SFIT4 – description of the forward model parameter

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Boulder, 2019

General

- The main control file is **sfit4.ctl** which resides in the directory sfit4 is started in.
- The general format is **key1.key2.key3...**

General

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```
# General

file.in.stalayers                = station.layers
file.in.refprofile               = reference.prf
file.in.spectrum                 = spectrum
file.in.isotope                  = isotope.input
file.in.solarlines               = solar.dat
file.in.linelist                 = 00778.501722-01008.558278.hbin

file.out.ak_matrix= ak.out
file.out.k_matrix= k.out
file.out.g_matrix= g.out
file.out.kb_matrix= kb.out
file.out.sa_matrix= sa.out
file.out.retprofiles= rprfs.table
file.out.aprprofiles= aprfs.table
file.out.summary= summary
file.out.seinv_vector            = seinv.vector
file.out.pbpfile           = pbpfile
file.out.retprofiles       = rprfs.table
file.out.aprprofiles       = aprfs.table

# Definition for retrieval gases

gas.layers                  =              41
gas.profile.list            = O3 H2O O3668 O3686
gas.column.list             = CO2 C2H4
gas.profile.O3.correlation          =               F
gas.profile.O3.logstate             =               F
```

General

- The main control file is **sfit4.ctl** which resides in the directory sfit4 is started in.
- The general format is **key1.key2.key3...**
- This deals with some of the entries in the sections **fw** and **rt**
- **fw** defines how the forward models behaves, it includes parameters for the atmosphere, and the instrument.
- **rt** defines properties of the retrieval
- some of the parameters affecting the forward model and the retrieval are found in the section **band** and **sp**, e.g.:

band.zshift.apriori an band specific offset
band.wave_factor a scaling aplied to the spectrum, multiplied to the shift.
band.opd, band.fov properties of the instrument
sp.snr noise (deweighting) defined on some region of the spectrum

Apodisation and Phase error

Apodisation and Phase Function

In FT spectrometry an interferogram is Fourier transformed to get a spectrum

$$S(\nu) = \int_0^\infty I(\Delta x)\cos(2\pi\nu x)dx \tag{1}$$

Caveats:

- Interferogram finite
- Interferogram may not be strictly symmetrical
- Beam in interferometer not strictly parallel

Hence: Equation 1 has to be modified for real world spectra

- Apodisation and phase functions define the instrumental lineshape (ILS)
- inherent feature of the instrument
- the ILS affects the spectrum and has to be accounted for
- ILS effects can mask or emulate true atmospheric features

Apodisation and Phase Function

In FT spectrometry an interferogram is Fourier transformed to get a spectrum

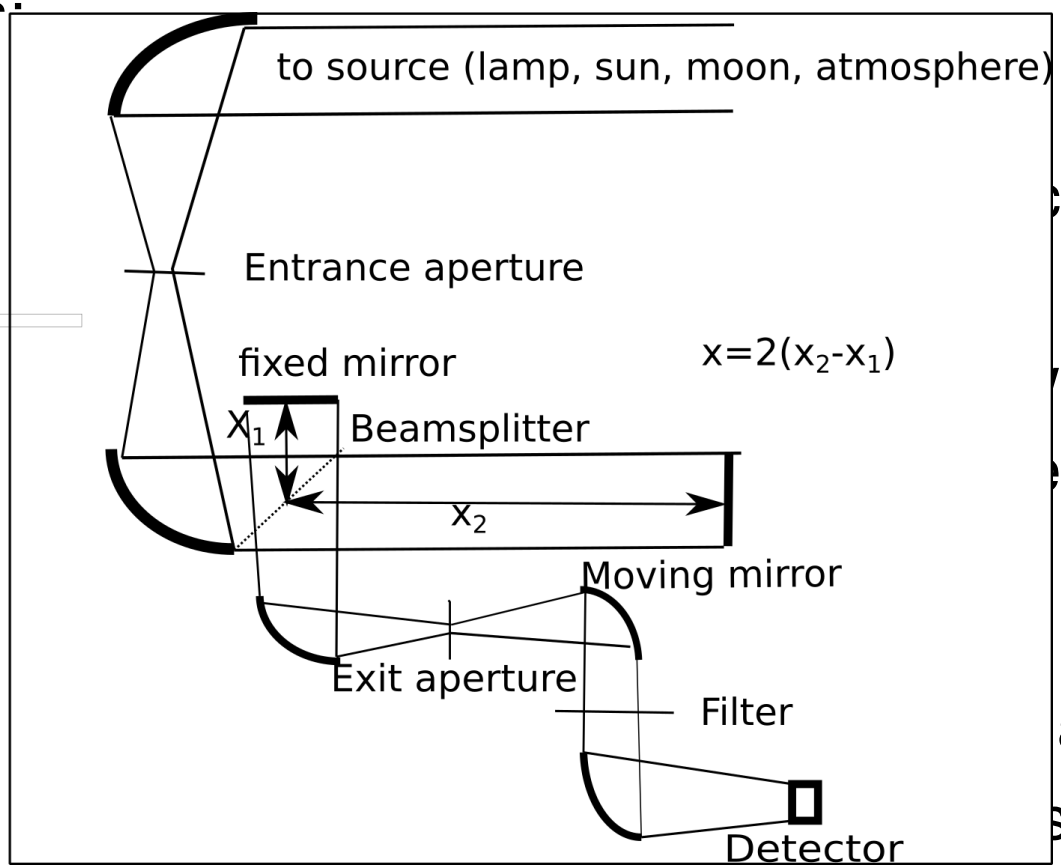
$$S(\nu) = \int_0^\infty I(\Delta x)\cos(2\pi\nu x)dx \qquad (1)$$

Caveat

- Int
- Int
- Be

Hence

- Ap
  lin
- inh
- the
- IL



cal

orld spectra

instrumental

accounted for

spheric features

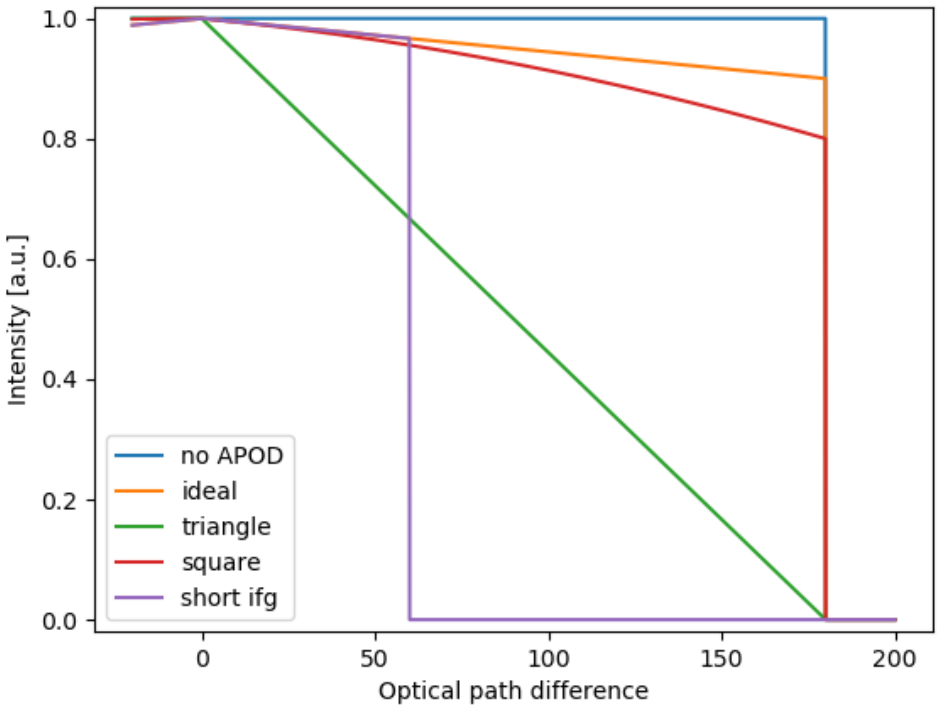
Apodisation and Phase Function

In FT spectrometry an interferogram is Fourier transformed to get a spectrum

$$S(\nu) = \int_0^{\infty} I(\Delta x) \cos(2\pi\nu x) dx \qquad (1)$$

Caveat:

- Int
- Int ...al
- Be
- Hence ...orld spectra
- Ap ... instrumental lin
- inh
- the ... accounted for
- ILS ... spheric features



Apodisation and Phase Function

How to account for the ILS in sfit4?

There are two 2 sources of apodisatioon

1. Apodisation applied while making the spectra: dealt with in band.GAS.apodization_code
2. Apodisation and phase error due to misalignement of the instrument

Here we are only concerned with point 2

fw.apod_fcn fw.apod_function = T
fw.apod_function.type = 0,1,2,3,4
fw.apod_function.order = 1,2,3,. . .

fw.phase_fcn fw.phase_function = T
fw.phase_function.type = 0,1,2,4
fw.phase_function.order = 1,2,3,. . . (no constant!!!)

rt.phase
- set as apriori value in rt.phase.apriori
- determines the constant phase offset
- the function determines in fw.phase_fcn is added to it

Apodisation and Phase Function

How to account for the ILS in sfit4?

The structure of the files file.in.modulation_fcn and file.in.phase_fcn is:

jeap
eapf(1) eapf(2) ... eapf(jeap)
[eapx(1) eapx(2) ... eapx(jeap)]

eapx is read only when ieap=1.

- jeap simply specifies the length of the following vectors. eapf is the vector of apodization parameters, whose meaning depends on ieap:

Apodisation and Phase Function

How to account for the ILS in sfit4?

ieap=1: eapf contains the values of the apodization function eapdz; in this case eapx contains the values of path difference at which the function is specified.

ieap=2: eapf contains the coefficients of a polynomial, defined by

$$eapdz = 1+(eapf(1)-1)*(x/xmax)+(eapf(2)-1)*(x/xmax)^2+\ldots$$

where x is the path difference

ieap=3: eapf contains the coefficients of a Fourier series

$$\begin{aligned} eapdz \quad = \quad & 1+(1-eapf(2))*sin(2*pi*eapf(1)*x/xmax)+ \\ & (1-eapf(3))*cos(2*pi*eapf(1)*x/xmax)+ \\ & (1-eapf(4))*sin(4*pi*eapf(1)*x/xmax)+ \\ & (1-eapf(5))*cos(4*pi*eapf(1)*x/xmax)+\ldots \end{aligned}$$

Apodisation and Phase Function

How to account for the ILS in sfit4?

ieap=1: eapf contains the values of the apodization function eapdz; in this case eapx contains the values of path difference at which the function is specified.

ieap=2: eapf contains the coefficients of a polynomial, defined by

$$eapdz = 1 + (eapf(1) - 1) * (x/xmax) + (eapf(2) - 1) * (x/xmax)^2 + \ldots$$

NOTE: a 1 means, the the respective coefficient is ZERO

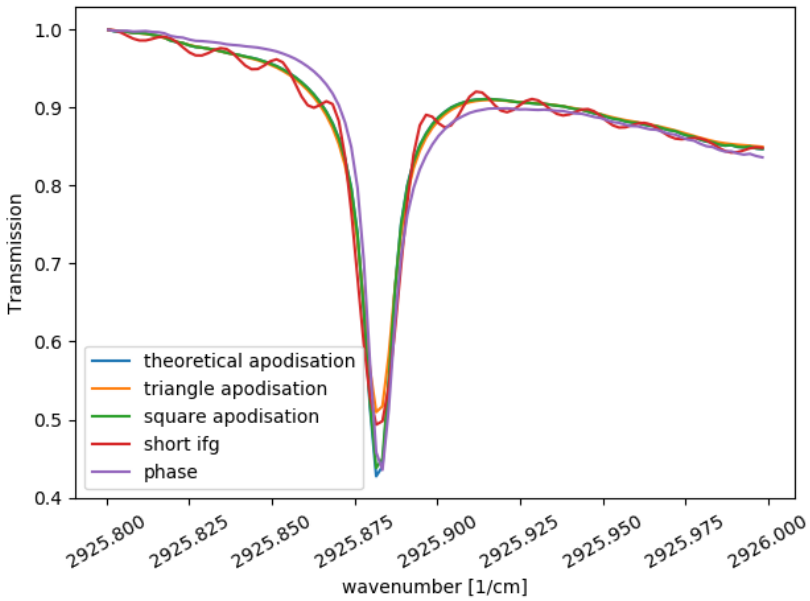
$\rightarrow$The parameter is the value, the ILS should have at MAX_OPD

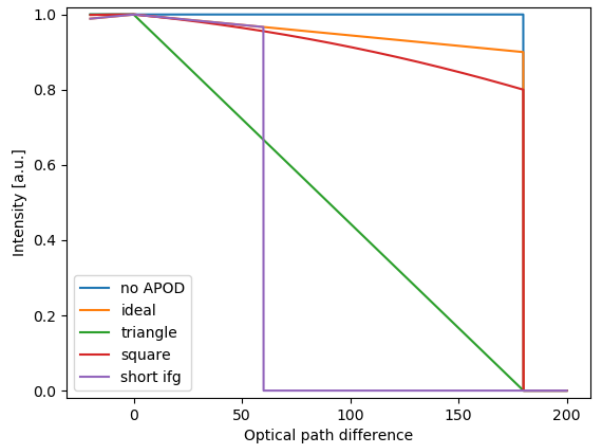
$$(1 - eapf(3)) * cos(2 * pi * eapf(1) * x/xmax) +$$
$$(1 - eapf(4)) * sin(4 * pi * eapf(1) * x/xmax) +$$
$$(1 - eapf(5)) * cos(4 * pi * eapf(1) * x/xmax) + \ldots$$

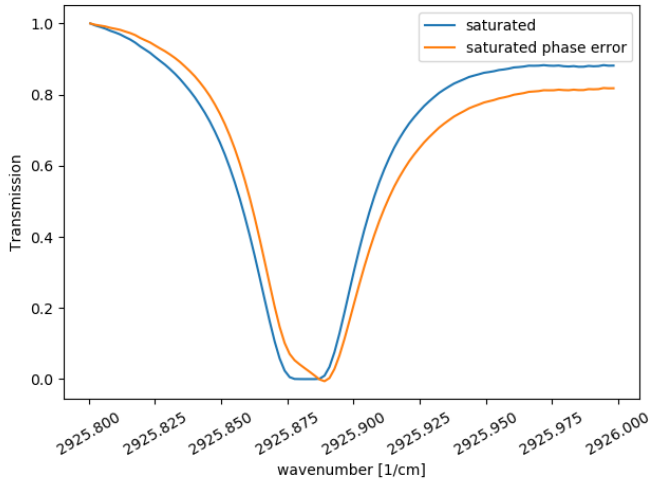
Apodisation and Phase Function

The effect of the ILS is to distort the measured spectrum: A line an be

- made broader
- made less deep
- made asymmetric
- leak to other spectral bins







Emission

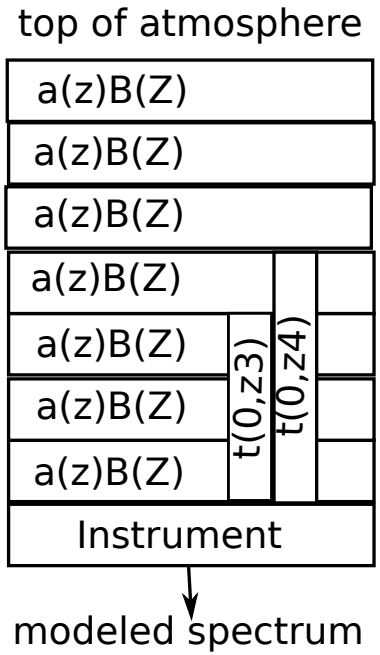
Cacluation of emission spectra

Atmospheric model

Radiance calculated by

$$I = B(\infty)\exp(-\tau(0,\infty)) + \int_0^\infty \underbrace{\alpha(z')B(z')}_{\text{Emission of layer z}} \exp(-\tau(0,z'))dz'$$

$$\tau(0,z) = \int_0^z \alpha(z')dz' \qquad \alpha(z) = \sum_{l=1}^{N} x_{a,l}(z)\alpha_l(z)$$



B(z) Planck function

Emission by Kirchhoff's law

$$e(\nu) = \alpha(\nu, P, T)B(\nu, T)$$

Transmission $\in [0, 1]$

$$T(0,z) = \exp(-\tau(0,z))$$

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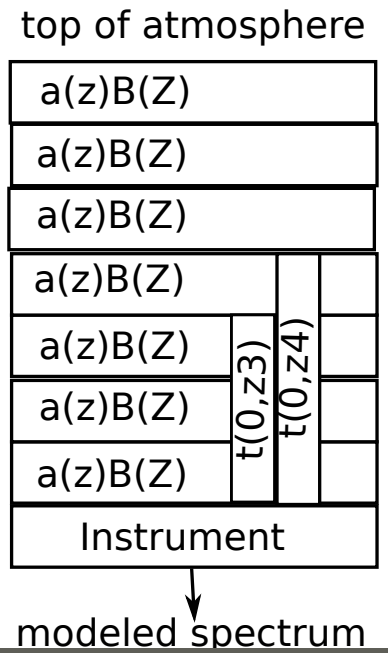

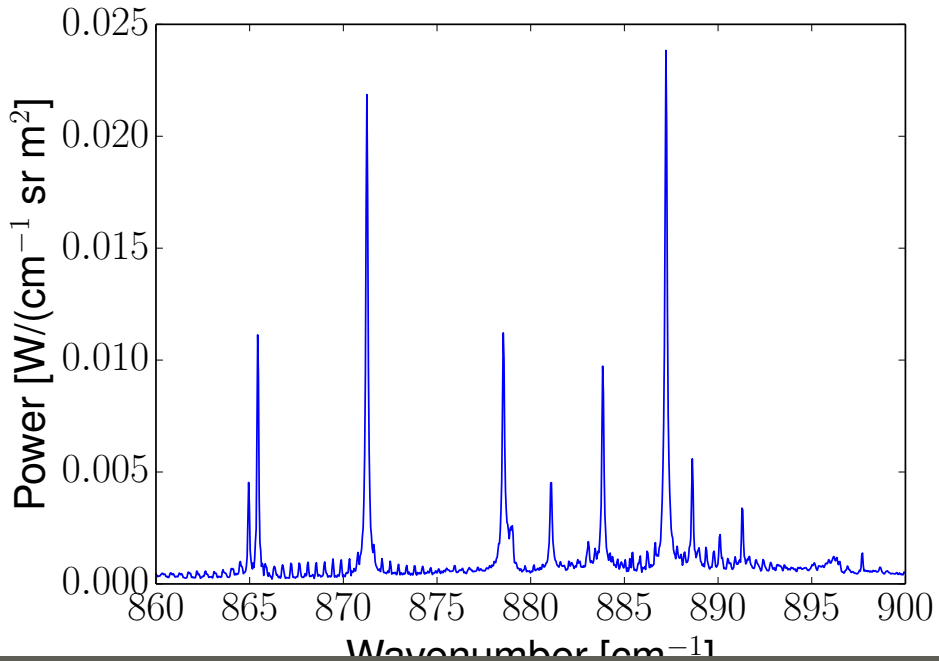

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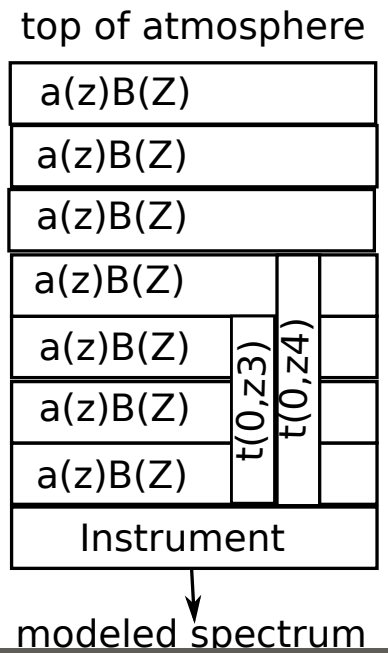
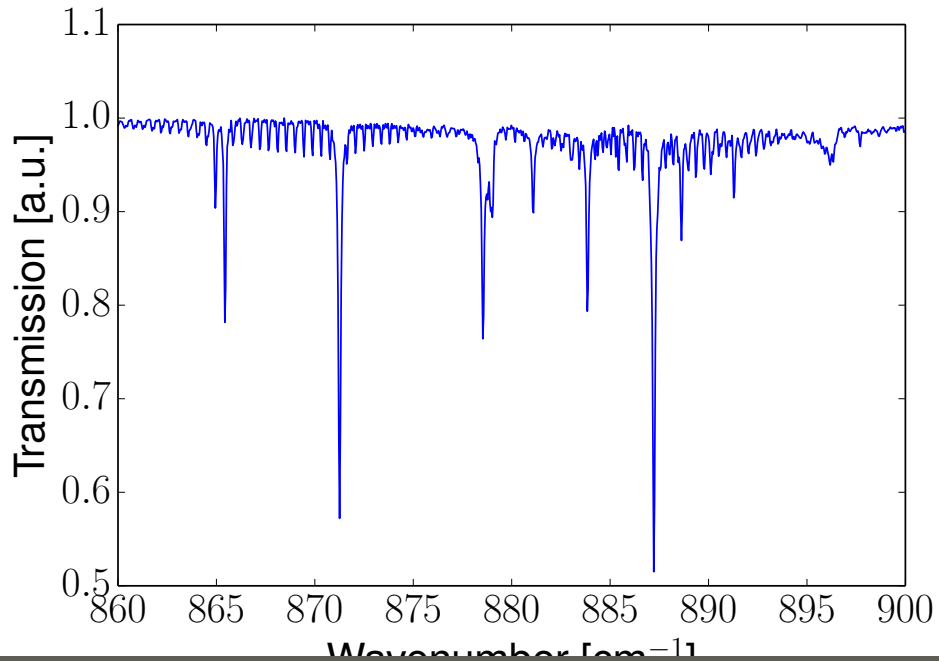




Cacluation of emission spectra

The calculation of the full radiativ transfer is switched on by fw.emission = T
The unit is the spectra is $\frac{W}{m^2 srcm^{-1}}$. The other parameters are

fw.emission.T_infinity the temperature of the radiations source outside the atmosphere. This can be

outer space: The temperature is currently (and for another while) 2.7K.

Sun: The effective temperature of the sun is 6700K. The result is the same as for the transmission spectra, but the unit is $\frac{W}{m^2 srcm^{-1}}$.

Moon The temperature of the moon is 370.0K. Above about 3000 cm^{-1} reflection of solar light is larger than the blackbody emission

Cacluation of emission spectra

fw.emission.object used to include reflection of solar light

.e. no reflection calculated

.m. reflection of solar light on the moon calculated

fw.emission.normalized The spectra are normalized to 1. This can be used to correct spectra recorded with the moon as the light source for atmospheric emission.

this option is very seldom used, only if one has lunar measurements in transmission.

Line shape options

Line shape options

fw.lshapemodel this option offers the choice to enforce a certain lineshape model to be used.

- = 0 default and historical value. The line shape model is chosen according the spectral values available.
- = 1 enforce use of Voigt model, regardless of extra line parameters
- = 2 use Galatry if BETA_T is given, if not Voigt
- = 3 LM calculation uing an adapted Voigt profile
- = 4 pCqSDHC line shape

fw.lineshapemodel.sdv use the SDV approximation in the pCqSDHC model

fw.linemixing switch on line mixing calculation (currently only 1st order)

fw.linemixing.gas currently not used

Line shape modeling

Assumptions required to arrive at the Voigt function and LBL radiative transfer

1. Binary impact theorem
   -> Only two molecules interact at one time
2. Sudden impact theorem
   -> The molecules are considered to be hard spheres
3. Translational and collisional effects are independent
   -> Gauss and Lorentz line shape, respectively
   -> Combination is Voigt line shape

$$L_V = L_G * L_L \tag{2}$$

4. Pressure broadening not a function of speed of active molecule -> Lorentz function
5. Transitions do not interact with each other
   -> line-by-line calculation

Assumption: Translational and collisional effects are independent

Dicke narrowing

Assumption: The molecules are moving at a constant speed on a straight line

Correct: Collisions may change the velocity of the molecule during the lifetime of the state

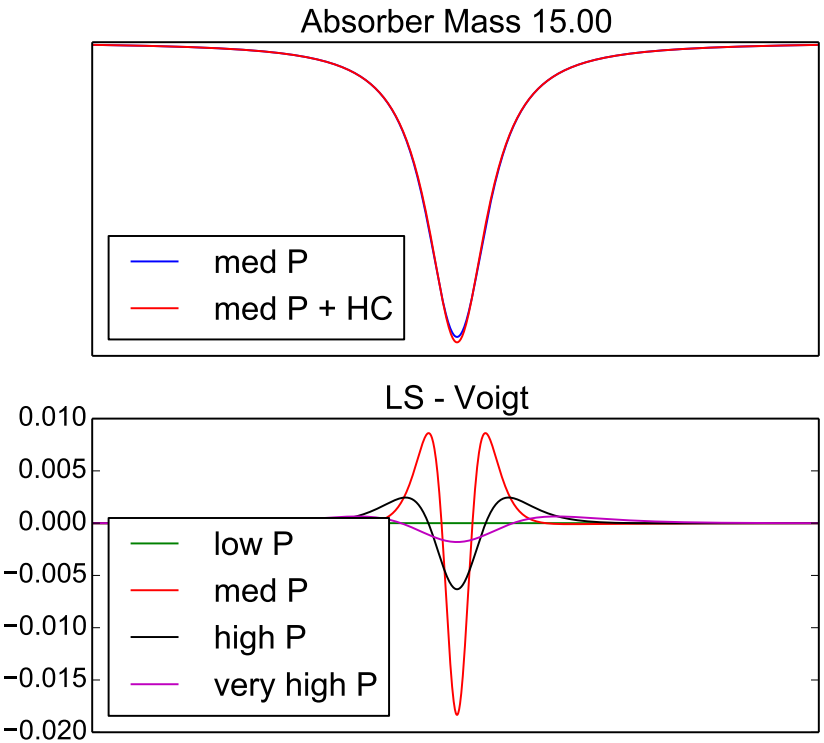
-> Collisions lead to a Lorentz shape of the transition(Dicke, 1953)

-> More frequent collisions lead to a narrower Doppler broadening.

Hard collision model	Soft collision model
Velocity after a collision is completely unrelated to the speed and direction before the collision	Each collision changes the velocity of the molecule only a bit, depending on the ratio (active molecule)/(perturbing molecule)
Rautian and Sobel`man (1967)	Galatry (1961)

Dicke narrowing

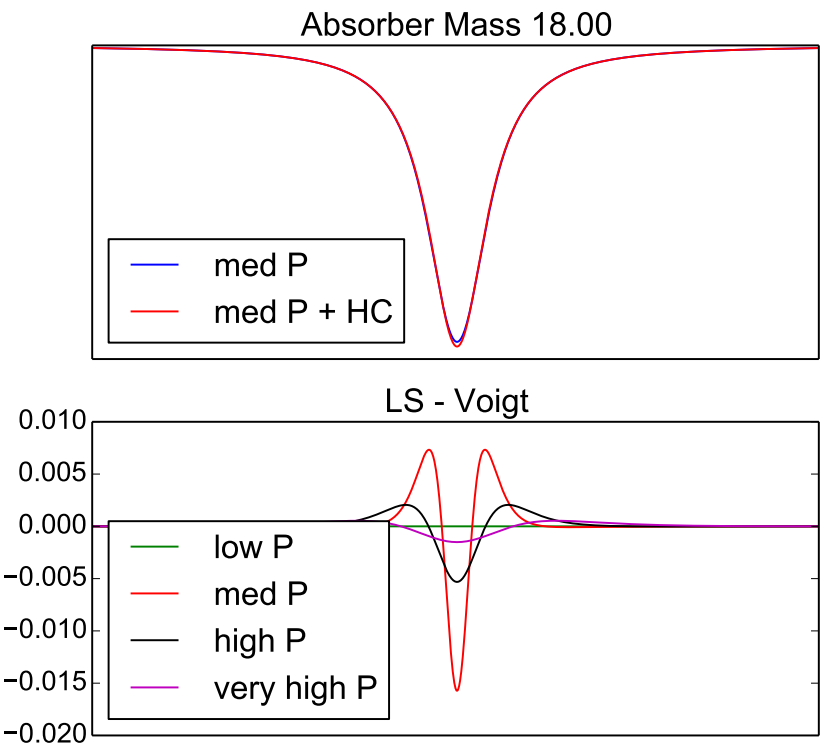
Dependency of Dicke narrowing on pressure



- Dicke narrowing modeled using hard collision model
- Effect is only present at a certain density
- At higher pressure Dicke narrowing becomes less important
- Effect most prominent if the active molecule is relatively light

Dicke narrowing

Dependency of Dicke narrowing on pressure



- Dicke narrowing modeled using hard collision model
- Effect is only present at a certain density
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Dicke narrowing

Due to lack of parameters for the hard collision model, Dicke narroing is modelled only using the GALATRY lineshape model (fw.lshapemodel = 3) and for HCL and HF.
In sfit4.ctl:
fw.lshapemodel = 2
The spectroscopic input parameters are chosen in hbin.input
hitran.files = 99
. . .
014_HF/14_hit12.par
015_HCL/15_hit12.par
. . .
aux = gal
aux.gal.nr = 2
aux.gal.files =
014_HF/14_hit12_Galatry.txt
015_HCL/15_hit12_Galatry.txt
. . .

Dicke narrowing

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In sfit4.ctl:

fw.lshapemodel = 2

The spectroscopic input parameters are chosen in hbin input

hitran.f

```
READING SOLAR LINE LIST FILE...
  CALCULATION OF ASTRONOMICAL QUANTITIES ...
 BAND, # SOLAR LINES FOUND                                  :  1    269
 BAND, # SOLAR LINES FOUND                                  :  2    202
 BAND, # SOLAR LINES FOUND                                  :  3    179
READING ATMOSPHERIC LINE LIST FILE...
 HITRAN FILE : 02723.671422-02930.058578.hbin
   GALATRY FLAG & LINES WITH GALATRY PARAMETERS FOUND       :  T      6
   FCIA FLAG & FCIA LINES FOUND                             :  F      0
   SCIA FLAG & SCIA LINES FOUND                             :  F      0
   SDV FLAG & LINES WITH SDV PARAMETERS FOUND               :  F      0
   LINEMIXING FLAG & LINES WITH LINEMIXING PARAMETERS FOUND :  F      0
COMPUTING CROSS-SECTIONS...
```

...

014_H

015_H

...

aux = gal

aux.gal.nr = 2

aux.gal.files =

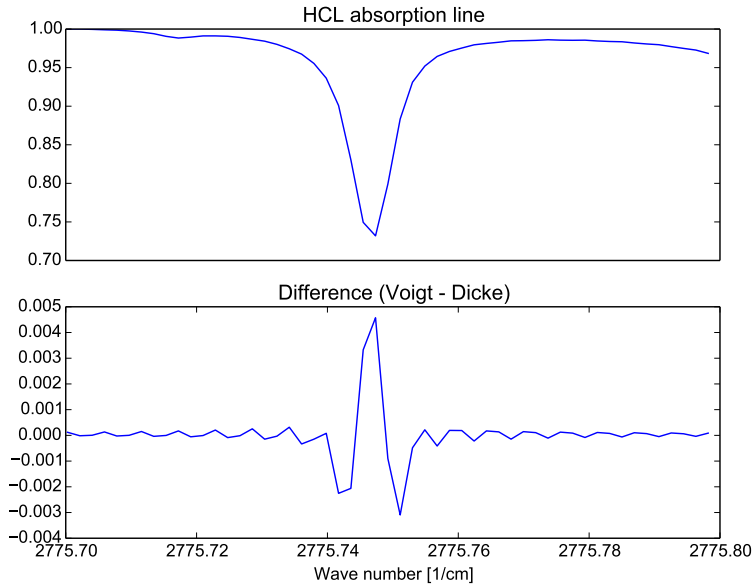
014_HF/14_hit12_Galatry.txt

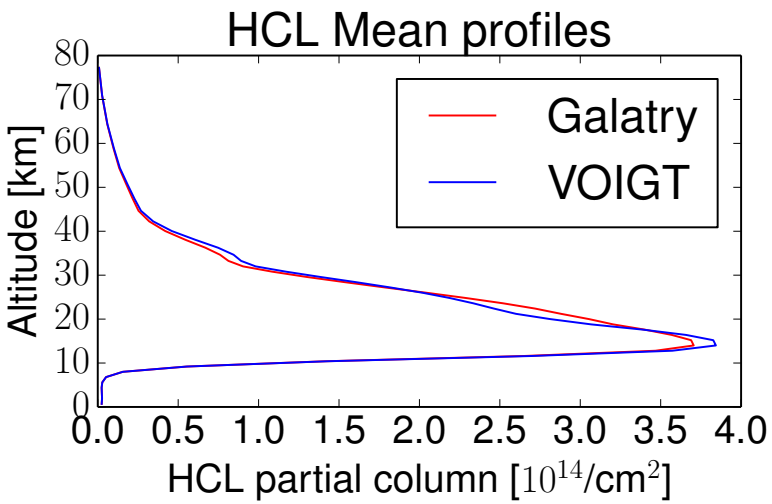
015_HCL/15_hit12_Galatry.txt

...

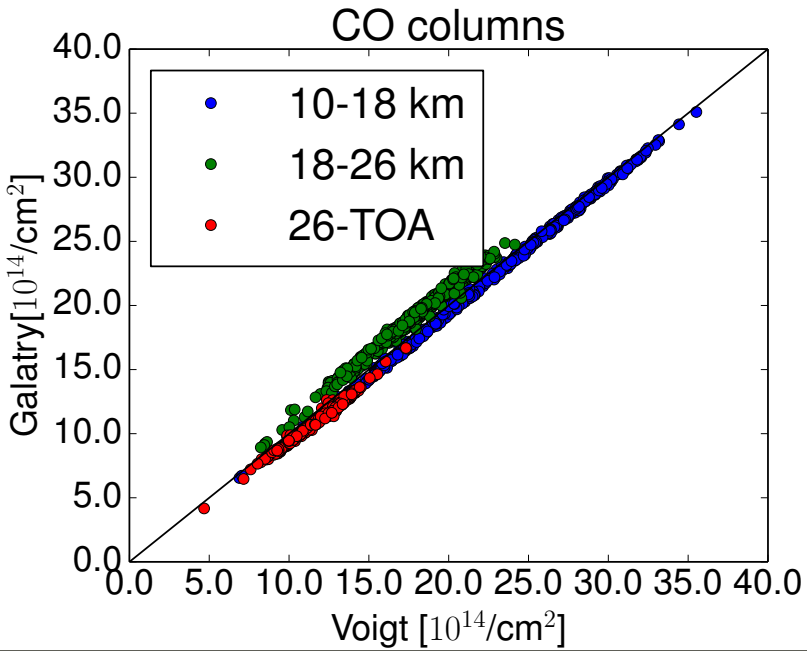
Dicke narrowing

Example: HCL





- Theoretically calculated lines with and without Dicke narrowing for the same atmospheric conditions.
- Total column does not differ, but profile



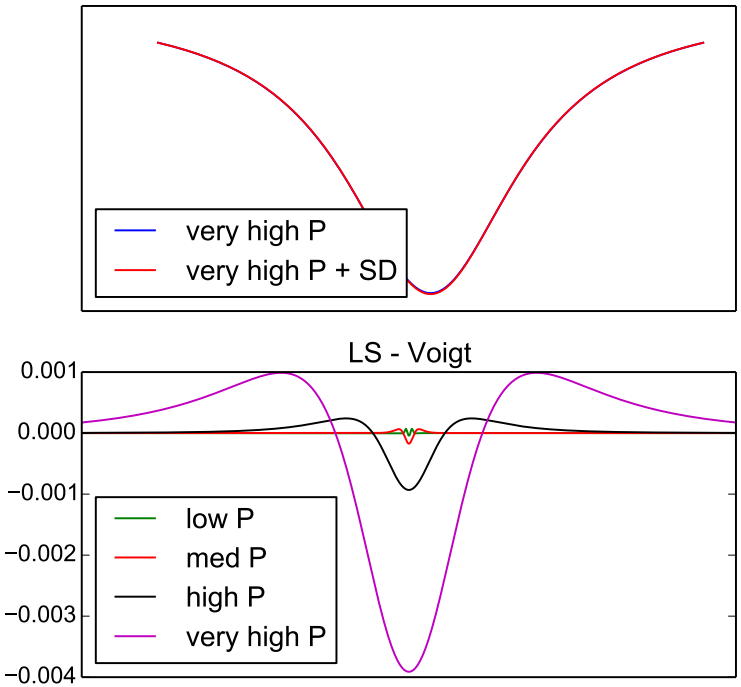
Speed dependence of pressure broadening

Assumptions: Pressure broadening not depending on speed of the molecules.
More correct: Pressure broadening depends on speed of the active molecule:

- Relative speed between active and perturbing molecules is not Maxwell Boltzmann distributed but skewed to higher velocities
- The mean of the relative speed is not given by the thermal mean of the perturber speed anymore.
- The line shape can be described by a weighted sum over Lorentz functions for different speed classes.

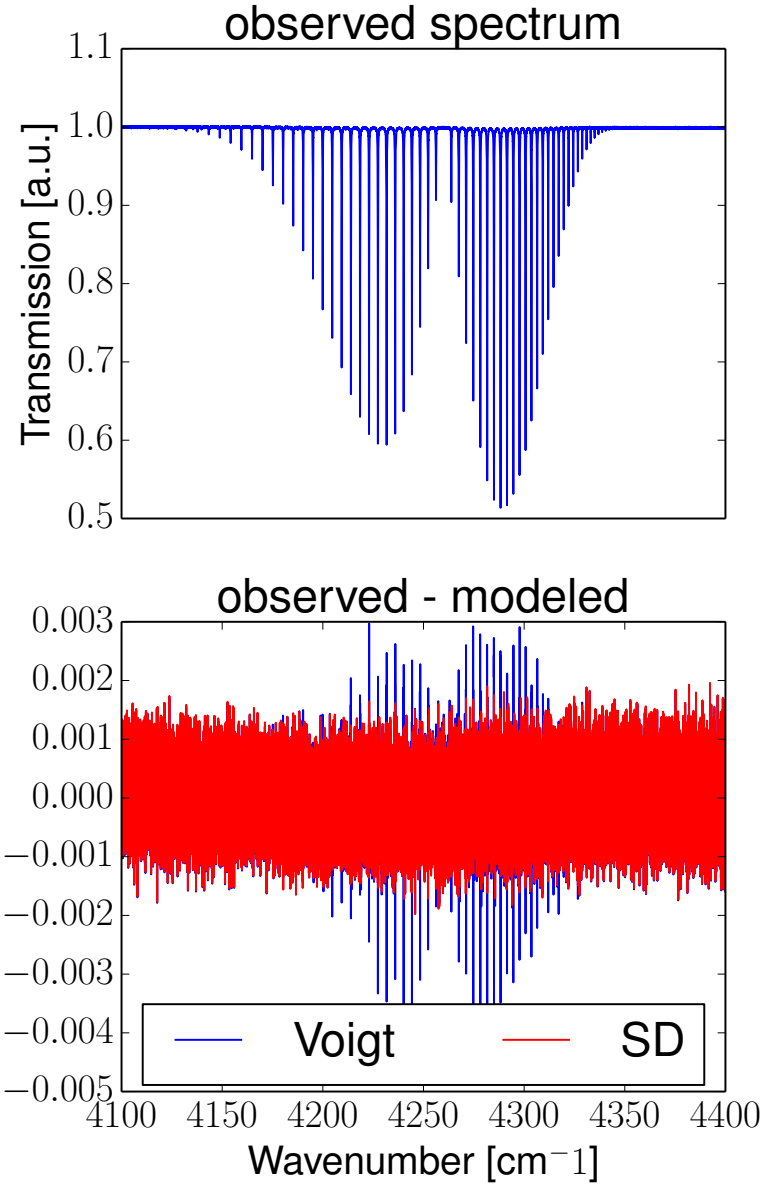
Speed dependence of pressure broadening

Dependency of effect on pressure



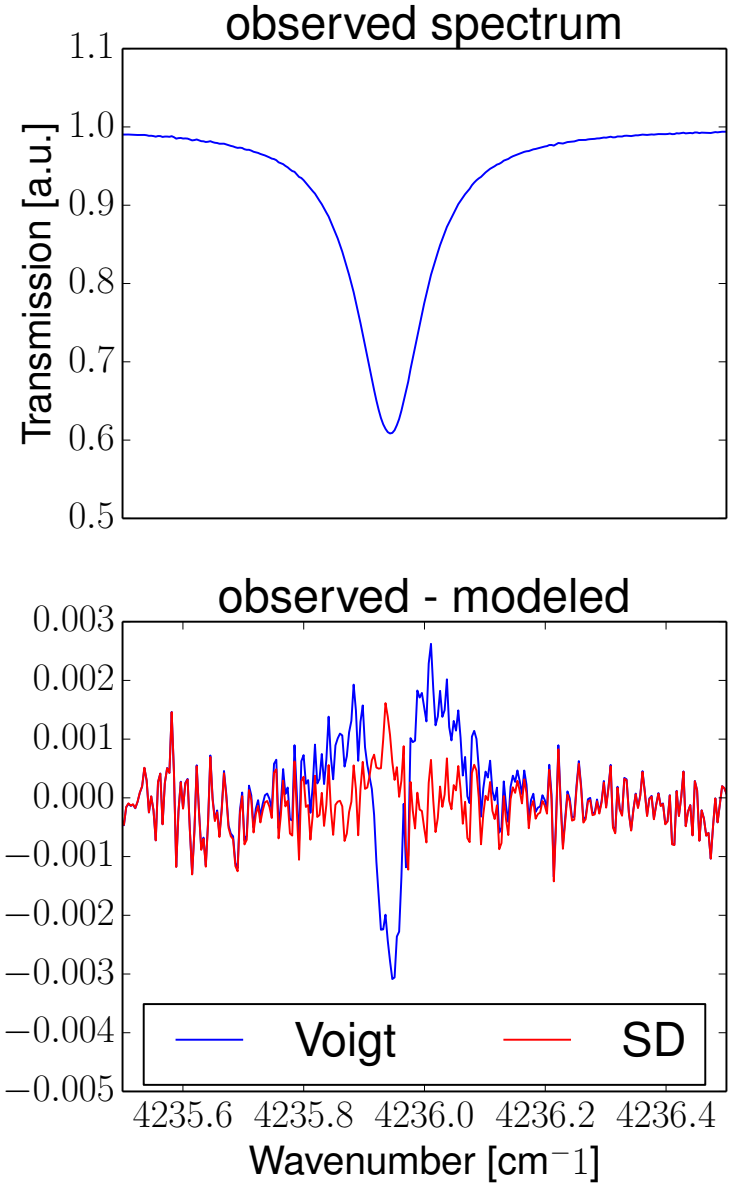
- independent on mass of molecule
- effect increases with pressure
- effect most important for gas with high abundance in troposphere

Speed dependence of pressure broadening



- Example CO
- Spectrum courtesy of M. Devy
- P = 943 hPa; T = 298 K
- Spectral data taken from HITRAN 2012
- Difference in line center about 0.5 %

Speed dependence of pressure broadening



- Example CO
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- P = 943 hPa; T = 298 K
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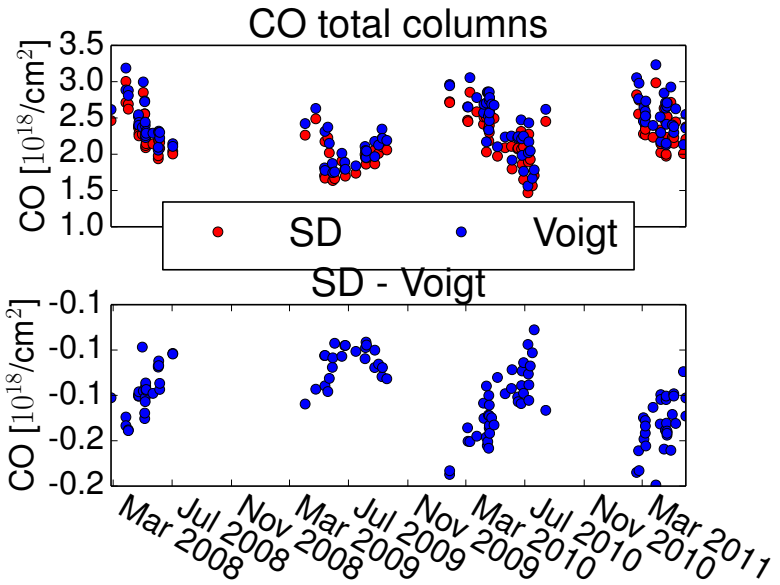
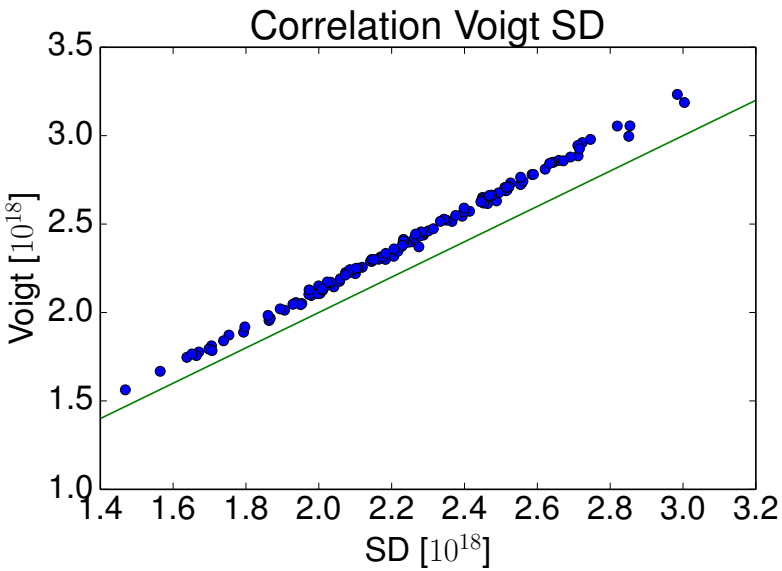
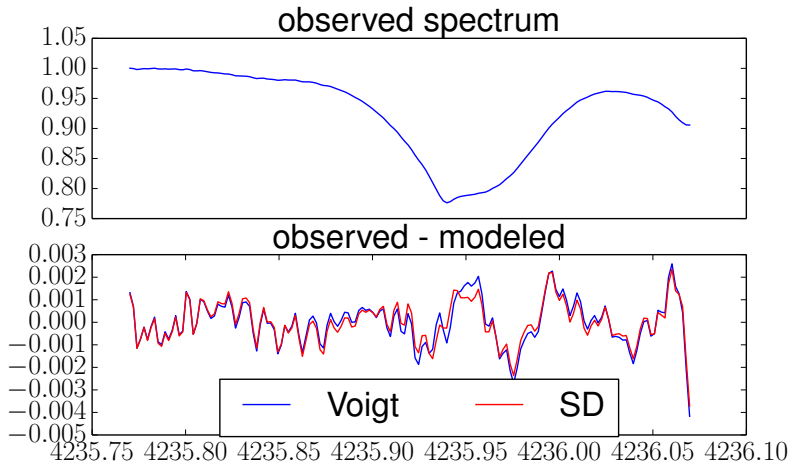
- Difference in line center about 0.5 %

Effect of speed dependence of pressure broadening on CO



- Total CO above Bremen
- Spectrum fitted equally well
- Difference in total column about 1%
- Difference can be corrected by scaling





Effect of speed dependence of pressure broadening on CO

Only few molecules in HITRAN have parameters for speed dependency. It seems only CO by the time being.
in sfit4.ctl:
fw.lshapemodel = 4
fw.lshapemodel.sdv = T
The spectroscopic input parameters chosen in hbin.input
hitran.files = 99
. . .
005_CO/05_hit12.par . . .
aux = . . . sdv . . .
aux.sdv.nr = 1
aux.sdv.files =
005_CO/05_hit12_SDV.txt . . .

Effect of speed dependence of pressure broadening on CO

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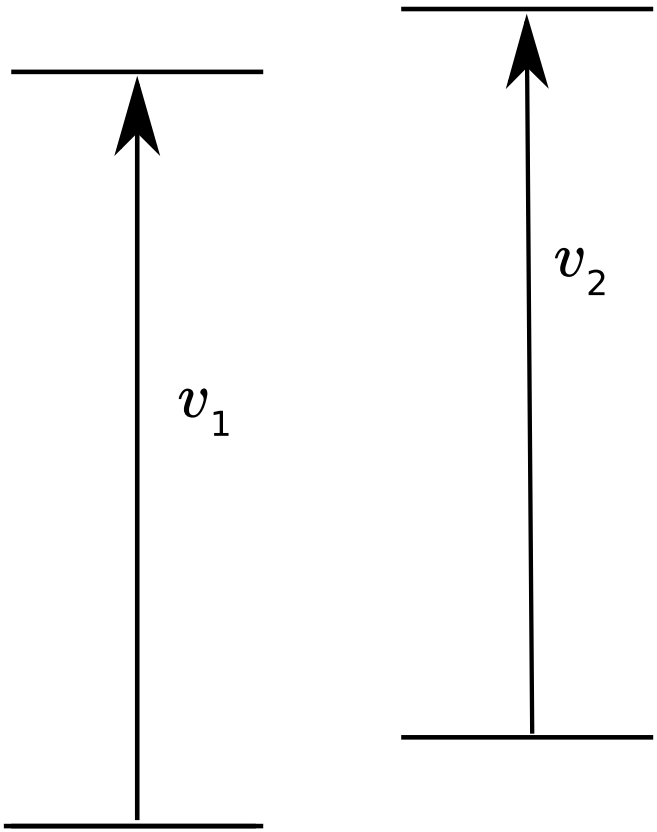
in sfit4.ctl:
fw.lshapemodel = 4
fw.lsha
The sp
hitran.f

```
READING ATMOSPHERIC LINE LIST FILE...
 HITRAN FILE : 04095.941722-04404.058278.hbin
   GALATRY FLAG & LINES WITH GALATRY PARAMETERS FOUND       :  F      0
   FCIA FLAG & FCIA LINES FOUND                             :  F      0
   SCIA FLAG & SCIA LINES FOUND                             :  F      0
   SDV FLAG & LINES WITH SDV PARAMETERS FOUND               :  T    100
   LINEMIXING FLAG & LINES WITH LINEMIXING PARAMETERS FOUND :  F      0
COMPUTING CROSS-SECTIONS...
```

. . .
005_CO/05_hit12.par . . .
aux = . . . sdv . . .
aux.sdv.nr = 1
aux.sdv.files =
005_CO/05_hit12_SDV.txt . . .

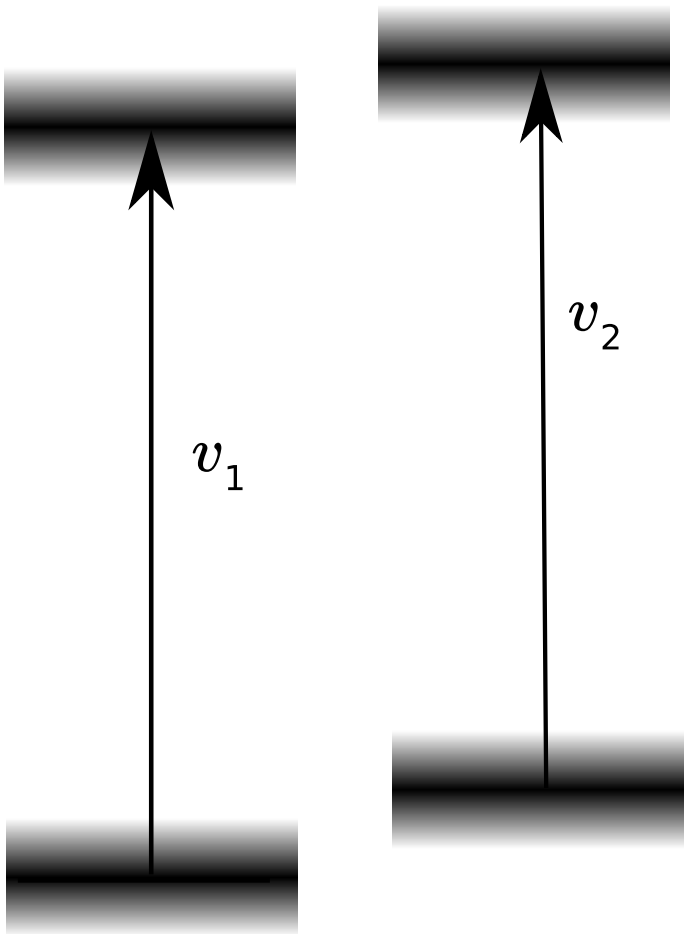
Assumption: Lines do not influence each other

Line mixing



- Absorption of photon leads to a transition from state 1 to state 2.

Line mixing



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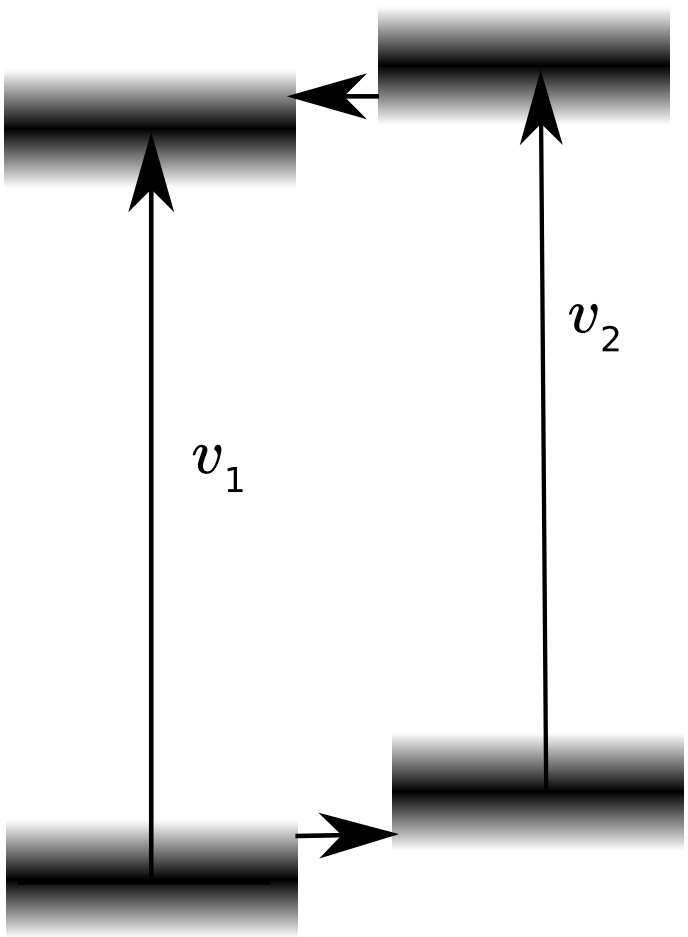

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- The statistical weight of the transitions defines, which transition, ν_1 or ν_2 is more likely.
- Collision couples different states in the same molecule

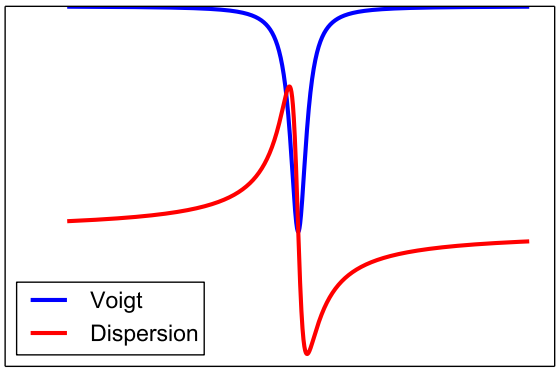
Modeling of line mixing

A band can be calculated (Berman, 1998) using

$$\alpha(\nu) = \frac{N}{\pi} \sum_i p_i \underbrace{\frac{\gamma_i}{(\nu - \nu_i)^2 + \gamma_i^2}}_{\text{Lorentz shape}} + q_i \underbrace{\frac{(\nu - \nu_i)}{(\nu - \nu_i)^2 + \gamma_i^2}}_{\text{Dispersion shape}} \quad (3)$$

The quantities p_i, q_i, γ_i and ν_i define the resulting line shape.
Rosenkrantz model (first order expansion):

Parameter	Isolated	Rosenkrantz
p	S	S
q	0	PYS
γ	$P\gamma_0$	$P\gamma_0$
ν_i	$\nu_0 P\delta$	$\nu_0 P\delta$



Modeling of line mixing

In SFIT4 the linemixing is calculated by

$$a(\nu) = \Re(\mathrm{LSMODEL}) + Y_P \Im(\mathrm{LSMODEL})$$

The traditional routine in SFIT4 to calculate the Voigt function does not calculate the imaginary part of the Voigt function. Two ways aroung:

fw.lshapemodel = 3 A modified Voigt rountine to incorporate line mixing

fw.lshapemodel = 4 the pCqSDHC model returns real and imaginary part and can therefor be used to calculate the line mixing.

Modeling of line mixing

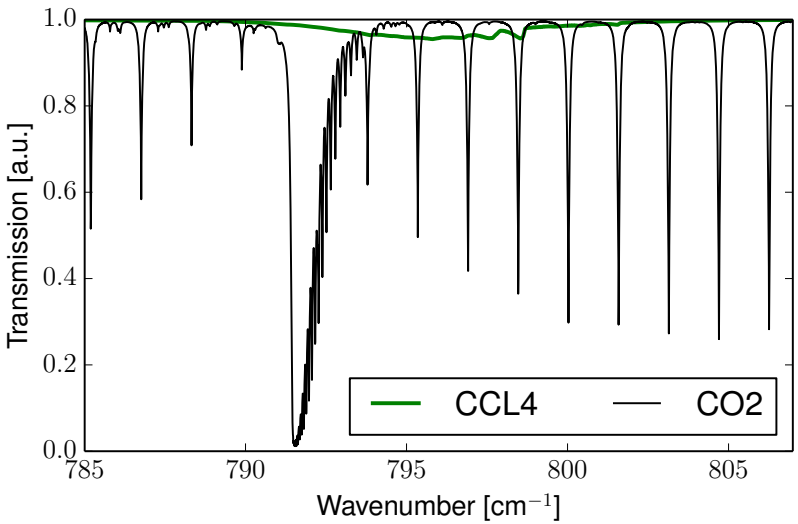
In sfit4.ctl:
fw.lshapemodel = 3 or 4
fw.linemixing = T
The spectroscopic paramater Y together with parameters describing the dependency on the pressure P is given in the hbin file:
hitran.files = 99
. . .
002_CO2/02_hit08_f53.par 005_CO/05_hit12.par . . .
aux = . . . lm . . .
. . .
aux.lm.nr = 2
aux.lm.files =
002_CO2/02_hit08_f53_LM1ST.par
005_CO/05_hit12_LM1ST.txt
. . .

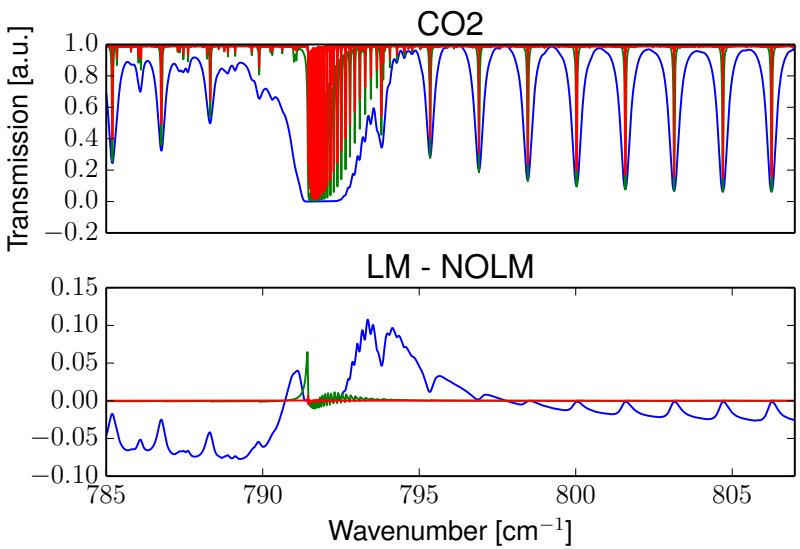
Modeling of line mixing

In sfit4.ctl:
fw.lshapemodel = 3 or 4
fw.linemixing = T
The spectroscopic paramater *Y* together with parameters describing the dependency on the pressure *P* is given in the hbin fil
hitran.f
. . .
002_C
aux = .
. . .
aux.lm
aux.lm.files =
002_CO2/02_hit08_f53_LM1ST.par
005_CO/05_hit12_LM1ST.txt
. . .

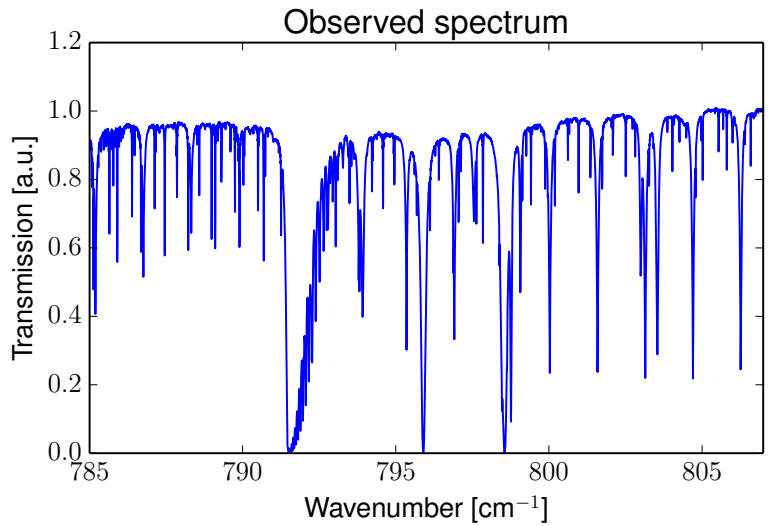
```
 READING ASCII SPECTRA FILE: spectrum
NFIT  BAND  SCAN/BAND  SCAN_ID  SCAN_CODE    SPACING     NSPAC
 RANGE     INIT_SNR
   1     1          1        1      80257  0.0061000         7     785.000 -
307.000   150.00000
   JJB-S12C01AF.DAT 01 DEC 2012  6.1000mK 2.50 mm Ap.ZA=80.257 S/N= 1264 h= 9.1
 READING SOLAR LINE LIST FILE...
   CALCULATION OF ASTRONOMICAL QUANTITIES ...
  BAND, # SOLAR LINES FOUND                                    :  1    236
 READING ATMOSPHERIC LINE LIST FILE...
  HITRAN FILE : 00780.871900-00811.128100.hbin
    GALATRY FLAG & LINES WITH GALATRY PARAMETERS FOUND         :  F      0
    FCIA FLAG & FCIA LINES FOUND                               :  F      0
    SCIA FLAG & SCIA LINES FOUND                               :  F      0
    SDV FLAG & LINES WITH SDV PARAMETERS FOUND                 :  F      0
    LINEMIXING FLAG & LINES WITH LINEMIXING PARAMETERS FOUND   :  T    378
 COMPUTING CROSS-SECTIONS...
```

Effect of line mixing in CO2 on retrieval of CCL4





- Artificial spectra of CCL4 and CO2
- Line mixing parameters by Frank Hase (KIT)
- Line mixing increasing with pressure
- Mismatch "resembles" CCL4 band



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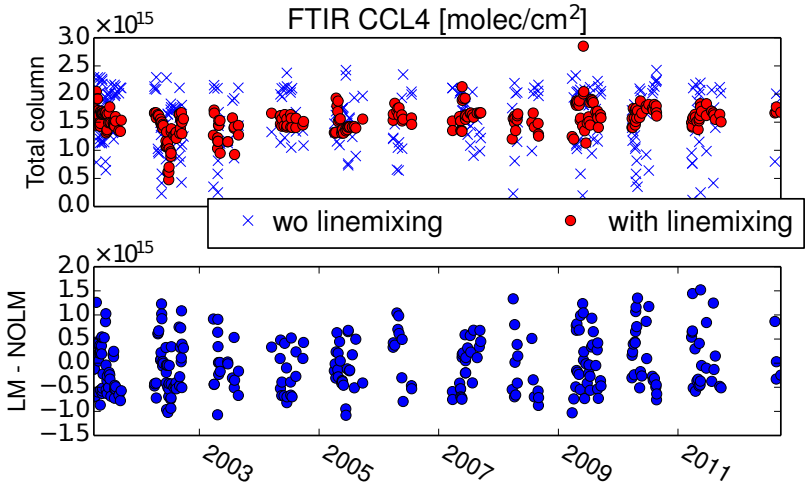
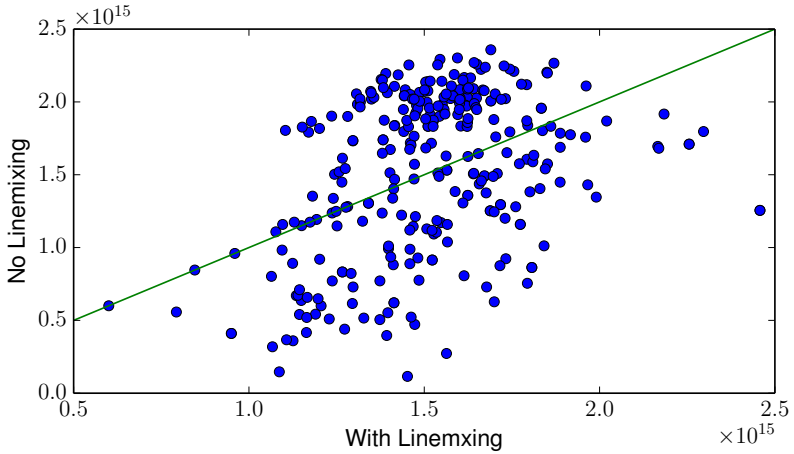
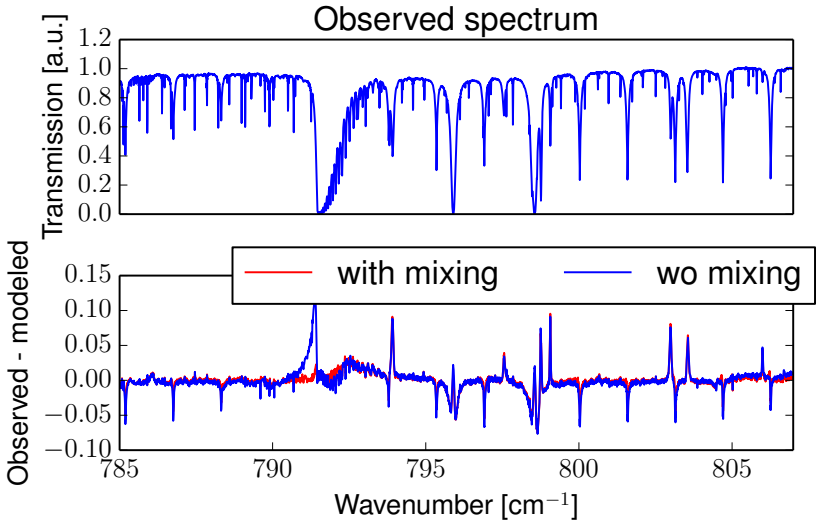


- CCl4 above Ny Alesund, Spitsbergen
- Mismatch in CO2 changes the retrieved value, seasonality and trend in CCL4.
- No easy correction possible.





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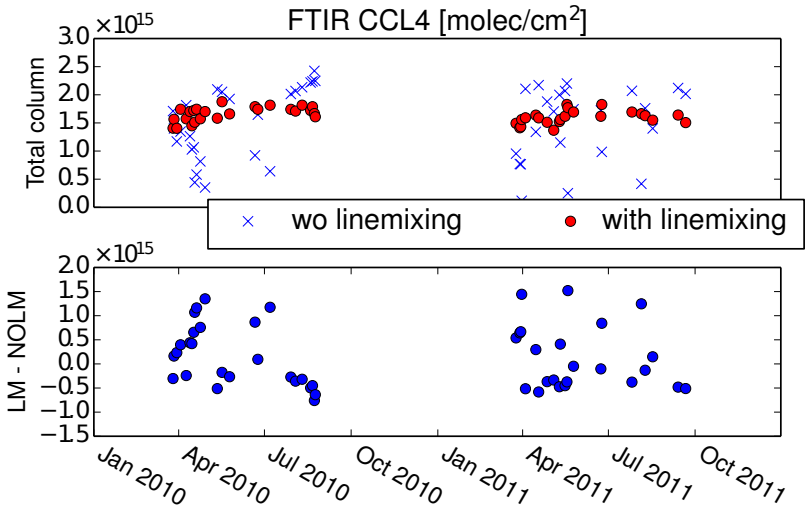

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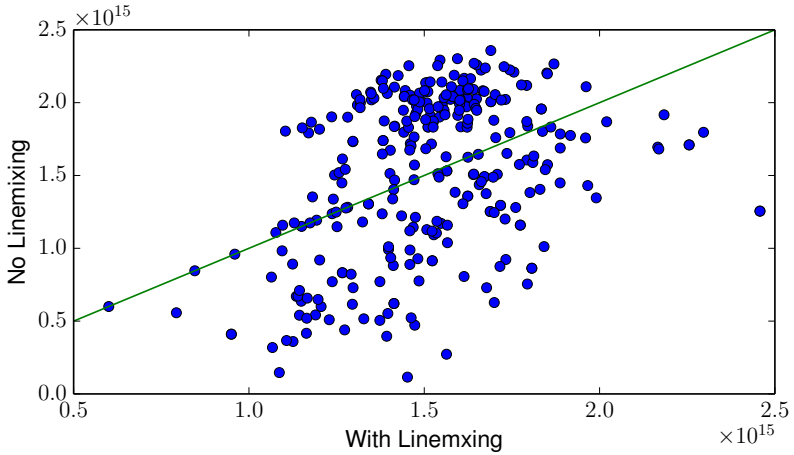

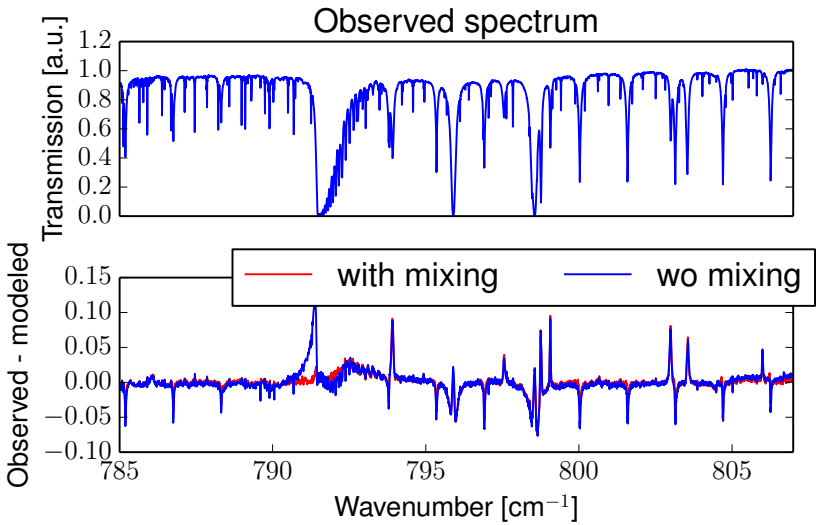

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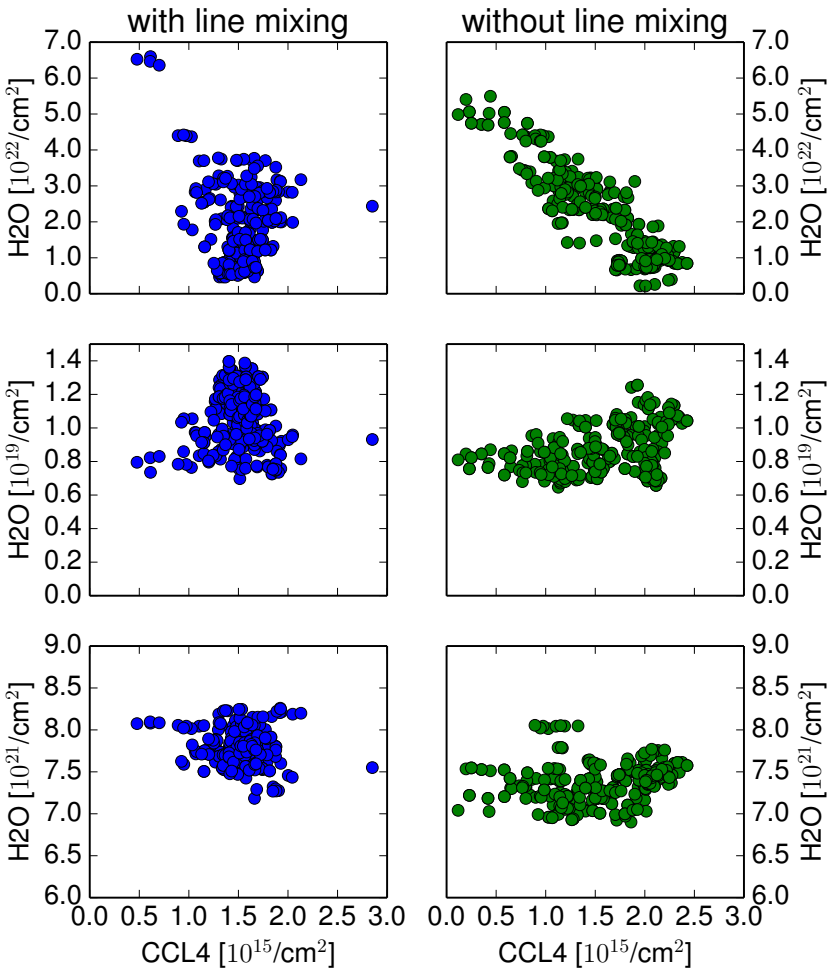
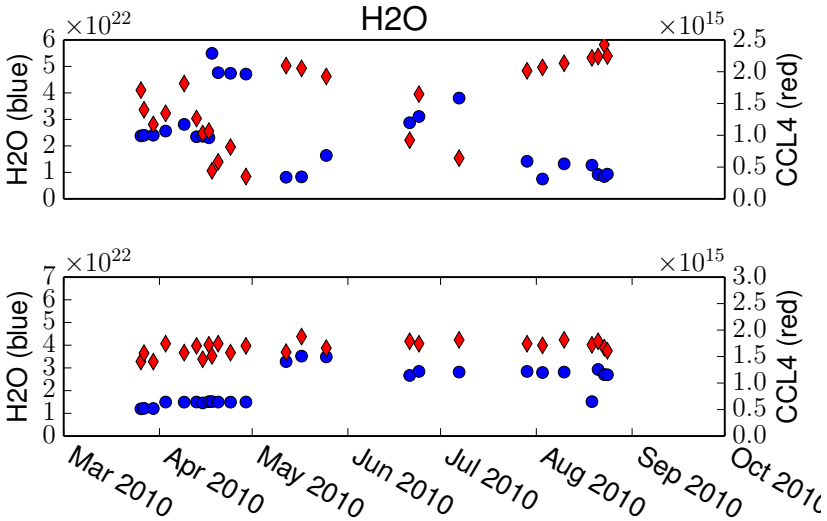


- Disregarding linemixing effects causes strong anti correlation with H2O which is not expected, because CCL4 is a very stable and long-lived gas.



pCqSDHC - partially Correlated quadratic Speed Dependent Hard Collision model

pCqSDHC

- The pCqSDHC function has been proposed by Ngo et.al., 2013 as a replacement for the Voigt line shape model

  HC - hard collision model
  qSD - quadratic speed dependency
  pC - partially correlation of translational and de-phasing effects of collisions

- The model can be used can be used to calculate line mixing in the Rosenberg approximation

$$S(\nu) = \mathrm{Re}(\mathrm{pCqSDHC}) + \gamma \mathrm{Im}(\mathrm{pCqSDHC}) \qquad (4)$$

  -> line-by-line calculation with correction due to line mixing

- The computational effort is about twice as high as evaluating the Voigt function because speed broadening is modeled as a weigthed sum of two Voigt functions
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- ONE PROFILE FOR ALL MOLECULES !!!

Literatur (not complete)