SFIT4 – Retrieval parameters

Mathias Palm

Institute of Environmental Physics
Universität Bremen
Germany

Boulder, 2019

Retrieval parameters

Retrieval parameters

Overview

rt The main parameter rt can be used to switch off and one the retrieval altogether.

rt.lm Switches on or off the Levenberg-Marquardt iteration scheme.

rt.convergence the iteration is considered converged when rt.convergence > D_CHI = (CHI_2_MAX$_{i-1}$ - CHI_2_MAX$_i$)

rt.max_iteration maximum number of iterations

Retrieval parameters

Overview

ITER	FIT_RMS	GAMMA	CHI^2_X	CHI^2_Y	CHI^2	CHI^2_OLD	DCHI^2
1	25.5294	1.00E+05	0.000	886.616			
2	15.7601	1.00E+05	0.000	332.528	332.528	886.616	554.088226
3	9.8038	1.00E+04	0.004	134.162	134.166	332.528	198.361710
4	5.1080	1.00E+03	0.038	32.608	32.646	134.166	101.519910
5	2.6411	1.00E+02	0.105	6.402	6.507	32.646	26.139551
6	1.9136	1.00E+01	0.217	2.831	3.048	6.507	3.458828
7	1.8797	1.00E+00	0.281	2.594	2.875	3.048	0.172872
8	1.8844	1.00E-01	0.300	2.573	2.873	2.875	0.002286

FINAL: MEAN_SNR= 86.6267 MEAN_FIT_RMS(%)= 1.88443 NVAR= 185 NFIT= 3477

BAND	SCAN	RMSSNR (CALCULATED)	(EFFECTIVE)	(RETRIEVED)	CHI^2
1	1	53.98	53.98	49.55	1.19
2	1	57.52	57.52	56.78	1.03
3	1	154.48	154.48	110.55	1.95
4	1	147.91	84.62	50.79	2.92

NEGATIVE MIXING RATIO VALUES FOUND FOR : O3668
NEGATIVE MIXING RATIO VALUES FOUND FOR : O3686

Retrieval parameters

Overview

rt The main parameter rt can be used to switch off and one the retrieval altogether.

rt.lm Switches on or off the Levenberg-Marquardt iteration scheme.

rt.convergence the iteration is considered converged when rt.convergence > D_CHI = (CHI_2_MAX$_{i-1}$ - CHI_2_MAX$_i$)

rt.max_iteration maximum number of iterations

For all retrieval parameters a apriori is given and a standard deviation sigma in the form

rt.x.apriori the apriori of a given value. It is actually applied in the forward calculation. Meaning it can also be used in forward calculations.

rt.x.sigma the entry in the S_A matrix corresponding to this parameter.

Retrieval parameters

Wave number scaling and shifting

rt.wshift wave number shift.

- Shift works on the internal grid **band.X.calc_point_space**
- This is only useful for microwindows (small) because the mismatch is a wavenumber dependent polynomial. For small wave number regions, this can be approximated by a shift.
- This is on top of rt.wave_factor, which is a scaling.
- The artificial grid needs to be more dense than the measured grid

rt.dwshift wave number shift for each retrieved gas separately, except the first retrieved one.

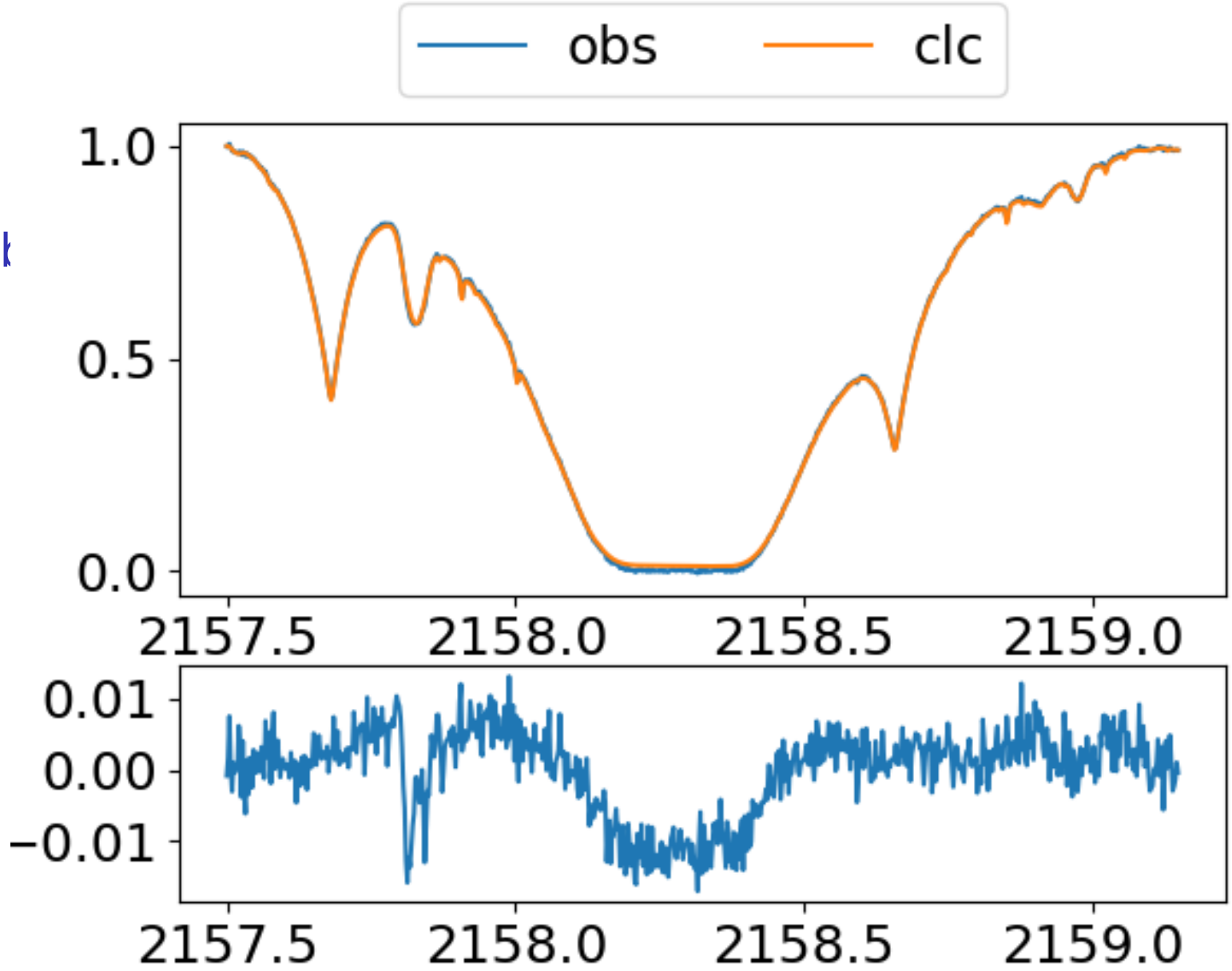
- all lines of each gas are shifted by the same amount (!!!)

offset in window

band.zshift calculates and retrieves an offset in the microwindow. Two types:

.type = 1 retrieves the offset in this MW ONLY ONE!!!

offset in window



offset in window

band.zshift calculates and retrieves an offset in the microwindow. Two types:

- .type = 1 retrieves the offset in this MW ONLY ONE!!!
- .type = 2 uses the offset which is retrieved in another microwindow. THIS MUST BE LATER THAN THE MW USED FOR **ZSHIFT.TYPE=1**

band.zshift.apriori is also an **FW parameter**

offset in window

band.zshift calculates and retrieves an offset in the microwindow. Two types:

- .type = 1 retrieves the offset in this MW ONLY ONE!!!
- .type = 2 uses the offset which is retrieved in another microwindow. THIS MUST BE LATER THAN THE MW USED FOR **ZSHIFT.TYPE=1**

band.zshift.apriori is also an **FW parameter** RETRIEVAL ONLY POSSIBLE IF THERE IS AN SATURATED PART IN THE MW.

channeling in window

The channeling in a MW is calculated via

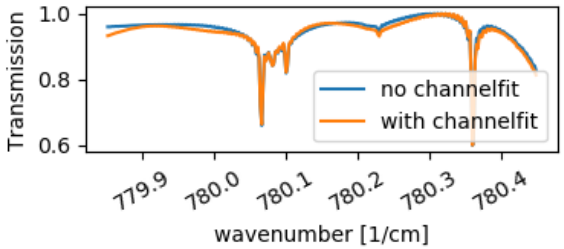
band.x.beam = 1,2 The beams with the numbers 1 and 2 are caclulated

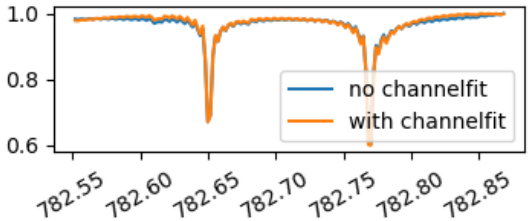
band.x.beam.model = IP, PS which one is better has to be checked.

band.x.beam.1.apriori = AMP, FREQ,PHAS,SLOPE defines the apriori values of the beam 1

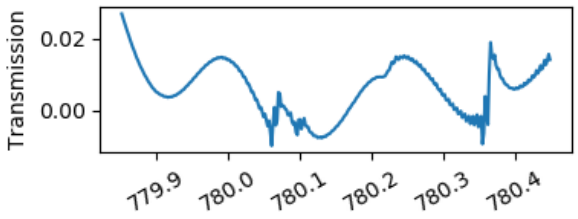
band.x.beam.1.sigma standard deviations for all parameters, i sigma = 0, parameter is not retrieved,

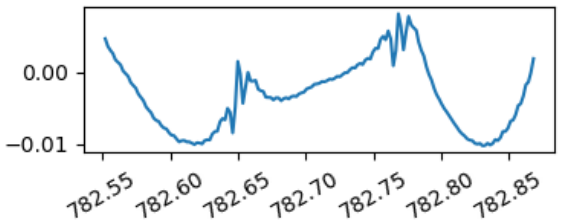
channeling in window





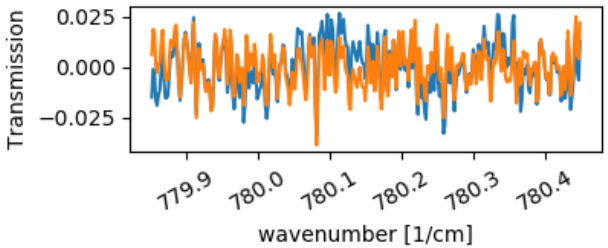
and 2 are

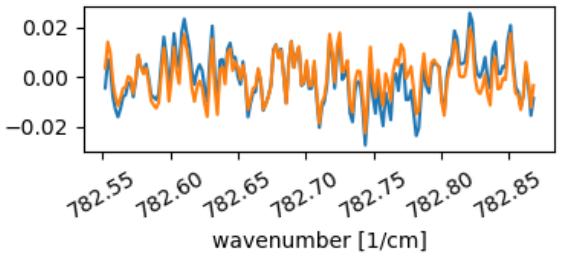




s to be

E defines





rameters, i

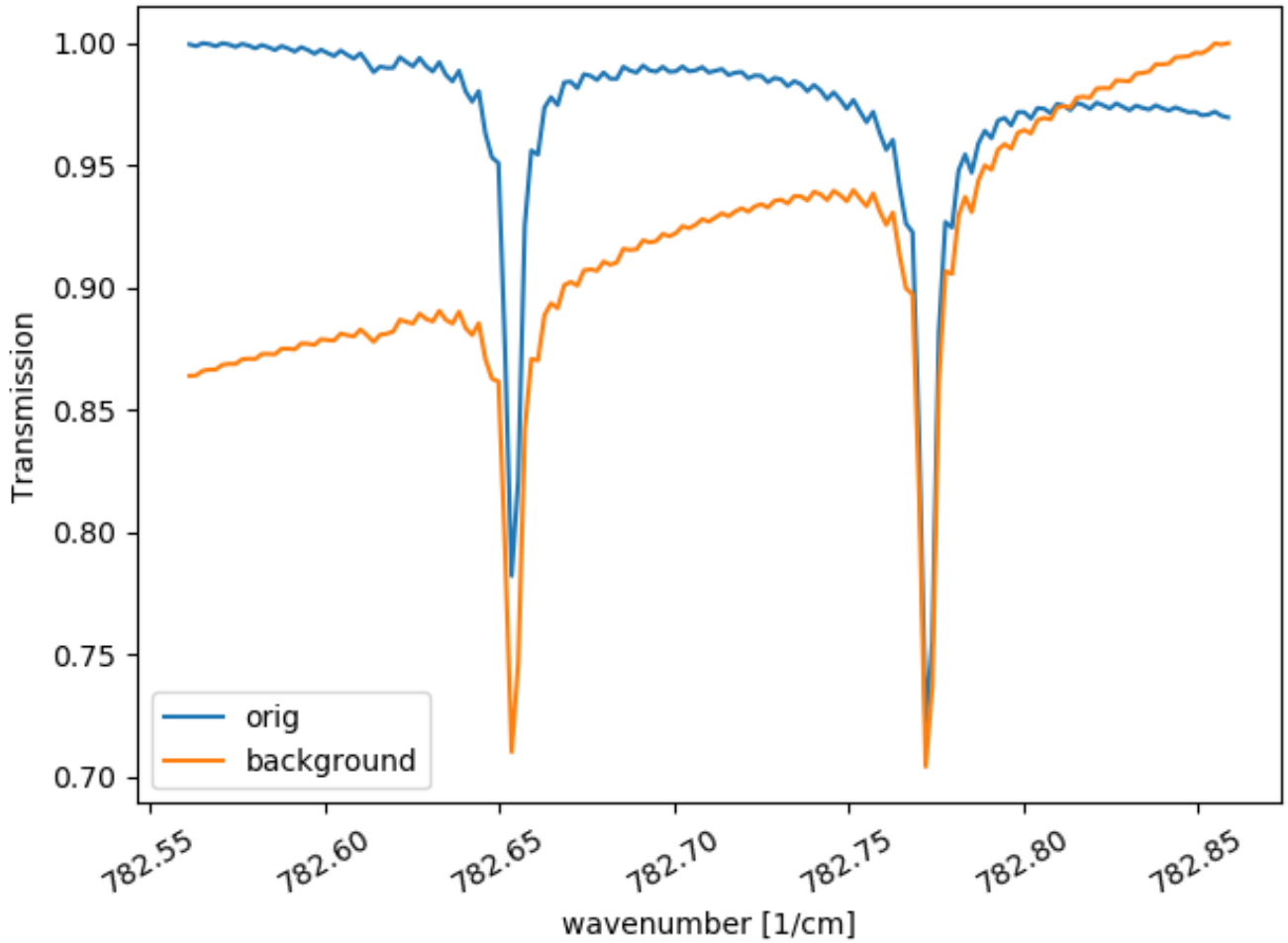
rt.slope and rt.background

rt.slope and rt.background can be used to model a sensitivity function of the instrument, caused by a filter or the wave number dependent sensitivity of the instrument itself.
A function

$$\text{rt.slope} * \nu + \text{rt.background} * \nu^2 \tag{1}$$

is multiplied to the calculated spectrum.

rt.slope and rt.background



sensitivity
*w*ave
lf.

(1)

Retrieval parameters

Construction of the S_A matrix.

The S_A matrix is constructed from the sigma values given. How this is actually done, depends on the parameters. In principle the S_A is constructed as a diagonal matrix and inverted in the code to yield the S_A^{-1} matrix. Some caveats:

gas.profile.x.correlation off diagonals using the sigma values as maxima

- .type = 1 gaussian with FWHM = .width
- .type = 2 exponentially with FWHM = .width
- .type = 3 not used
- .type = 4 the S_A matrix is read in from file.sa_matrix
- .type = 5 the S_A^{-1} matrix is read in from file.sa_matrix

Retrieval parameters

Construction of the S_A matrix.

The S_A matrix is constructed from the sigma values given. How this is actually done, depends on the parameters. In principle the S_A is constructed as a diagonal matrix and inverted in the code to yield the S_A^{-1} matrix. Some caveats:

gas.profile.x.regmethod lets you chose between OE optimization and the Thikonov-Phillips regularization with L1 constraint (smoothness constraint)

.type = 'OE' optimal estimation (Rodgers, 2000)

.type = 'TP' Thikonov-Phillips with smoothness constraint

.lambda strength of the regularization in TP. The higher the value the less is the regularization.

The smoothness constraint is calculated from file.stalayers in order to adapt for non-unique altitude layering. The matrix is scaled using the gas.profile.x.sigma values.

Retrieval parameters

SFIT

```
ITER   FIT_RMS      GAMMA   CHI^2_X   CHI^2_Y      CHI^2 CHI^2_OLD       DCHI^2
   1   25.5294  1.00E+05     0.000   886.616
   2   15.7601  1.00E+05     0.000   332.528   332.528   886.616   554.088226
   3    9.8038  1.00E+04     0.004   134.162   134.166   332.528   198.361710
   4    5.1080  1.00E+03     0.038    32.608    32.646   134.166   101.519910
   5    2.6411  1.00E+02     0.105     6.402     6.507    32.646    26.139551
   6    1.9136  1.00E+01     0.217     2.831     3.048     6.507     3.458828
   7    1.8797  1.00E+00     0.281     2.594     2.875     3.048     0.172872
   8    1.8844  1.00E-01     0.300     2.573     2.873     2.875     0.002286

FINAL:    MEAN_SNR= 86.6267  MEAN_FIT_RMS(%)= 1.88443  NVAR= 185  NFIT= 3477

  BAND   SCAN   RMSSNR (CALCULATED)   (EFFECTIVE)   (RETRIEVED)         CHI^2
     1      1                53.98         53.98         49.55          1.19
     2      1                57.52         57.52         56.78          1.03
     3      1               154.48        154.48        110.55          1.95
     4      1               147.91         84.62         50.79          2.92

NEGATIVE MIXING RATIO VALUES FOUND FOR : O3668
NEGATIVE MIXING RATIO VALUES FOUND FOR : O3686
```

FIT_RMS mean variance of the residuum

GAMMA the Levenberg Marquardt Parameter

CHI_2_X A measure of the deviation of the retrieved state from the A PRIORI

Retrieval parameters

SFIT

```
ITER   FIT_RMS      GAMMA   CHI^2_X   CHI^2_Y      CHI^2 CHI^2_OLD       DCHI^2
   1   25.5294  1.00E+05     0.000   886.616
   2   15.7601  1.00E+05     0.000   332.528   332.528   886.616   554.088226
   3    9.8038  1.00E+04     0.004   134.162   134.166   332.528   198.361710
   4    5.1080  1.00E+03     0.038    32.608    32.646   134.166   101.519910
   5    2.6411  1.00E+02     0.105     6.402     6.507    32.646    26.139551
   6    1.9136  1.00E+01     0.217     2.831     3.048     6.507     3.458828
   7    1.8797  1.00E+00     0.281     2.594     2.875     3.048     0.172872
   8    1.8844  1.00E-01     0.300     2.573     2.873     2.875     0.002286

FINAL:    MEAN_SNR= 86.6267  MEAN_FIT_RMS(%)= 1.88443  NVAR= 185  NFIT= 3477

  BAND   SCAN   RMSSNR (CALCULATED)   (EFFECTIVE)   (RETRIEVED)         CHI^2
     1      1                53.98         53.98         49.55          1.19
     2      1                57.52         57.52         56.78          1.03
     3      1               154.48        154.48        110.55          1.95
     4      1               147.91         84.62         50.79          2.92

NEGATIVE MIXING RATIO VALUES FOUND FOR : O3668
NEGATIVE MIXING RATIO VALUES FOUND FOR : O3686
```

CHI_2_Y A measure for the retrieval quality

$$\chi^2_Y = \frac{(y_M - y_C)^T S_\epsilon (y_M - y_C)}{m}$$

$\chi^2_Y = 1$ if the residuum is reduced to the noise as specified in S_ϵ

Retrieval parameters

SFIT

```
ITER   FIT_RMS      GAMMA   CHI^2_X   CHI^2_Y      CHI^2 CHI^2_OLD       DCHI^2
   1   25.5294  1.00E+05     0.000   886.616
   2   15.7601  1.00E+05     0.000   332.528   332.528   886.616   554.088226
   3    9.8038  1.00E+04     0.004   134.162   134.166   332.528   198.361710
   4    5.1080  1.00E+03     0.038    32.608    32.646   134.166   101.519910
   5    2.6411  1.00E+02     0.105     6.402     6.507    32.646    26.139551
   6    1.9136  1.00E+01     0.217     2.831     3.048     6.507     3.458828
   7    1.8797  1.00E+00     0.281     2.594     2.875     3.048     0.172872
   8    1.8844  1.00E-01     0.300     2.573     2.873     2.875     0.002286

FINAL:    MEAN_SNR= 86.6267  MEAN_FIT_RMS(%)= 1.88443  NVAR= 185  NFIT= 3477

  BAND   SCAN   RMSSNR (CALCULATED)   (EFFECTIVE)   (RETRIEVED)          CHI^2
     1      1                53.98         53.98         49.55           1.19
     2      1                57.52         57.52         56.78           1.03
     3      1               154.48        154.48        110.55           1.95
     4      1               147.91         84.62         50.79           2.92

NEGATIVE MIXING RATIO VALUES FOUND FOR : 03668
NEGATIVE MIXING RATIO VALUES FOUND FOR : 03686
```

- In the lower half, the retrieval diagnostics for the last calculation are shown for each MW.
- A warning if retrieved profiles have negative parts

Retrieval parameters

SFIT

```
ITER   FIT_RMS      GAMMA   CHI^2_X   CHI^2_Y      CHI^2 CHI^2_OLD       DCHI^2
   1   25.5294  1.00E+05     0.000   886.616
   2   15.7601  1.00E+05     0.000   332.528   332.528   886.616   554.088226
   3    9.8038  1.00E+04     0.004   134.162   134.166   332.528   198.361710
   4    5.1080  1.00E+03     0.038    32.608    32.646   134.166   101.519910
   5    2.6411  1.00E+02     0.105     6.402     6.507    32.646    26.139551
   6    1.9136  1.00E+01     0.217     2.831     3.048     6.507     3.458828
   7    1.8797  1.00E+00     0.281     2.594     2.875     3.048     0.172872
   8    1.8844  1.00E-01     0.300     2.573     2.873     2.875     0.002286

FINAL:    MEAN_SNR= 86.6267  MEAN_FIT_RMS(%)= 1.88443  NVAR= 185  NFIT= 3477

  BAND   SCAN   RMSSNR (CALCULATED)   (EFFECTIVE)   (RETRIEVED)         CHI^2
     1      1                53.98         53.98         49.55          1.19
     2      1                57.52         57.52         56.78          1.03
     3      1               154.48        154.48        110.55          1.95
     4      1               147.91         84.62         50.79          2.92

NEGATIVE MIXING RATIO VALUES FOUND FOR : O3668
NEGATIVE MIXING RATIO VALUES FOUND FOR : O3686
```

Iteration stopped if either DCHI < rt.convergence or ITER > rt.max_iteration, what ever comes first.

The finish

```
  BAND   SCAN   RMSSNR (CALCULATED)   (EFFECTIVE)   (RETRIEVED)         CHI^2
     1      1                138.44        138.44        113.72          1.48
     2      1                146.53        146.53        143.52          1.04
     3      1                327.50        327.50        185.55          3.12
     4      1                319.57        146.69         81.72          2.40

NEGATIVE MIXING RATIO VALUES FOUND FOR : H2O
NEGATIVE MIXING RATIO VALUES FOUND FOR : C2H4

 O3     : T  H2O    : T  CO2    : F  O3668  : F  O3686  : F  C2H4   : F
 9.5734E+18  5.2139E+22  7.9696E+21  1.6077E+19  1.6077E+19  9.8413E+14
 1.0921E+19  4.1944E+22  1.4369E+22  1.6255E+19  1.5224E+19 -9.1080E+14

Itr/Mx:05/15 %RMS=1.125 FitPrm=117 CVRG:T DIVW:F DOFS=4.755 SNR=  162. CHI_2_Y=   2.2875

 RDRV: DONE. ELAPSED TIME =    200.01916800000001
```