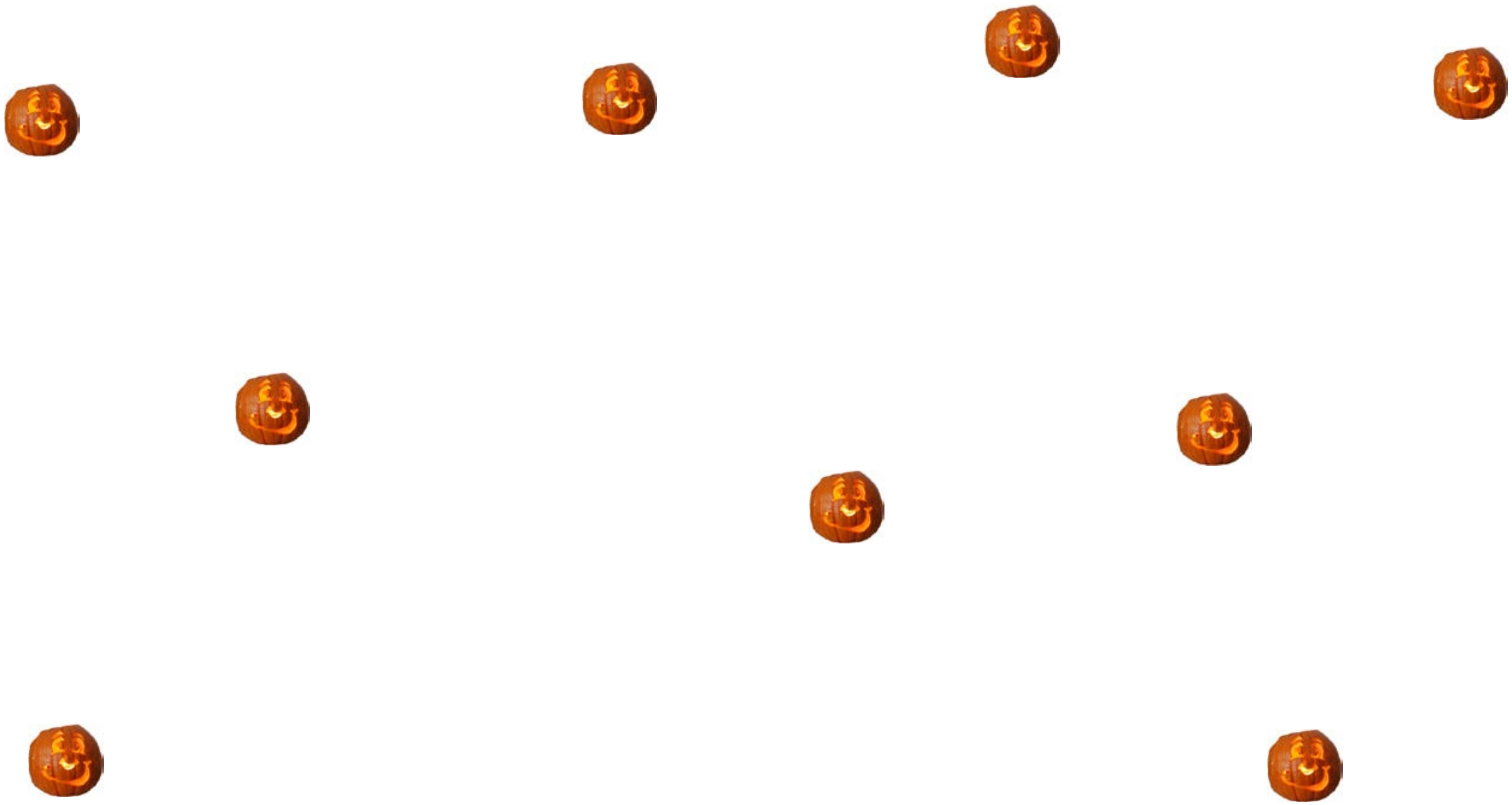
Absorption cross-section: $\sigma_{a,\lambda}$

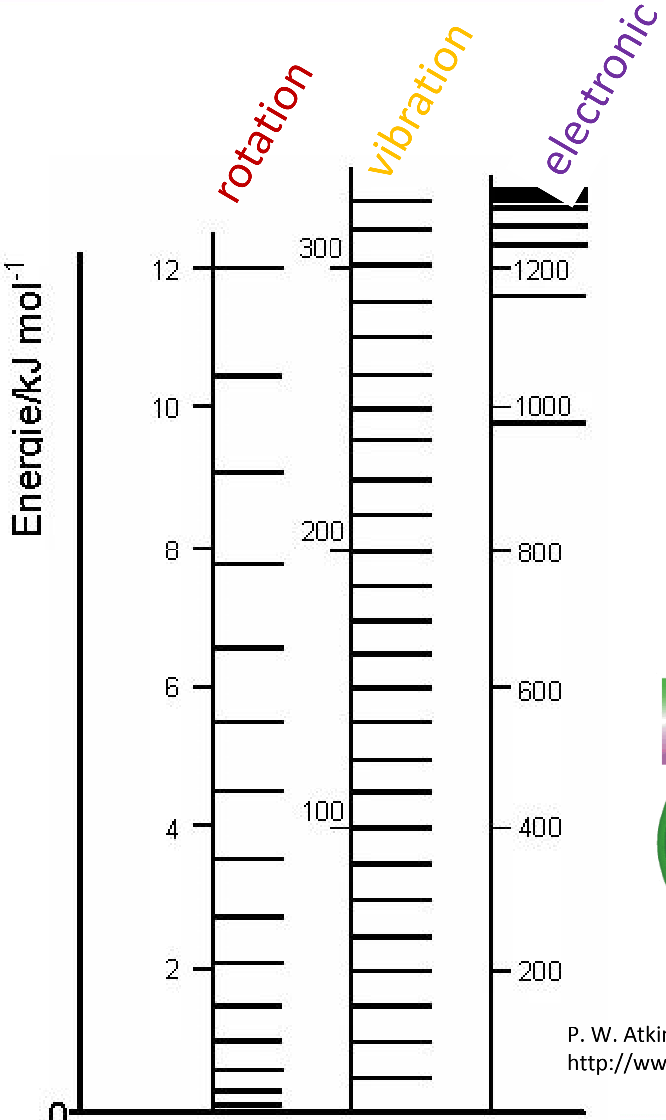
Number density: N

“Radiative” effective cross-section at stronly absorbing wavelength

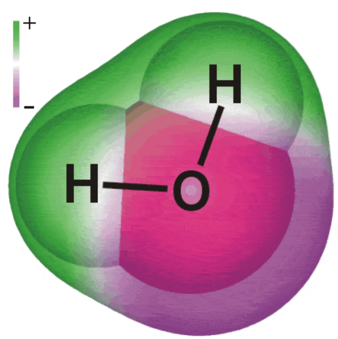


“Radiative” effective cross-section at weakly absorbing wavelength

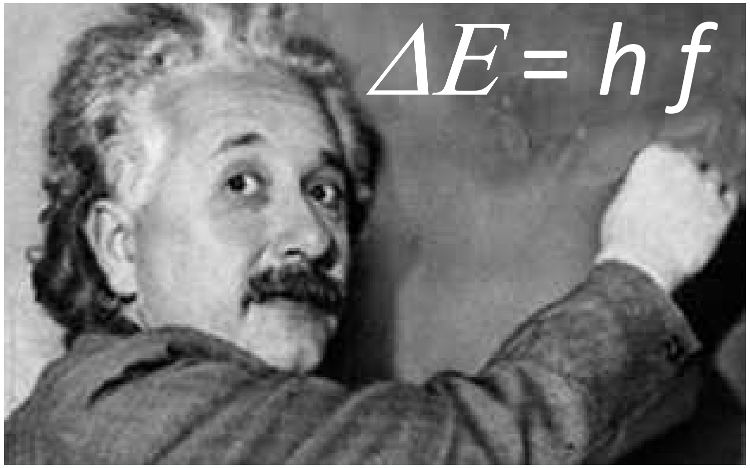




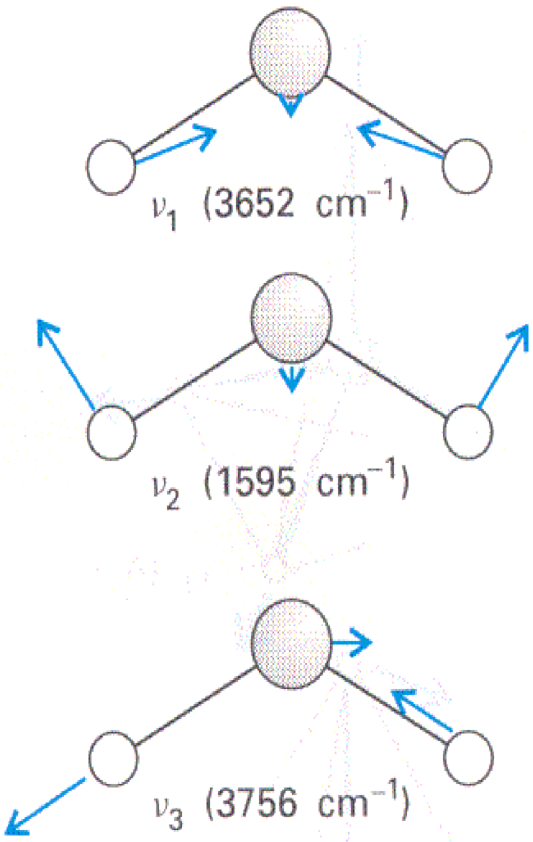
- Quantum mechanics: a bound microscopic system can only be in distinct rotational/vibrational/electronic states.
- Transfer from one to the other state can occur through emission/absorption of electromagnetic radiation (photon)
- Microwave: rotation of a molecule with static dipole moment
- IR: vibration of a molecule; changing dipole moment
- UV-VIS: electronic transitions



P. W. Atkins, Physikalische Chemie, 1996
http://www.polymere.uni-koeln.de/11572.html



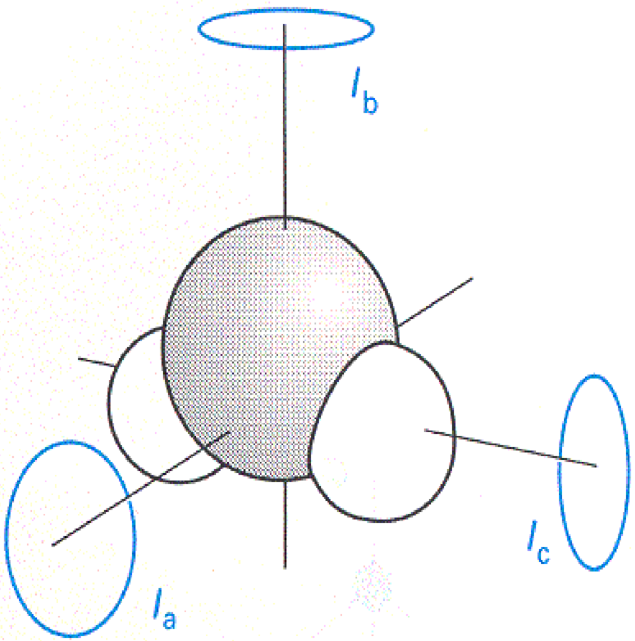
Beispiel: Schwingung und Rotation des H_2O-Moleküls



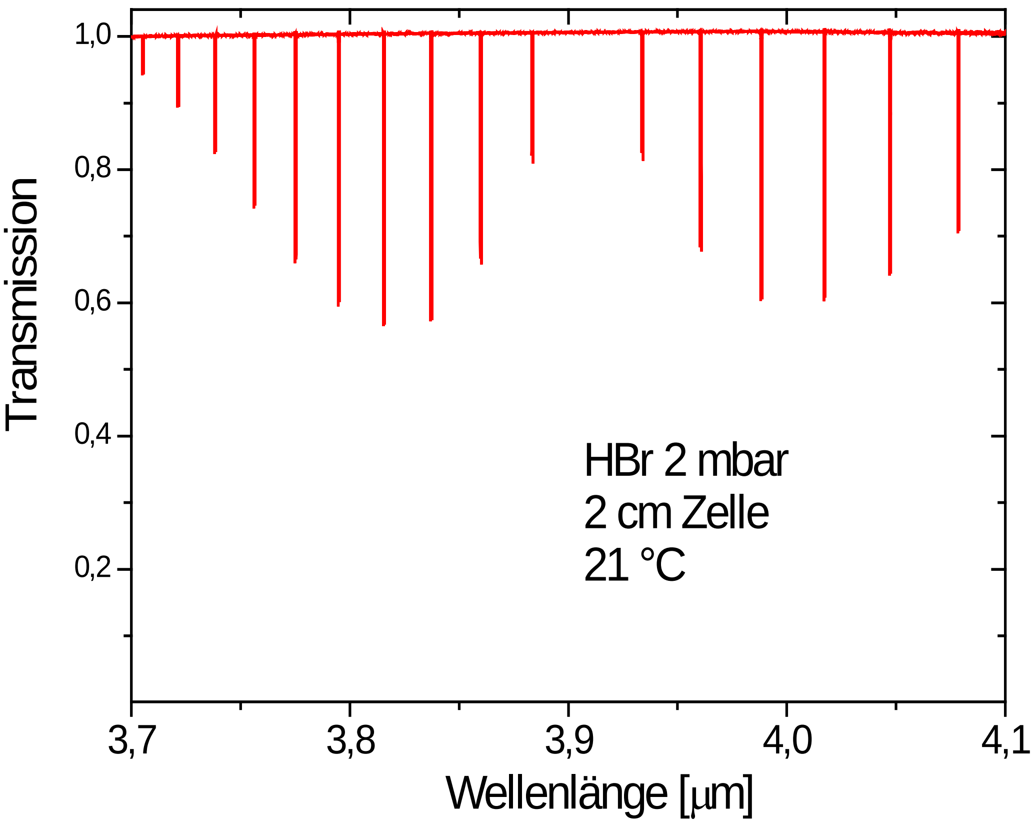
2.74 µm

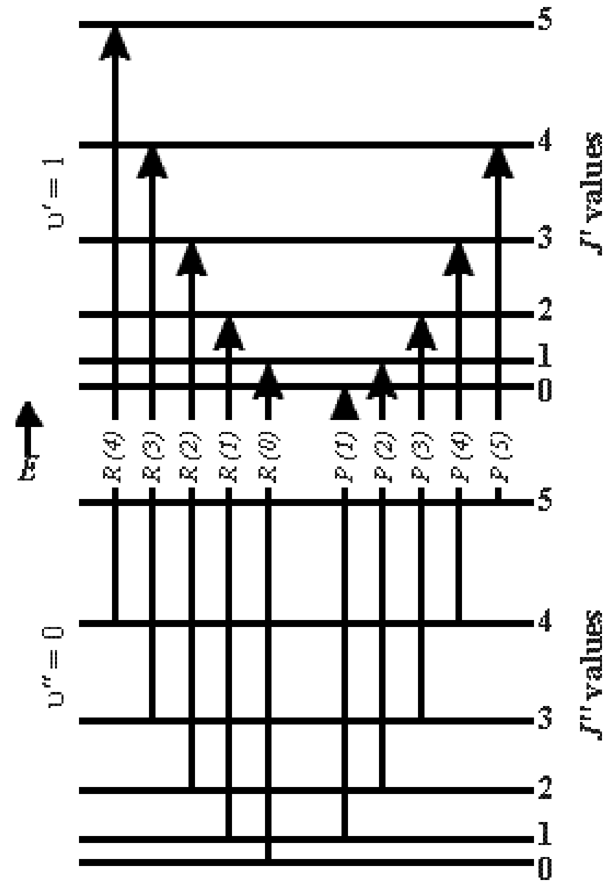
6.27 µm

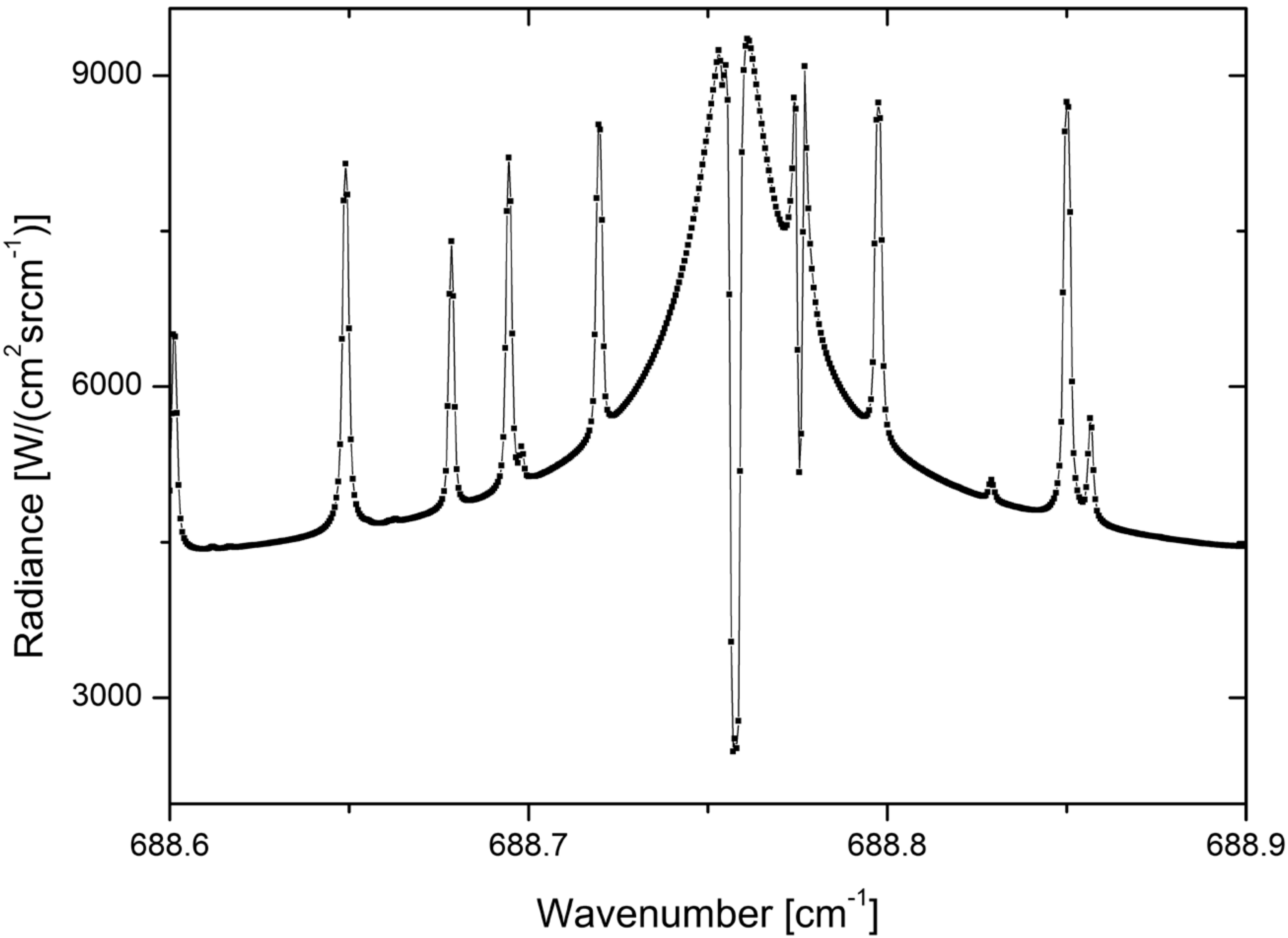
2.66 µm



Ro-vibrational transition in the mid-IR







9000
6000
3000
688.6
688.7
688.8
688.9
Radiance [W/(cm2srcm-1)]
Wavenumber [cm-1]

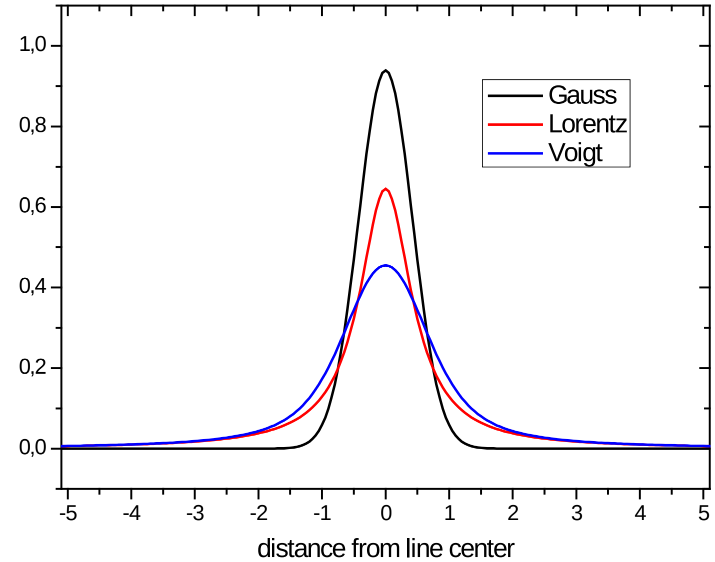
The finite width of spectral lines

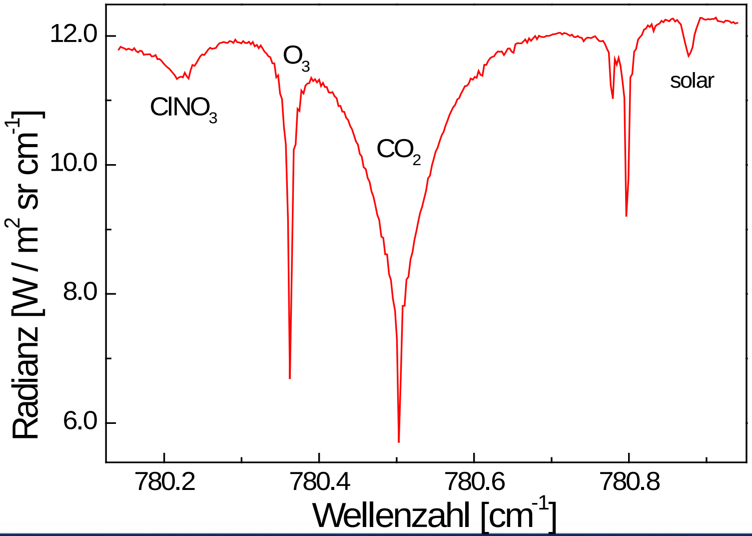
Doppler-broadening:

- Thermal movement of molecules along the line-of-sight
- Gaussian shape
- ~0.001 cm^{-1} @ 1000 cm^{-1}
- Proportional to the frequency

Pressure-broadening:

- Collisions with other molecules disturb their oscillation
- Transition frequency becomes ‘blurred’
- Lorentz shape
- ~0.05 cm^{-1} @ 1000 hPa
- Proportional to the collision rate (pressure)





http://www.cfa.harvard.edu/hitran/

Variable	Definition	Units	Comments
Mol	Molecule number	Unitless	Chronological assignment
I_a	Isotopologue number	Unitless	Ordering based on terrestrial values of atoms given in Ref. [389]
ν	Transition wavenumber	cm^{-1}	Line position in vacuum
S	Intensity	$cm^{-1}/(molecule\,cm^{-2})$	At 296 K
A	Einstein *A*-coefficient	s^{-1}	See Ref. [387]
γ_{air}	Air-broadened half-width	$cm^{-1}\,atm^{-1}$	HWHM at 296 K
γ_{self}	Self-broadened half-width	$cm^{-1}\,atm^{-1}$	HWHM at 296 K
E''	Lower-state energy	cm^{-1}	Referenced to zero for lowest possible level
n_{air}	Temperature-dependence exponent of γ_{air}	Unitless	
δ_{air}	Air pressure-induced shift	$cm^{-1}\,atm^{-1}$	At 296 K
v', v''	Upper- and lower-state "global" quanta	Unitless	See Table 3 of Ref. [1]
q', q''	Upper- and lower-state "local" quanta	Unitless	See Table 4 of Ref. [1]
ierr	Uncertainty indices	Unitless	See Table 5 of Ref. [1]
iref	Reference indices	Unitless	Pointers to sources in *HITRAN*
g', g''	Upper- and lower-state statistical weights	Unitless	Includes state-independent factors in *HITRAN*, see Ref. [387]
Other properties or constants			
Q	Partition sum	Unitless	Function of temperature
h	Planck constant	erg s	$6.62606896(33) \times 10^{-27}$
c	Speed of light	$cm\,s^{-1}$	$2.99792458 \times 10^{10}$
k_B	Boltzmann constant	$erg\,K^{-1}$	$1.3806504(24) \times 10^{-16}$
T	Temperature	K	

Discretisation and measurement error

$$\hat{y} = \hat{F}(\hat{x})$$

$$\vec{y} = \vec{F}(\vec{x}) + \vec{\varepsilon}$$

Error (spectral noise)

Measurement vector (spectral channels)

Vector with altitude profiles (*n* points)

Radiative transfer model

Linearisation

$$\vec{y} = \vec{F}(\vec{x}) + \vec{\varepsilon}$$

$$\vec{y} = \vec{F}(\vec{x}_0) + \left.\frac{\partial \vec{F}(\vec{x})}{\partial \vec{x}}\right|_{\vec{x}_0} (\vec{x} - \vec{x}_0) + \vec{\varepsilon} = \vec{F}(\vec{x}_0) + \mathbf{K}(\vec{x} - \vec{x}_0) + \vec{\varepsilon}$$

First guess

Jacobi-Matrix (~weighting functions)

$$\mathbf{K} = \begin{pmatrix} \frac{\partial F_1}{\partial x_1} & . & . & . & \frac{\partial F_1}{\partial x_n} \\ . & . & & & . \\ . & & . & & . \\ . & & & . & . \\ \frac{\partial F_m}{\partial x_1} & . & . & . & \frac{\partial F_m}{\partial x_n} \end{pmatrix}$$

Case 1: m = n = 1

$$\vec{y} = \vec{F}(\vec{x}_0) + \mathbf{K}(\vec{x} - \vec{x}_0) + \vec{\varepsilon}$$

$$y = f(x_0) + \left.\frac{df(x)}{dx}\right|_{x_0} (x - x_0) + \varepsilon$$

Newton-Iteration:

$$x_{i+1} = x_i + \frac{1}{\left.\frac{df(x)}{dx}\right|_{x_i}} (y - f(x_i))$$

Error estimation:

$$\sigma_x{}^2 = \frac{1}{\left(\frac{df}{dx}\right)^2} \sigma_y{}^2$$

Case 2: m =2 n = 1

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \underbrace{\begin{pmatrix} \left.\frac{dF_1(x)}{dx}\right|_{x_0} \\ \left.\frac{dF_2(x)}{dx}\right|_{x_0} \end{pmatrix}}_{\mathbf{K}} (x - x_0) + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \end{pmatrix}$$

K is vector and cannot be inverted

Way 1:

1. Calculate *x* separately for each *y* as in example 1
2. Calculate error for each x_i as in example 1 $\qquad \sigma_{x_1}, \sigma_{x_2}$
3. Calculate the result *x* as weighted mean
4. And the error of *x* as:

$$x = \frac{\frac{x_1}{\sigma_{x_1}^{\;2}} + \frac{x_2}{\sigma_{x_2}^{\;2}}}{\frac{1}{\sigma_{x_1}^{\;2}} + \frac{1}{\sigma_{x_2}^{\;2}}}$$

$$\sigma_x^{\;2} = \left(\frac{1}{\sigma_{x_1}^{\;2}} + \frac{1}{\sigma_{x_2}^{\;2}} \right)^{-1}$$

Way2:

Case 2: m =2 n = 1

Least-squares inversion

Minimise the weighted quadratic differences:

$$\left[\vec{y}-\vec{F}(x)\right]^T S_y^{-1}\left[\vec{y}-\vec{F}(x)\right]=\left[\vec{y}-\left(\vec{F}(x_0)+\mathbf{K}(x-x_0)\right)\right]^T S_y^{-1}\left[\vec{y}-\left(\vec{F}(x_0)+\mathbf{K}(x-x_0)\right)\right]$$

Covariance matrix of observations:

$$\mathbf{S}_y=\begin{pmatrix}\sigma_{y_1}^{\ 2} & 0\\ 0 & \sigma_{y_2}^{\ 2}\end{pmatrix}$$

Result of minimisation

$$x=x_0+\frac{1}{\frac{F_1'(x_0)^2}{\sigma_{y_1}^{\ 2}}+\frac{F_2'(x_0)^2}{\sigma_{y_2}^{\ 2}}}\left(\frac{F_1'(x_0)}{\sigma_{y_1}^{\ 2}}\left(y_1-F_1(x_0)\right)+\frac{F_2'(x_0)}{\sigma_{y_2}^{\ 2}}\left(y_2-F_2(x_0)\right)\right)$$

Same result as in way 1

Case 2: m =2 n = 1

$$x = x_0 + \frac{1}{\frac{F_1'(x_0)^2}{\sigma_{y_1}^{\;2}} + \frac{F_2'(x_0)^2}{\sigma_{y_2}^{\;2}}} \left(\frac{F_1'(x_0)}{\sigma_{y_1}^{\;2}} \left(y_1 - F_1(x_0)\right) + \frac{F_2'(x_0)}{\sigma_{y_2}^{\;2}} \left(y_2 - F_2(x_0)\right) \right)$$

For non-linear problems this can be written as iteration:

$$x_{i+1} = x_i + \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}\right)^{-1} \mathbf{K}^T \mathbf{S}_y^{-1} \left(\vec{y} - \vec{F}(x_i)\right)$$

Variance

$$\sigma_x^{\;2} = \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}\right)^{-1}$$

General case for m,n

$$\vec{x}_{i+1} = \vec{x}_i + \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}\right)^{-1} \mathbf{K}^T \mathbf{S}_y^{-1} \left(\vec{y} - \vec{F}(\vec{x}_i)\right)$$

$$\mathbf{S}_x = \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}\right)^{-1}$$

Regularization

- More unknowns than observations $n > m$
- $m >= n$ but linear dependent

↓

Introduction of constraints
(Regularization)

Tikhonov-Phillips regularization

The altitude profile should be "smooth"

Instead of:

$$\left[\vec{y}-\vec{F}(\vec{x})\right]^T S_y^{-1}\left[\vec{y}-\vec{F}(\vec{x})\right]$$

Minimize:

$$\left[\vec{y}-\vec{F}(\vec{x})\right]^T S_y^{-1}\left[\vec{y}-\vec{F}(\vec{x})\right]+\gamma\vec{x}^T\mathbf{L}^T\mathbf{L}\vec{x}$$

$$\mathbf{L}=\begin{pmatrix} -1 & 1 & 0 & 0 & \dots \\ 0 & -1 & 1 & 0 & \dots \\ . & . & . & . & \dots \\ . & . & & . & \dots \\ \dots. & \dots & 0 & -1 & 1 \end{pmatrix}$$

Solution:

$$\vec{x}_{i+1}=\vec{x}_i+\left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\gamma\mathbf{L}^T\mathbf{L}\right)^{-1}\left[\mathbf{K}^T\mathbf{S}_y^{-1}\left(\vec{y}-\vec{F}(\vec{x}_i)\right)+\gamma\mathbf{L}^T\mathbf{L}\left(\vec{x}_a-\vec{x}_i\right)\right]$$

Linear statistical regularization "optimal estimation"

Use statistical knowledge about atmospheric parameter x

$$\left[\vec{y}-\vec{F}(\vec{x})\right]^T S_y^{-1}\left[\vec{y}-\vec{F}(\vec{x})\right]$$

→

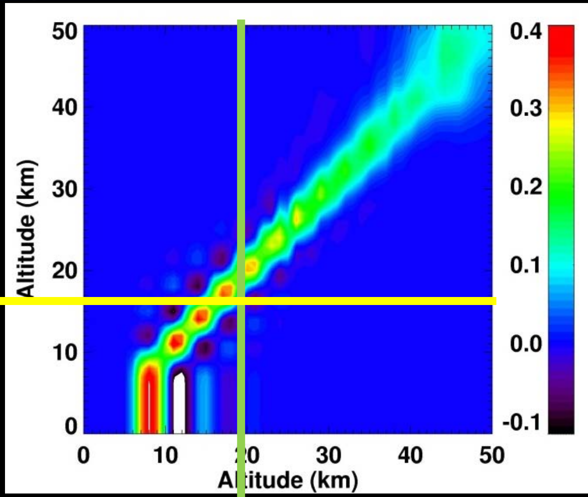
$$\left[\vec{y}-\vec{F}(\vec{x})\right]^T S_y^{-1}\left[\vec{y}-\vec{F}(\vec{x})\right]+(\vec{x}-\vec{x}_a)^T \mathbf{S}_a{}^{-1}(\vec{x}-\vec{x}_a)$$

a-priori covariance matrix

Solution:

$$\vec{x}_{i+1}=\vec{x}_i+\left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{S}_a^{-1}\right)^{-1}\left[\mathbf{K}^T\mathbf{S}_y^{-1}\left(\vec{y}-\vec{F}(\vec{x}_i)\right)+\mathbf{S}_a^{-1}\left(\vec{x}_a-\vec{x}_i\right)\right]$$

Averaging kernel matrix



MIPAS
ClONO2
Tikhonov
Regul.

Tikhonov-Phillips

$$\mathbf{A} = \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \gamma \mathbf{L}^T \mathbf{L}\right)^{-1} \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}$$

Optimal estimation

$$\mathbf{A} = \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \mathbf{S}_a^{-1}\right)^{-1} \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}$$

Column k: answer of the retrieval to a delta-function at altitude k

Row j: contribution of diffenent altitudes to the results in altitude j

Smoothing described by

$$\vec{x}_{inv} = \vec{x}_0 + \mathbf{A}(\vec{x}_{true} - \vec{x}_0)$$

Ozone inversion from ground-based FTIR

$$\vec{y} = \vec{F}(\vec{x})$$

$$K_{ij} = \partial y_i / \partial x_j$$

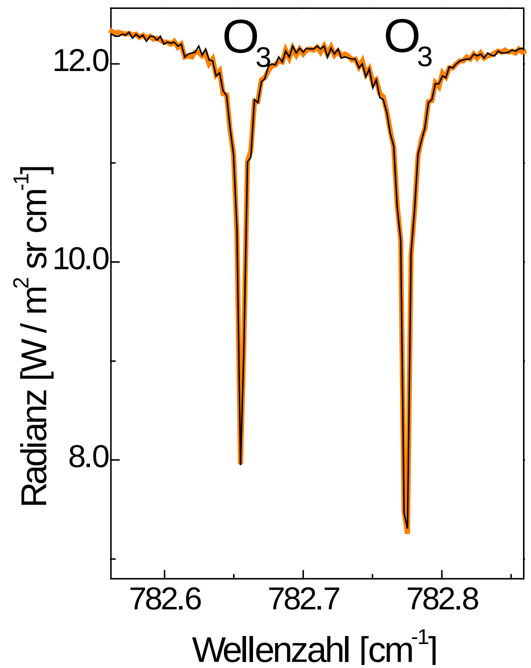
$$\Delta\vec{y} = \mathbf{K}\Delta\vec{x}$$

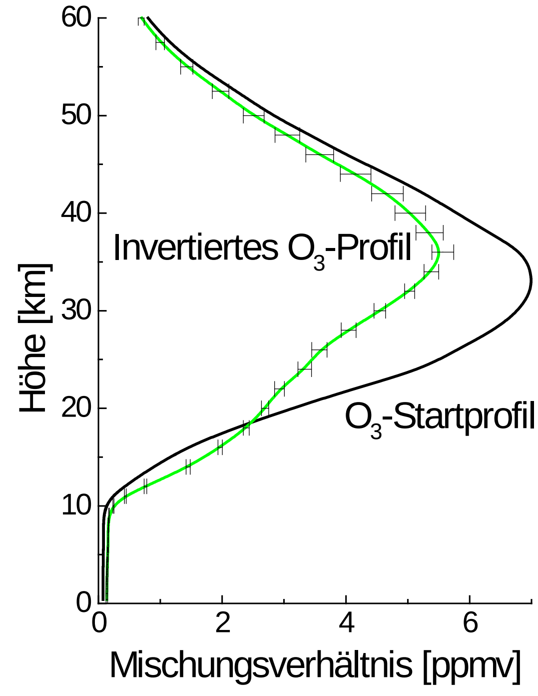
Iterative inversion of linearized problem:

Minimize:

$$\left[\vec{y} - \vec{F}(x)\right]^T S_y^{-1} \left[\vec{y} - \vec{F}(x)\right] + \gamma \vec{x}^T \mathbf{L}^T \mathbf{L} \vec{x}$$

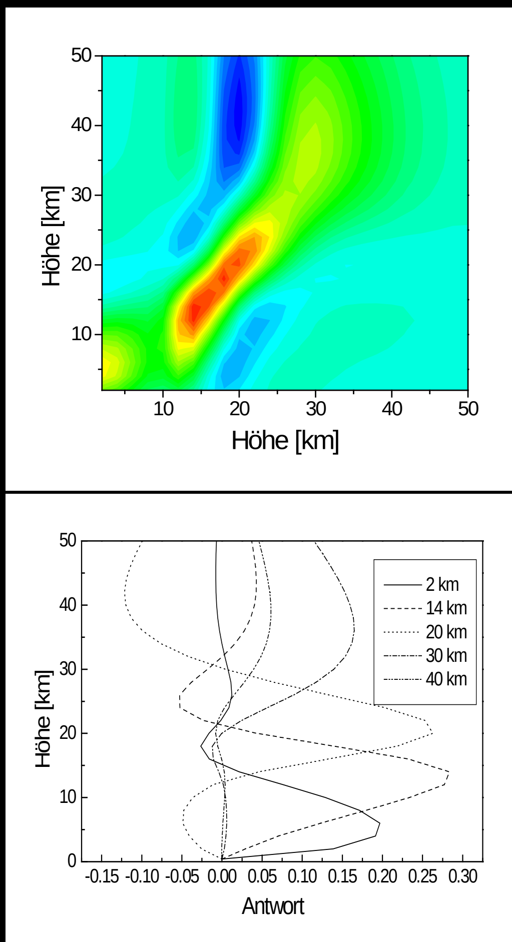
$$\vec{x}_{i+1} = \vec{x}_i + \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \gamma \mathbf{L}^T \mathbf{L}\right)^{-1} \left[\mathbf{K}^T \mathbf{S}_y^{-1} \left(\vec{y} - \vec{F}(\vec{x}_i)\right) + \gamma \mathbf{L}^T \mathbf{L} \left(\vec{x}_a - \vec{x}_i\right)\right]$$





Averaging kernel and vertical resolution

Ozone from ground-based FTIR



ClONO2 from MIPAS