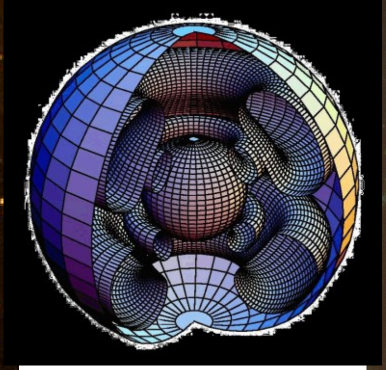
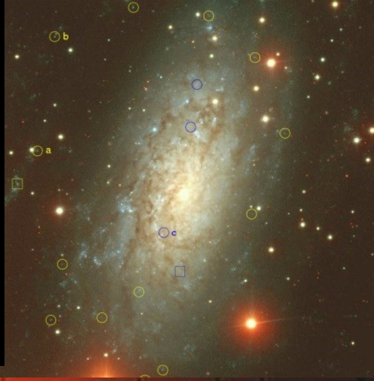
$$n_i \sum_{j\neq i}(R_{ij}+C_{ij}) = \sum_{j\neq i} n_j(R_{ji}+C_{ji})$$

$$\mu \frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu} = I_\nu - S_\nu$$





Sky Emission and Telluric Absorption Lines

Basics and Model-based Correction

Norbert Przybilla

Thanks: Wolfgang Kausch

Institute for Astro- and Particle Physics

universität innsbruck

Meet the Innsbruck ESO In-Kind Project
Main Actors

Stefan Kimeswenger

Wolfgang Kausch

Stefan Noll

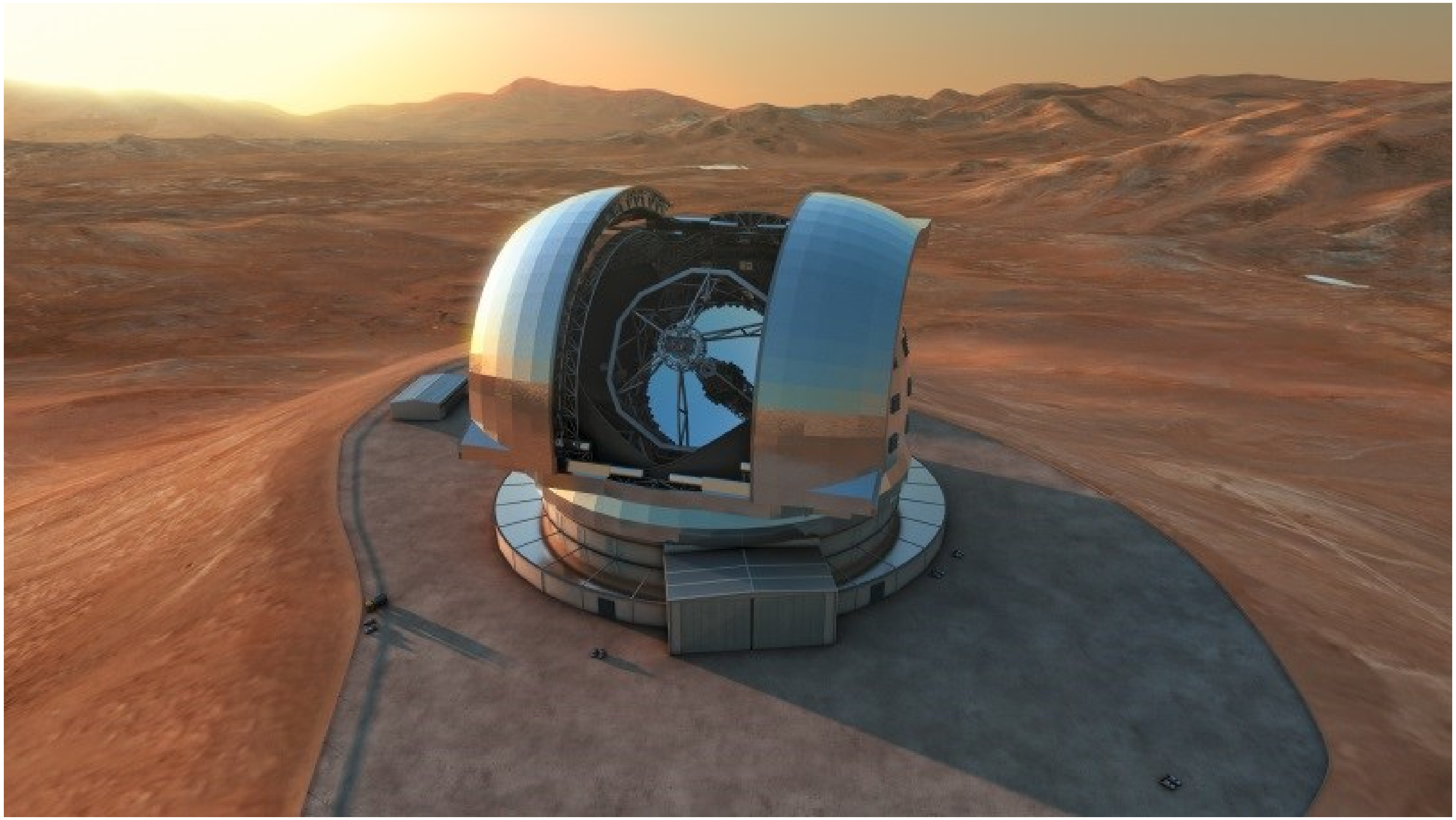
Amy M. Jones

Topics:

- sky model:
  Link **SkyCalc** on
  `www.eso.org/observing/etc/`
- telluric line correction
- sky emission correction

codes, manuals, tutorial download:
`http://www.eso.org/pipelines/skytools`

E-ELT



- mainly infrared telescope
- ground based ➔ light has to pass the Earth's atmosphere
- impact of atmosphere high in the IR, higher than in optical

➔ corrections required to recover astronomical spectra critical for observations with ELTs

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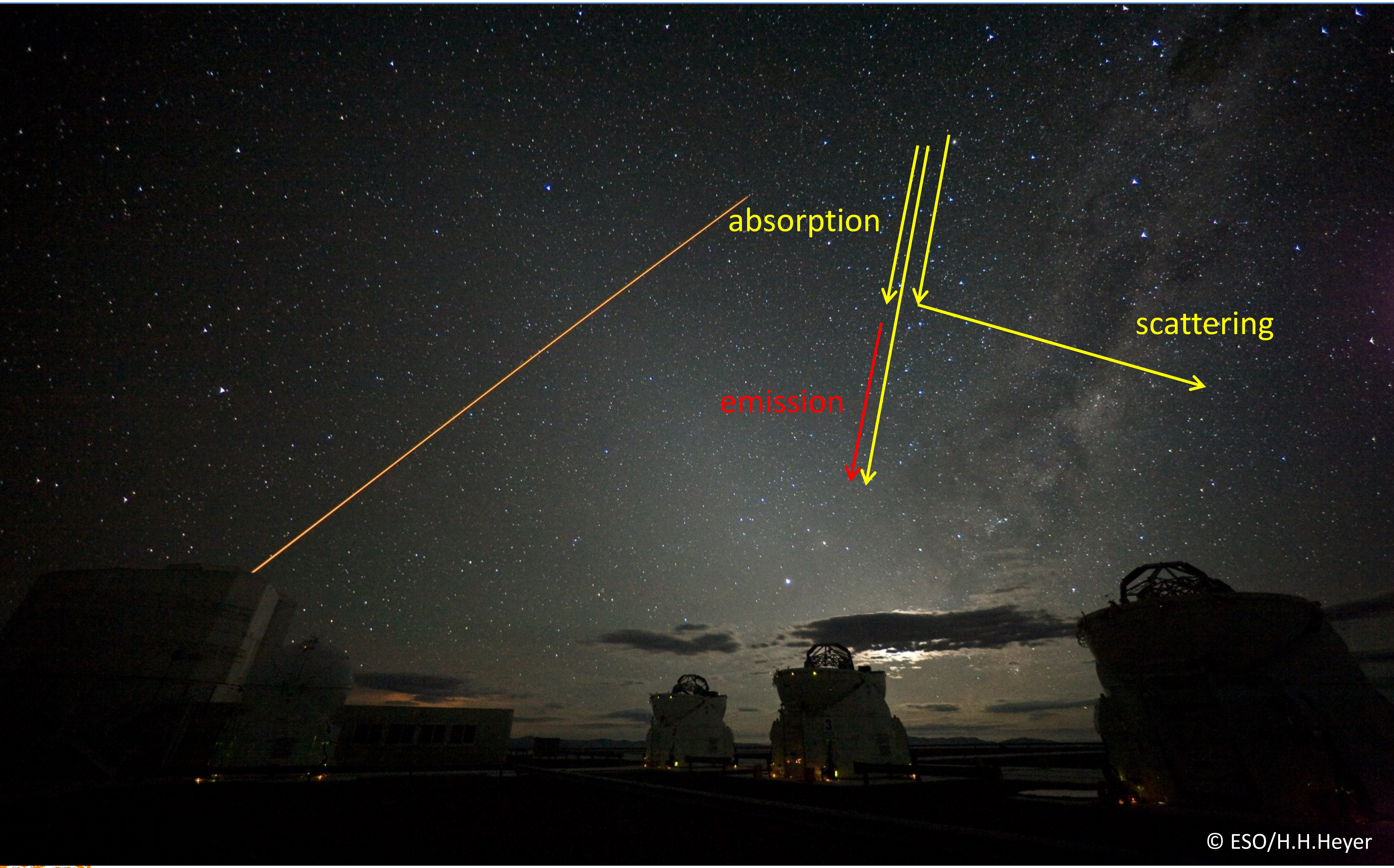
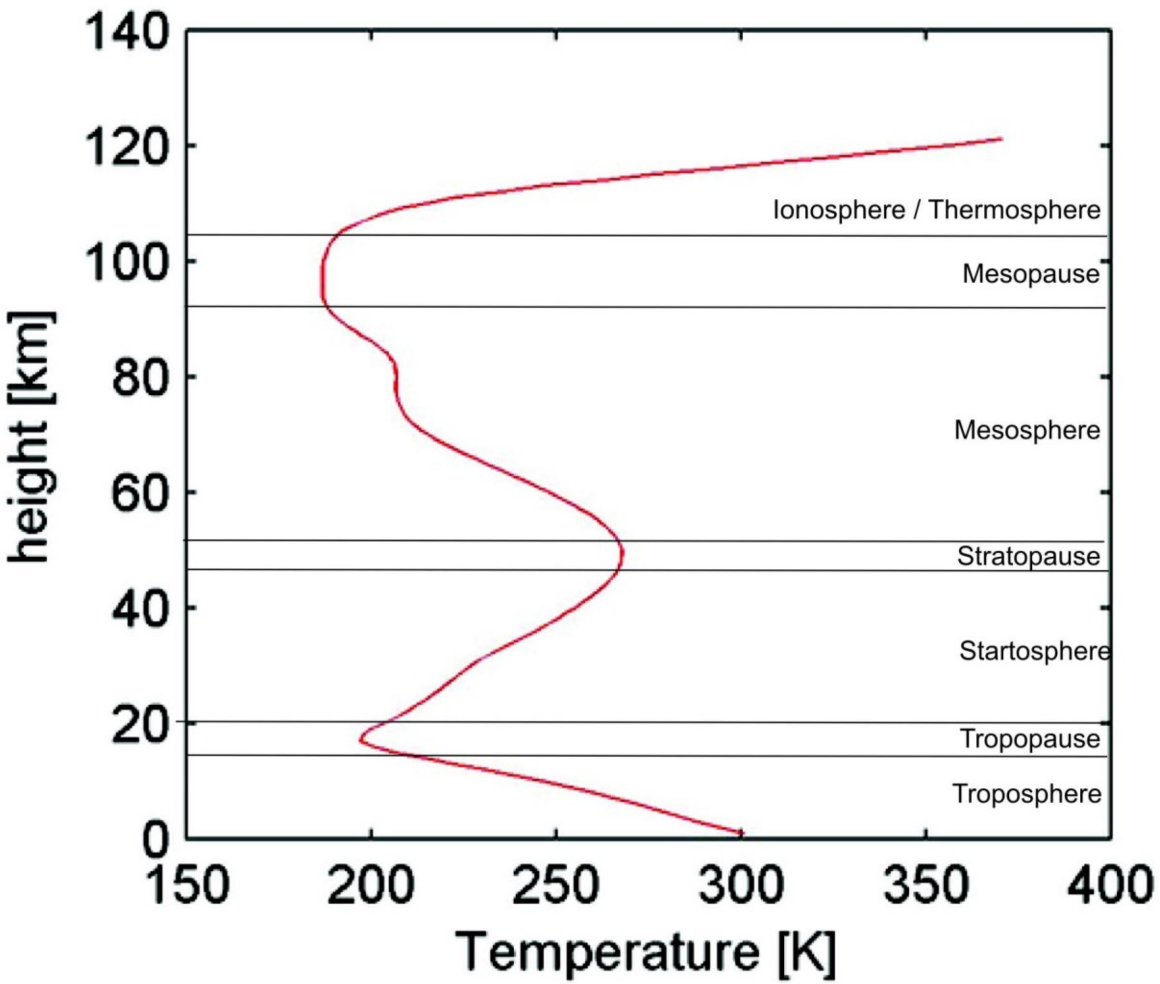
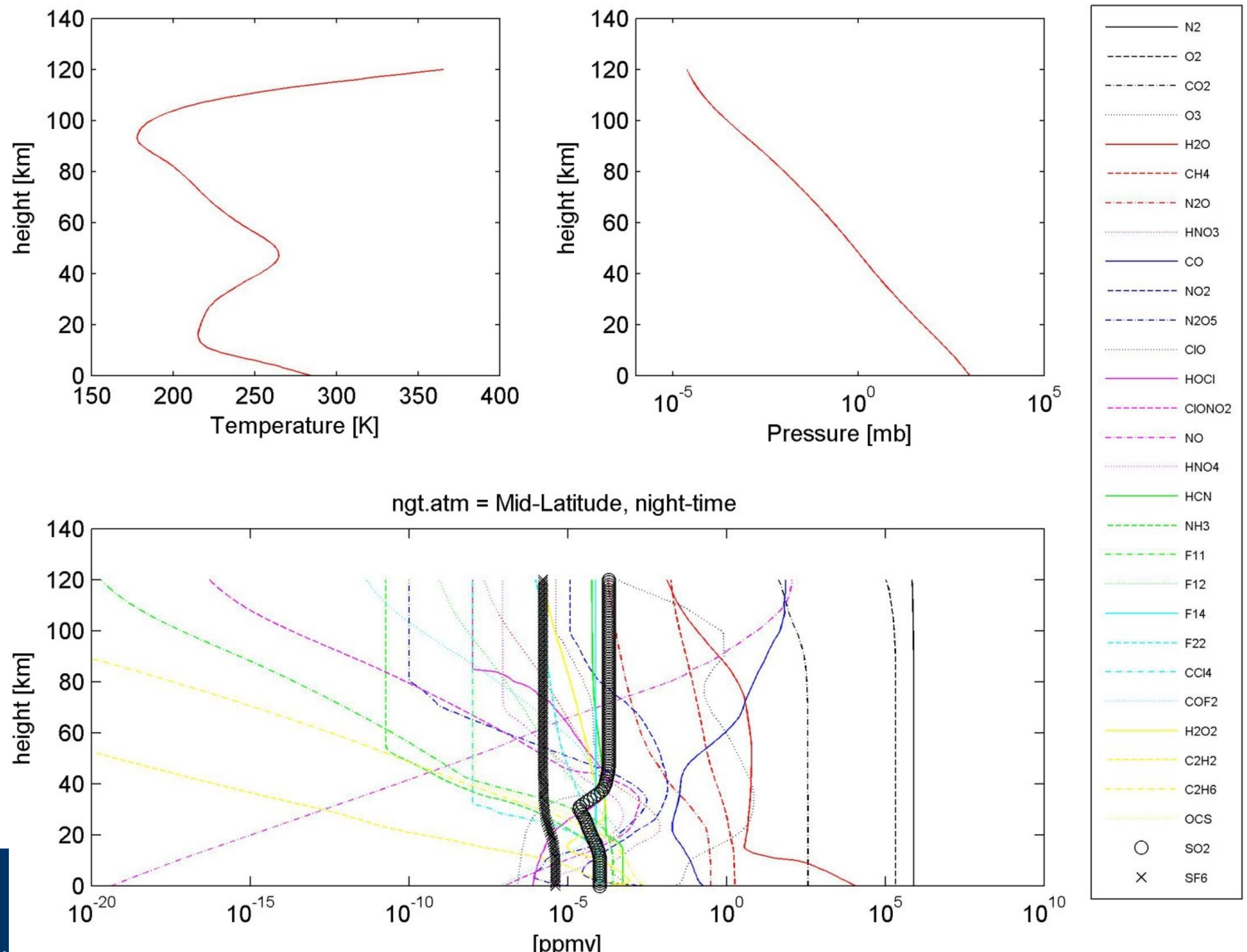
Earth‘s Atmosphere: Effects



Earth‘s Atmosphere: Layers



Standard Atmosphere
mid-latitude

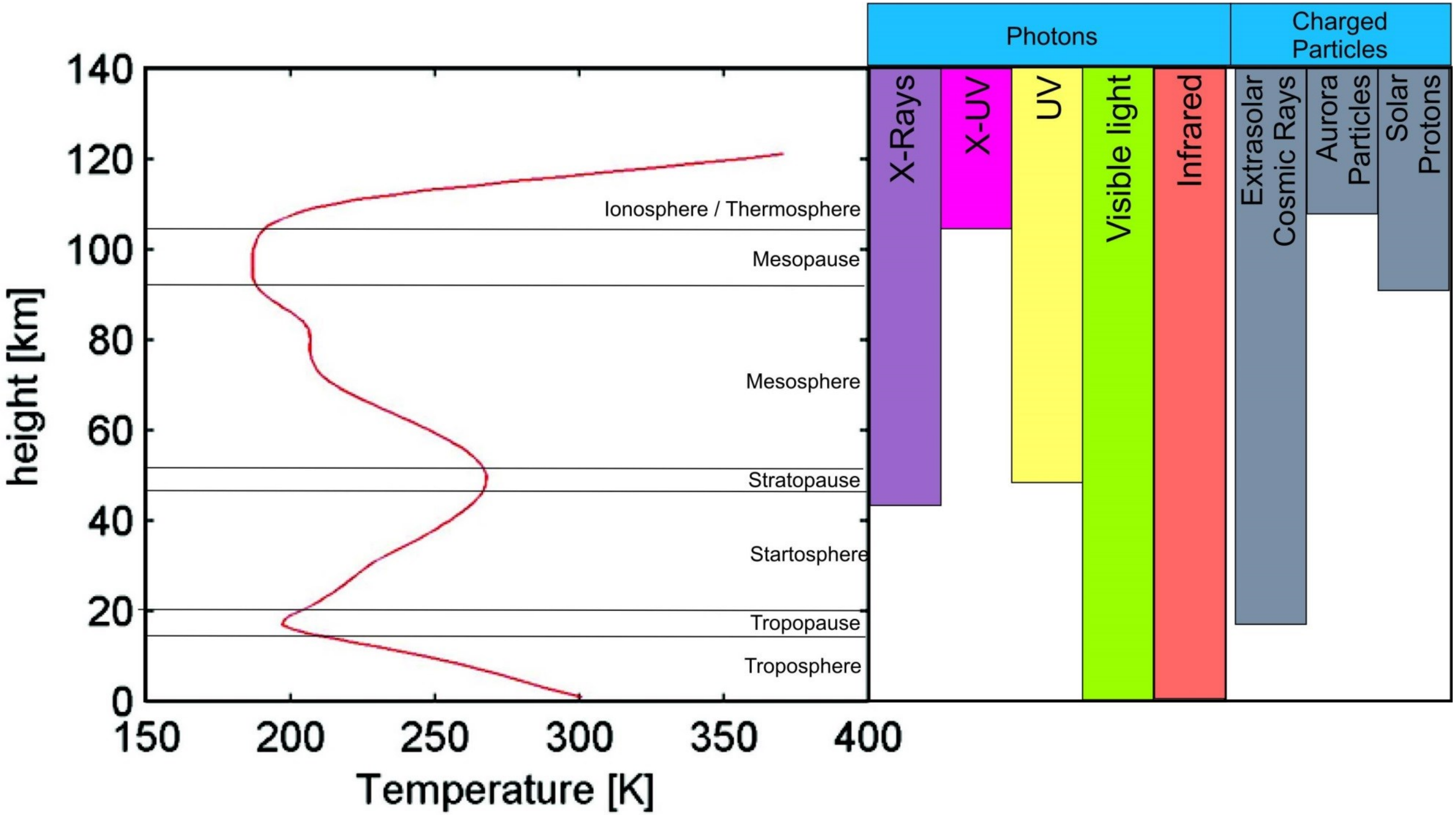


main components:

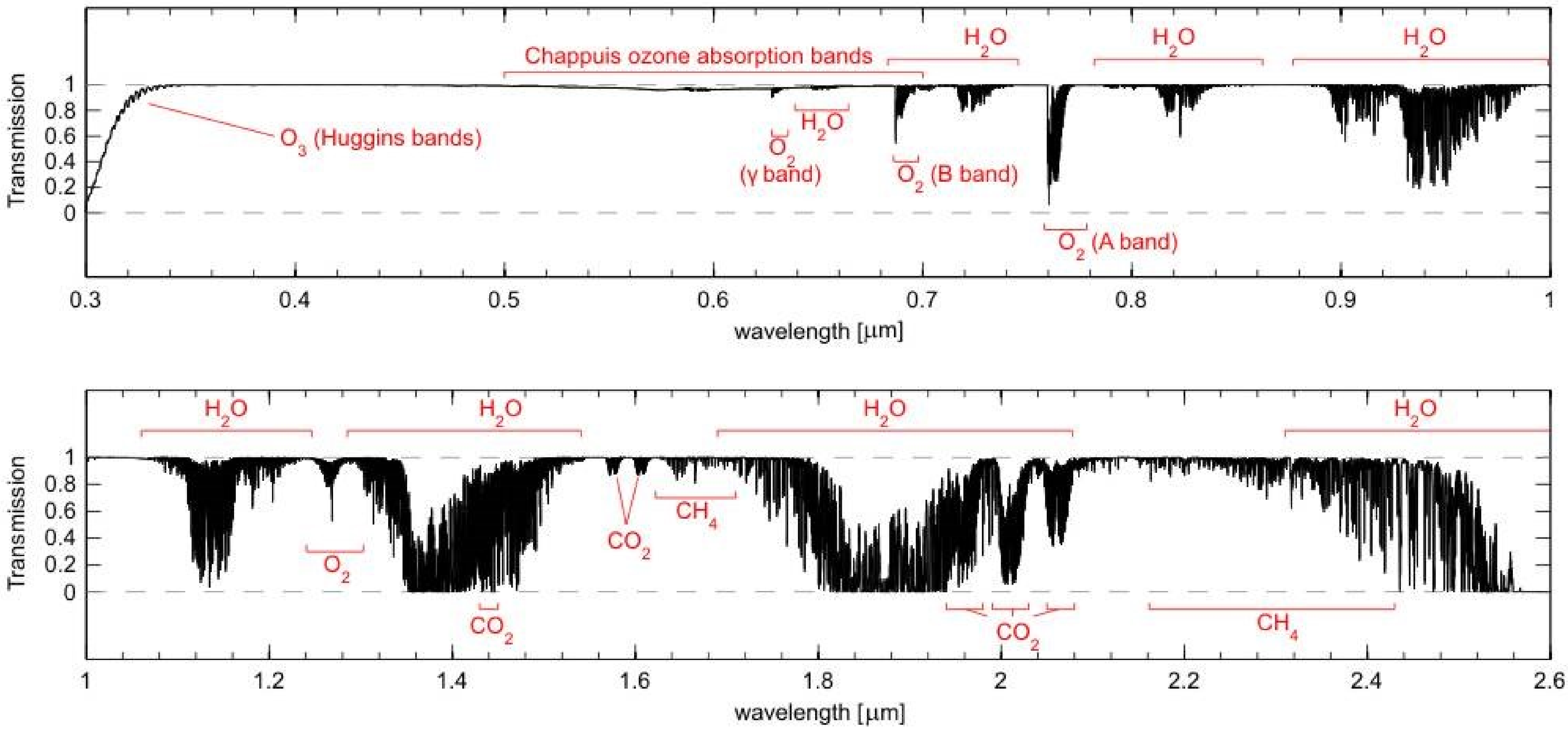
N_2: 78.084%
O_2: 20.946%
Ar: 0.934%
CO_2: ~0.04% !

http://www.atm.ox.ac.uk/RFM/atm/

Earth's Atmosphere
Interaction with Radiation and Charged Particles



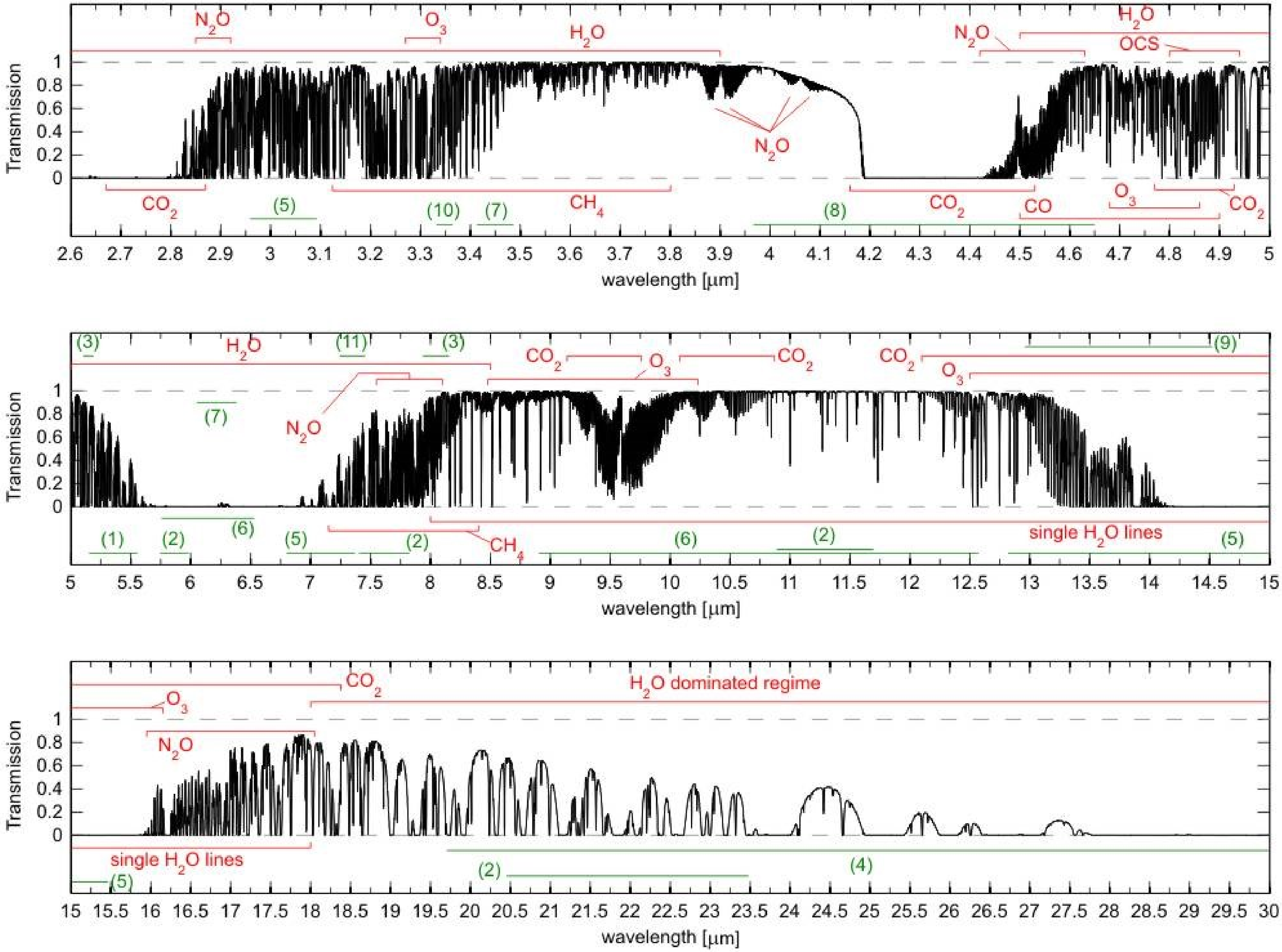
Atmospheric Absorption: Optical + NIR



Smette et al. 2015, A&A, 576, A77

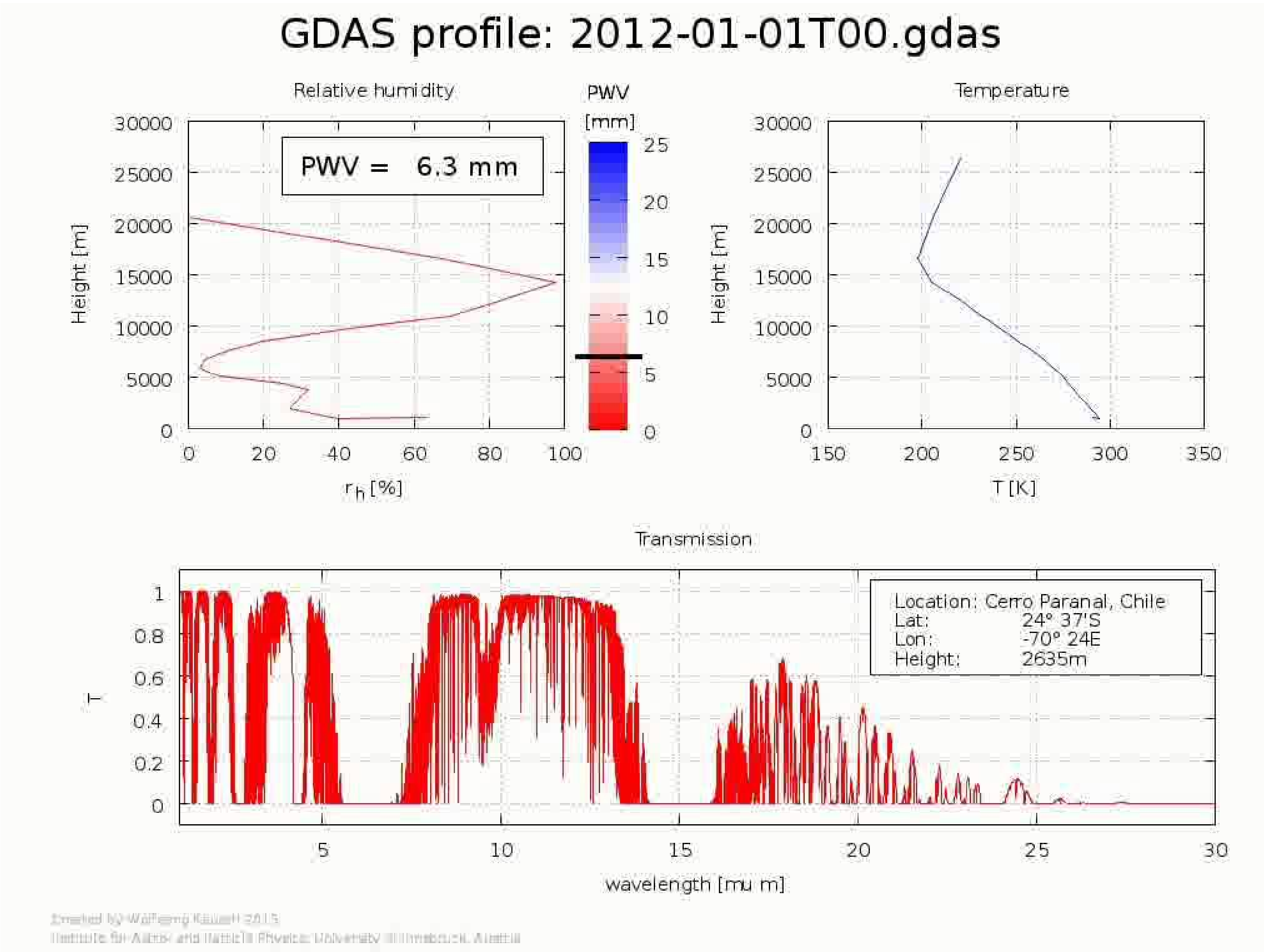
Atmospheric Absorption: MIR

Smette et al. 2015, A&A, 576, A77

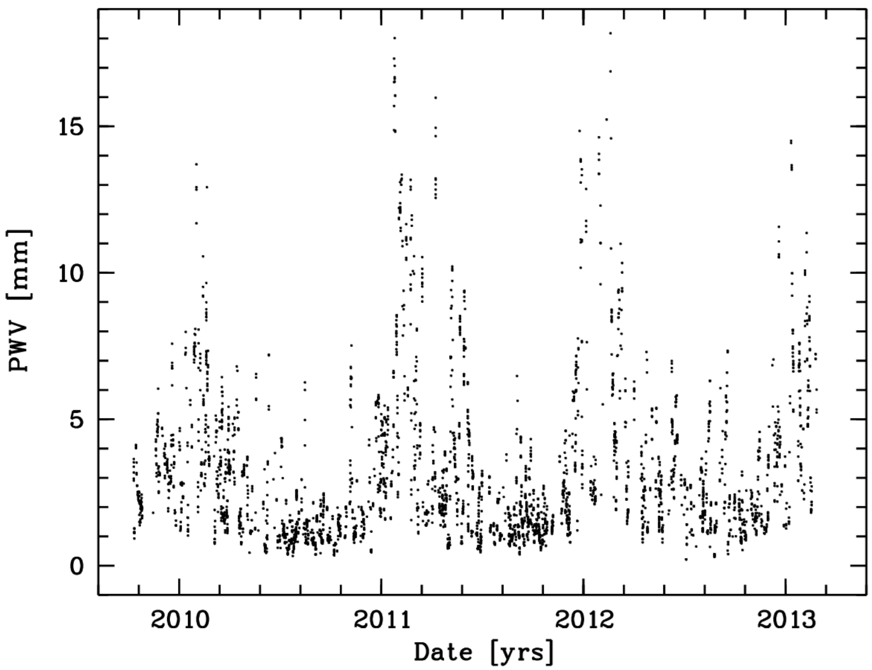


Trace gases: (1) NO, (2) HNO_3, (3) COF_2, (4) H_2O_2, (5) HCN, (6) NH_3, (7) NO_2, (8) N_2, (9) C_2H_2, (10), C_2H_6, (11) SO_2.

Variability: H_2O

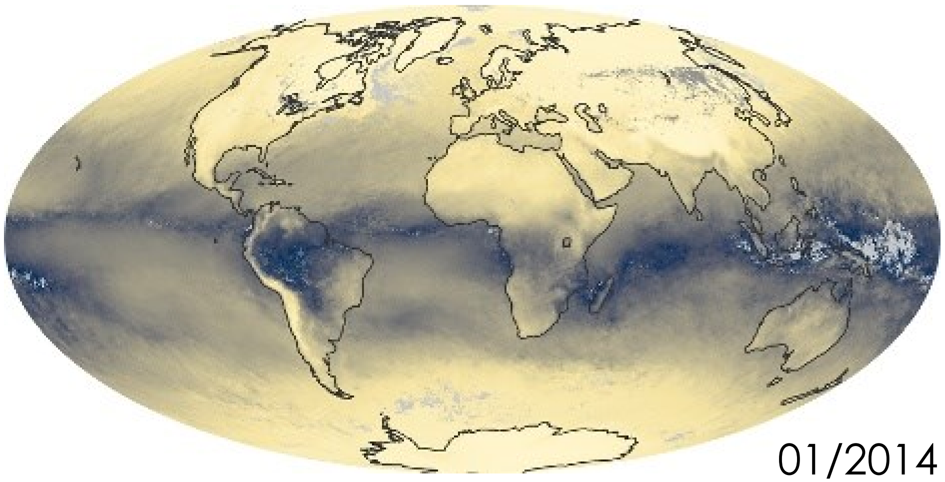


Variability: H_2O

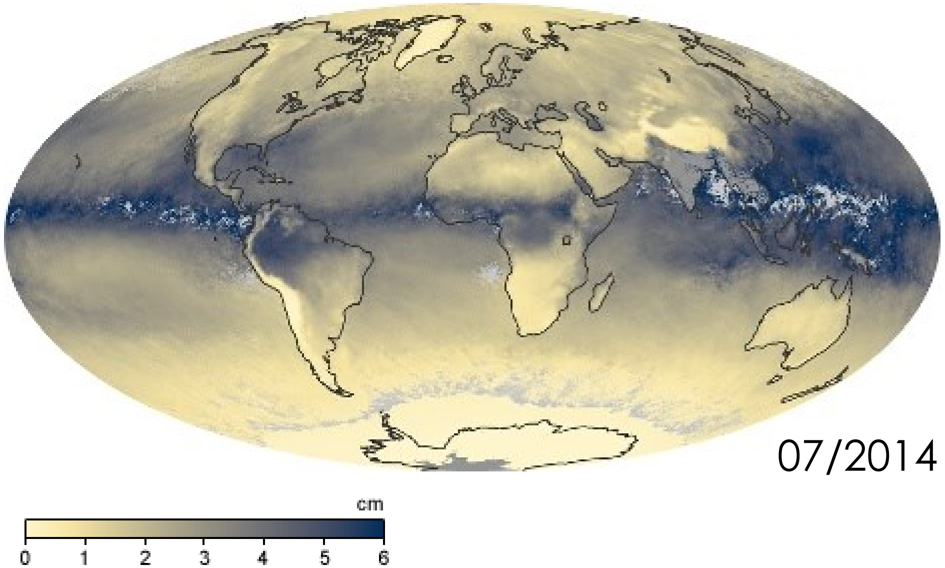


Cerro Paranal:
PWV from X-shooter echelle spectra

Kausch et al. 2015, A&A 576, A78



01/2014



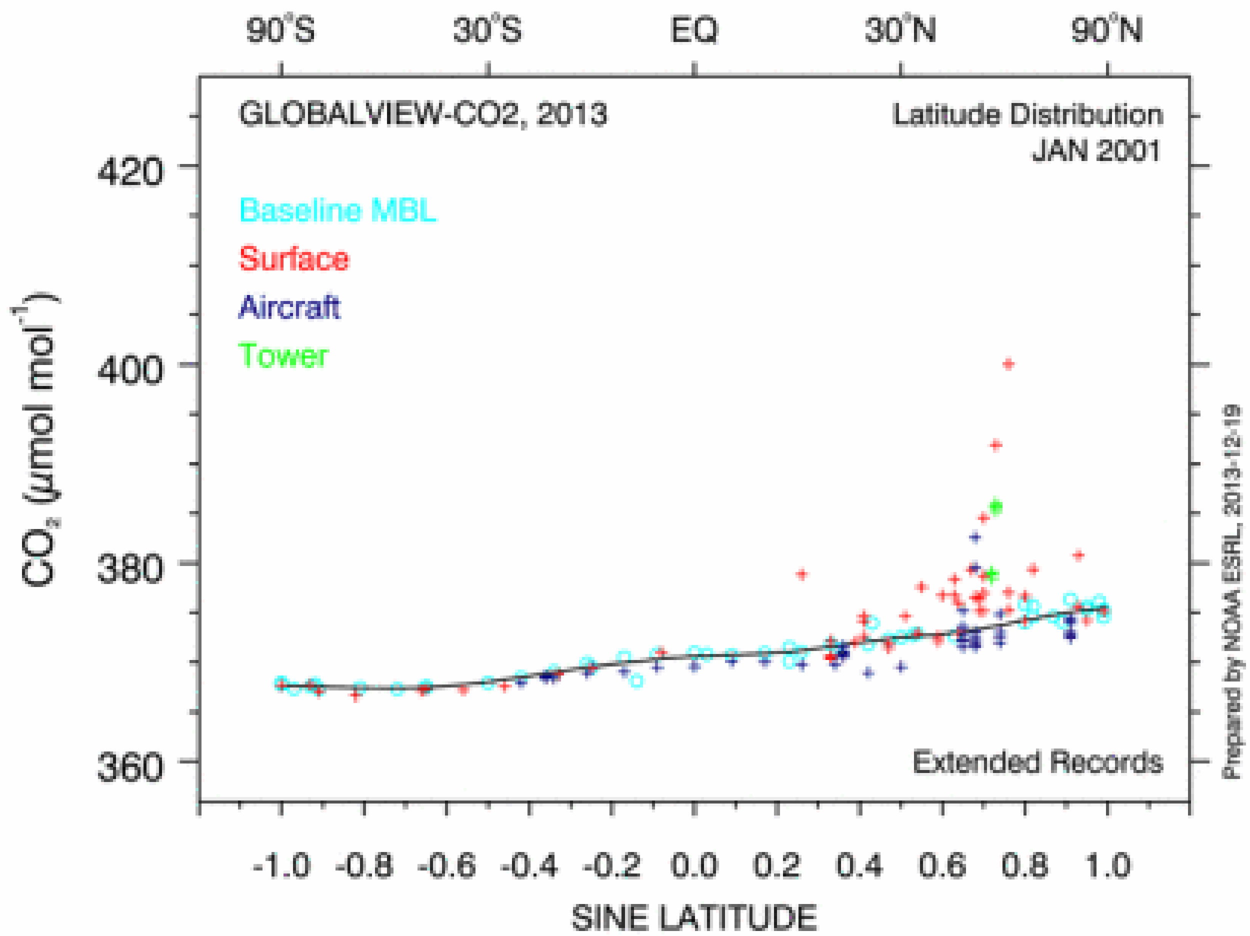
07/2014

Global Aqua/MODIS data for January and July 2014

http://earthobservatory.nasa.gov/

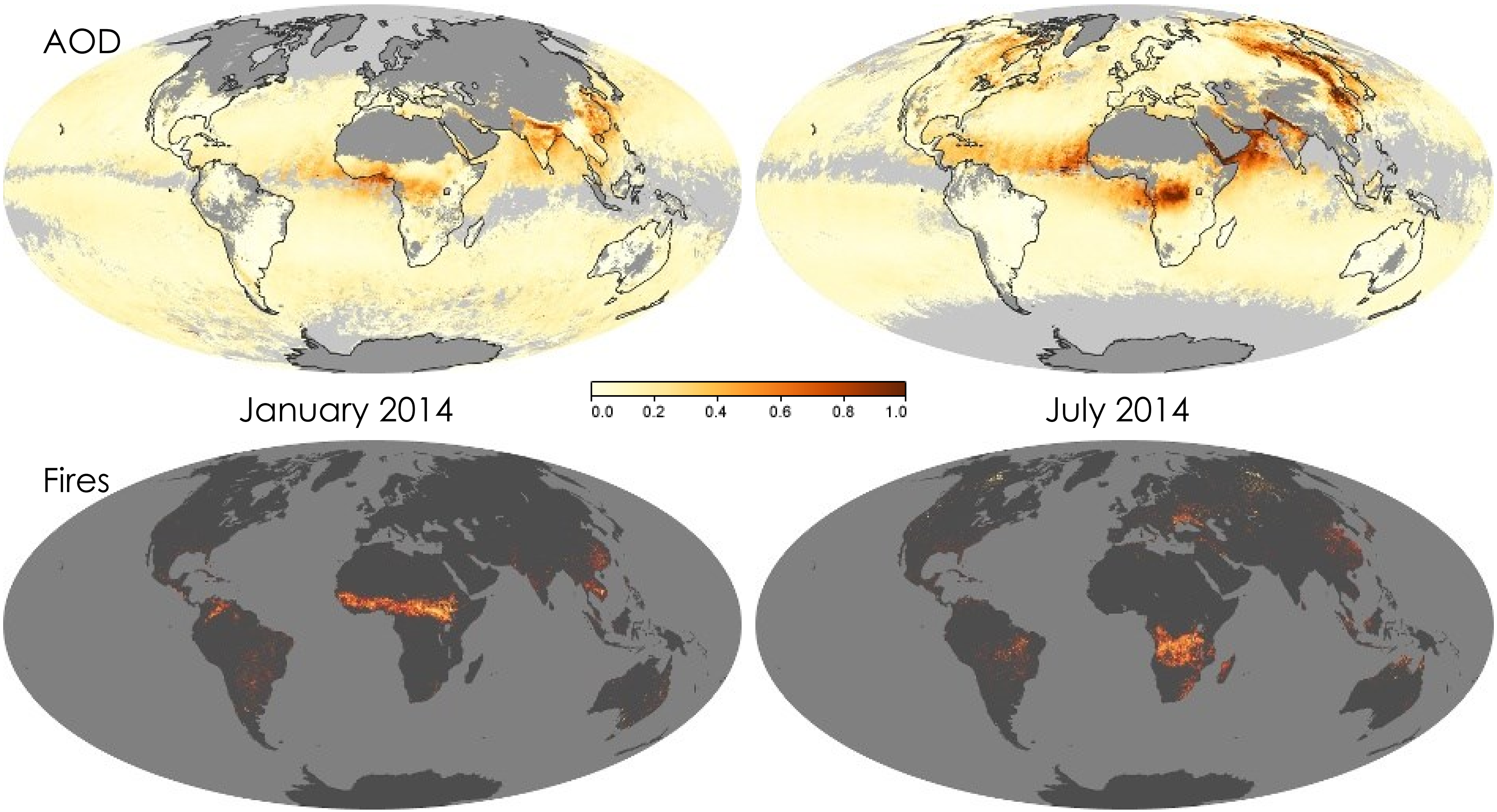
Variability: CO_2

Jan 2001 – Dec 2012



ESRL/NOAA
http://www.esrl.noaa.gov/gmd/ccgg/globalview/co2/co2_intro.html

Variability: Aerosols



Global Terra/MODIS aerosol optical depth (AOD)
and fire data for January and July 2014
http://earthobservatory.nasa.gov/

Variability

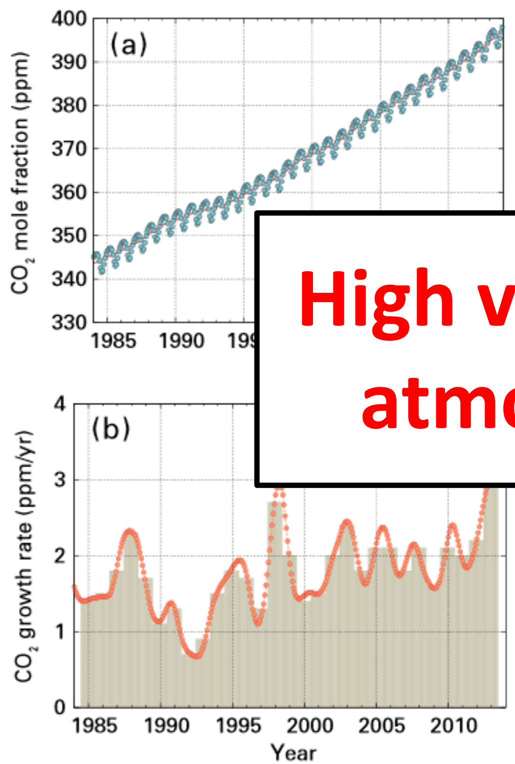


Figure 3. Globally averaged CO_2 mole fraction (a) and its growth rate (b) from 1984 to 2013. Differences in successive annual means are shown as shaded columns in (b).

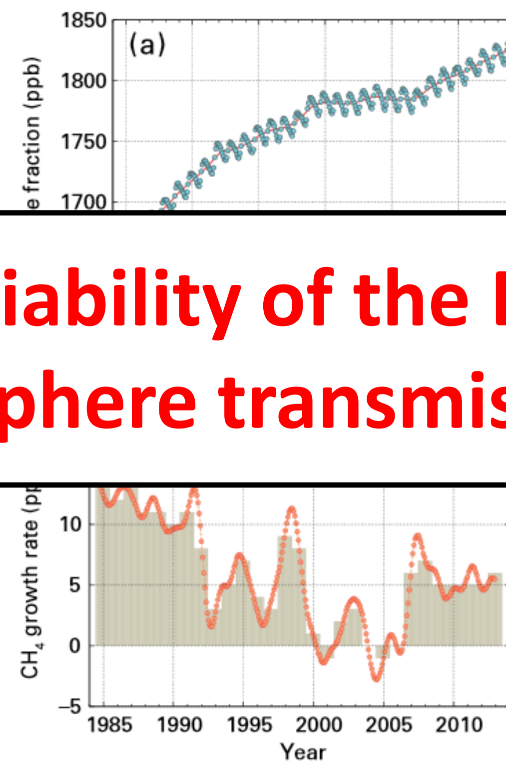


Figure 4. Globally averaged CH_4 mole fraction (a) and its growth rate (b) from 1984 to 2013. Differences in successive annual means are s
columns in (b).

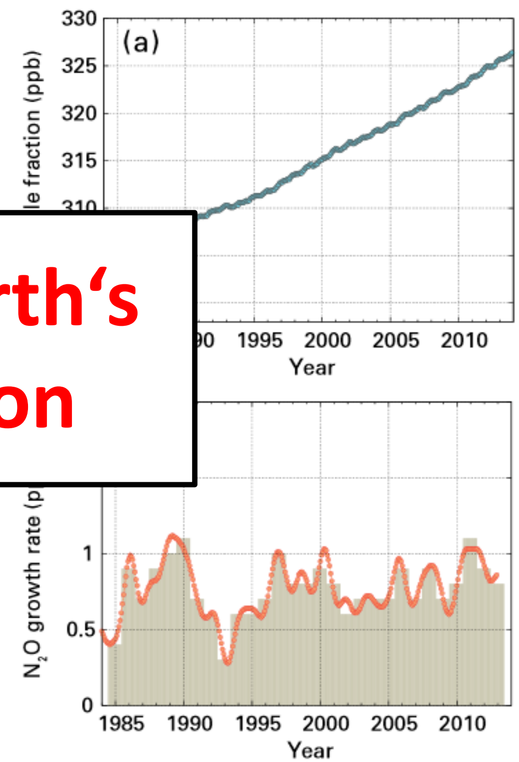


Figure 5. Globally averaged N_2O mole fraction (a) and its growth rate (b) from 1984 to 2013. Differences in successive

High variability of the Earth's atmosphere transmission

What about emission?

WMO Greenhouse Gas Bulletin No. 10, 6 Nov 2014

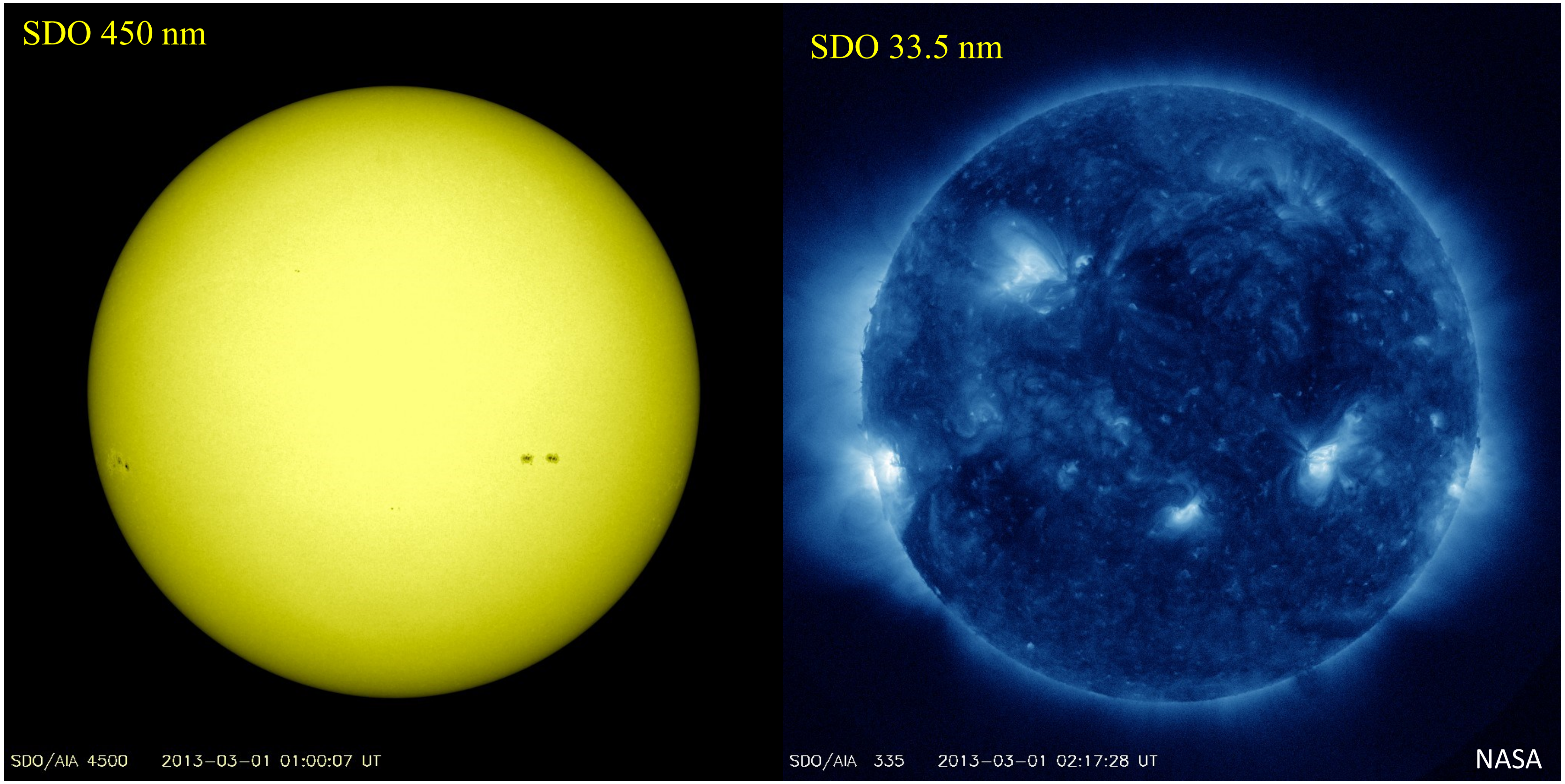
Airglow

= light emission by chemiluminiscence

- upper atmosphere (meso- to thermosphere)

Airglow

.....powered by the Sun's extreme UV photons



Solar UV photons can destroy molecules in the Earth's upper atmosphere.

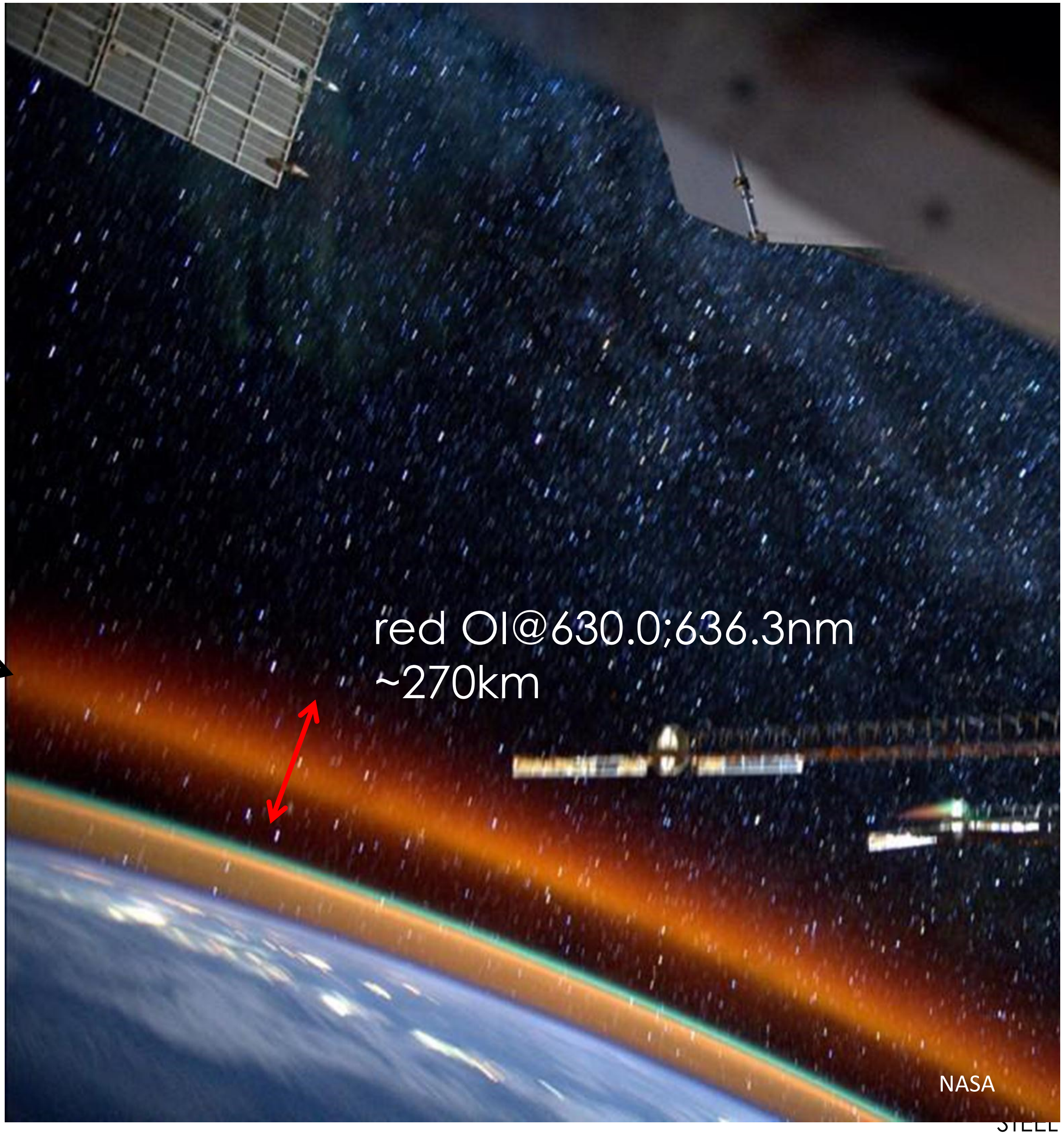
Airglow

Red OI airglow

Reaction:

$O_2^+ + e^- \rightarrow O + O(^1D)$
$O(^1D) \rightarrow O(^3P_2) + h\nu$ (630.0nm)
$O(^1D) \rightarrow O(^3P_1) + h\nu$ (636.3nm)

Bates (1982)



Airglow

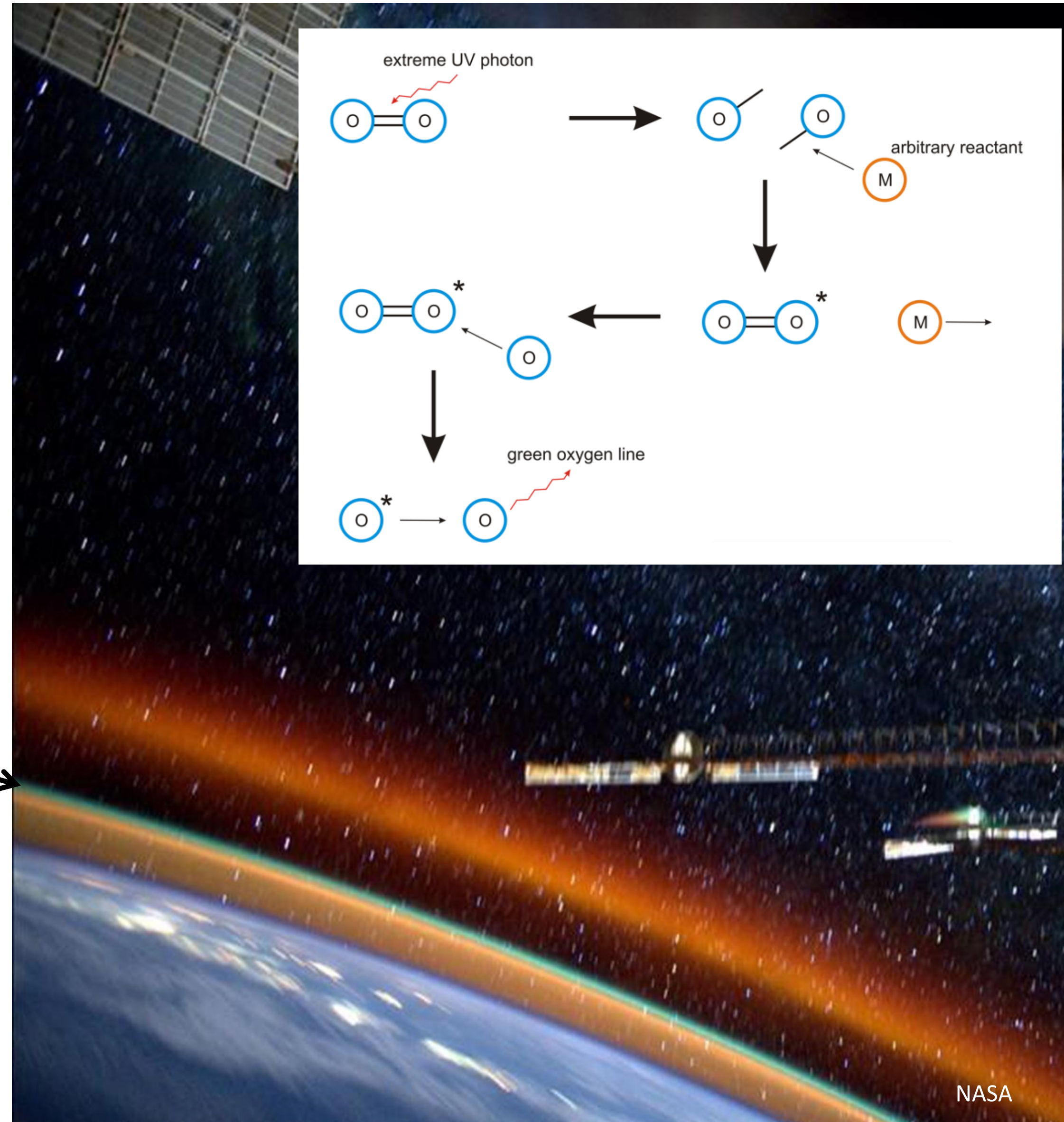
Oxygen airglow

Reaction:

$O_2 + h\nu\ (<0.24\mu m) \rightarrow O + O$
$O + O + M \rightarrow O_2^* + M$
$O_2^* + O \rightarrow O_2 + O^*(^1S)$
$O^*(^1S) \rightarrow O(1D) + h\nu$
(green 557.7nm)

~97km

Barth & Hildebrand (1961)



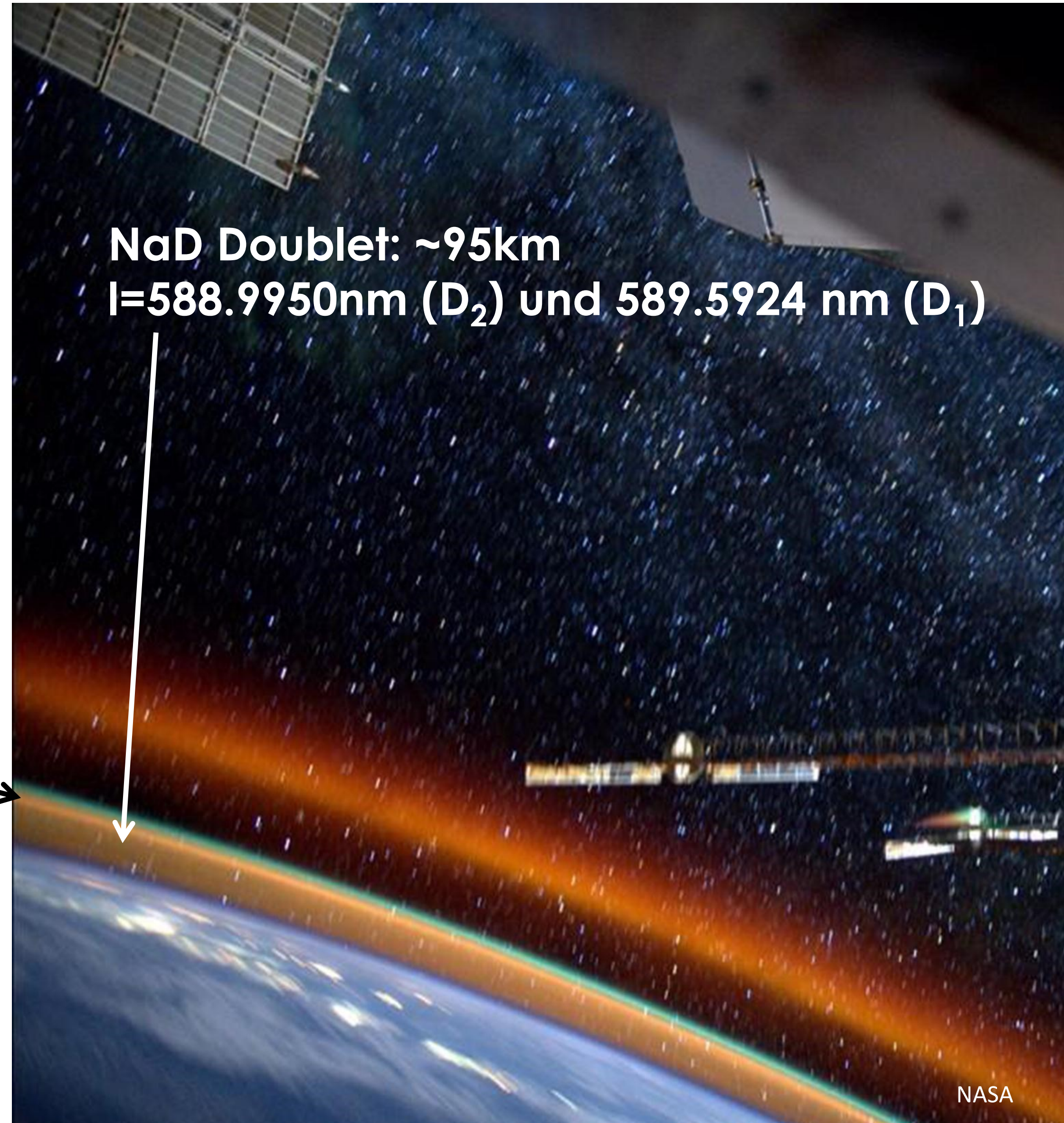
Airglow

NaD airglow

Reaction:

Na + O_3 → NaO + O_2
NaO +O → Na(^{2}P) + O_2
Na(^{2}P) → Na(^{2}S) + $h\nu$ (Doublet)

see Khomich (2008)
for an overview



Airglow

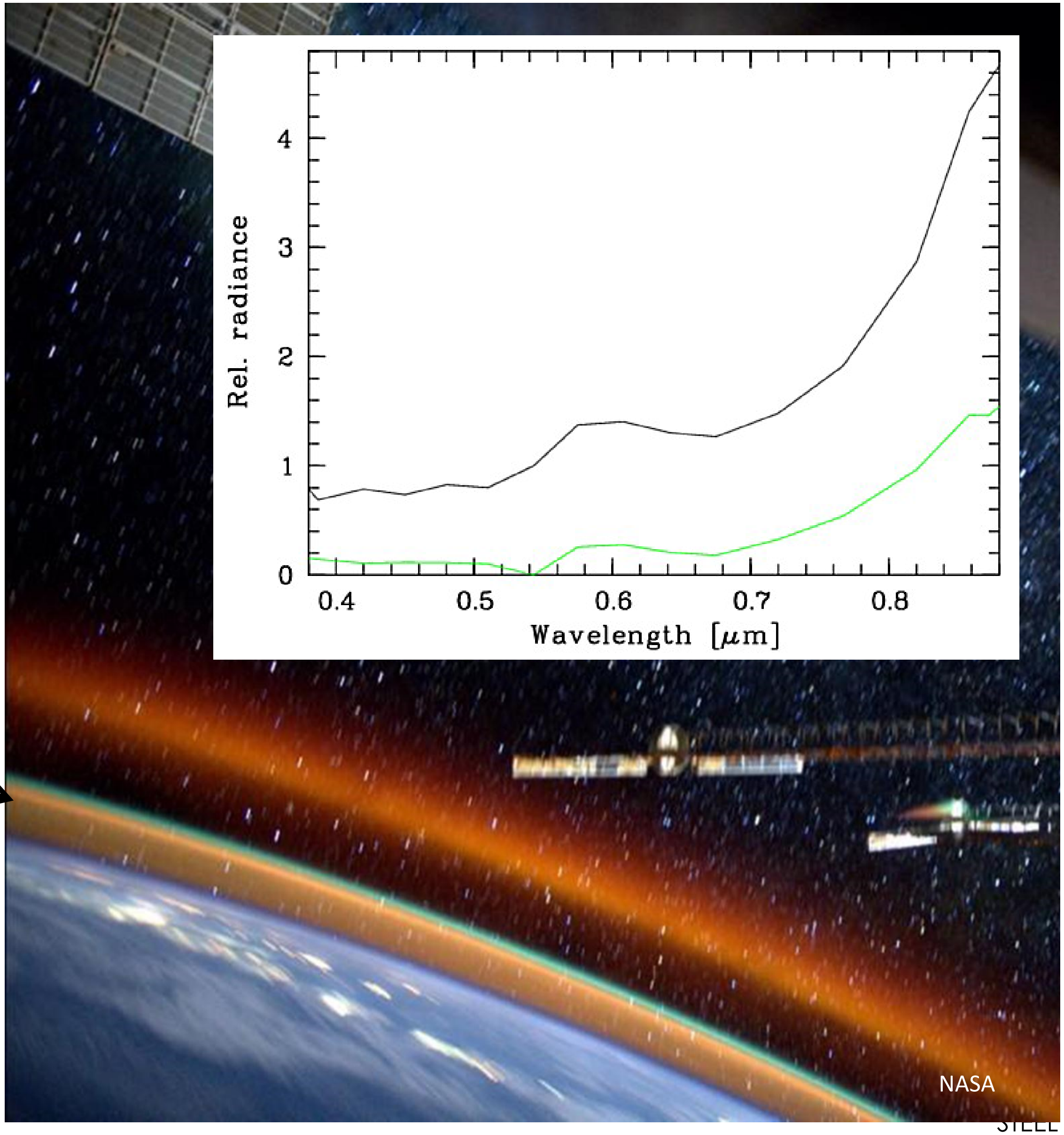
airglow continuum

Reaction:

$NO + O \rightarrow NO_2^*$
$NO_2^* \rightarrow NO_2 + h\nu$ (λ~0.6μm)
$NO_2 + O \rightarrow NO + O_2$
longer λ: probably $NO + O_3$
(not yet fully clarified)

~90km

Krassovsky (1951)



Airglow

Hydroxyl (OH) airglow

Reaction:

Dissociation of H_2O and O_2 → atomic O and H

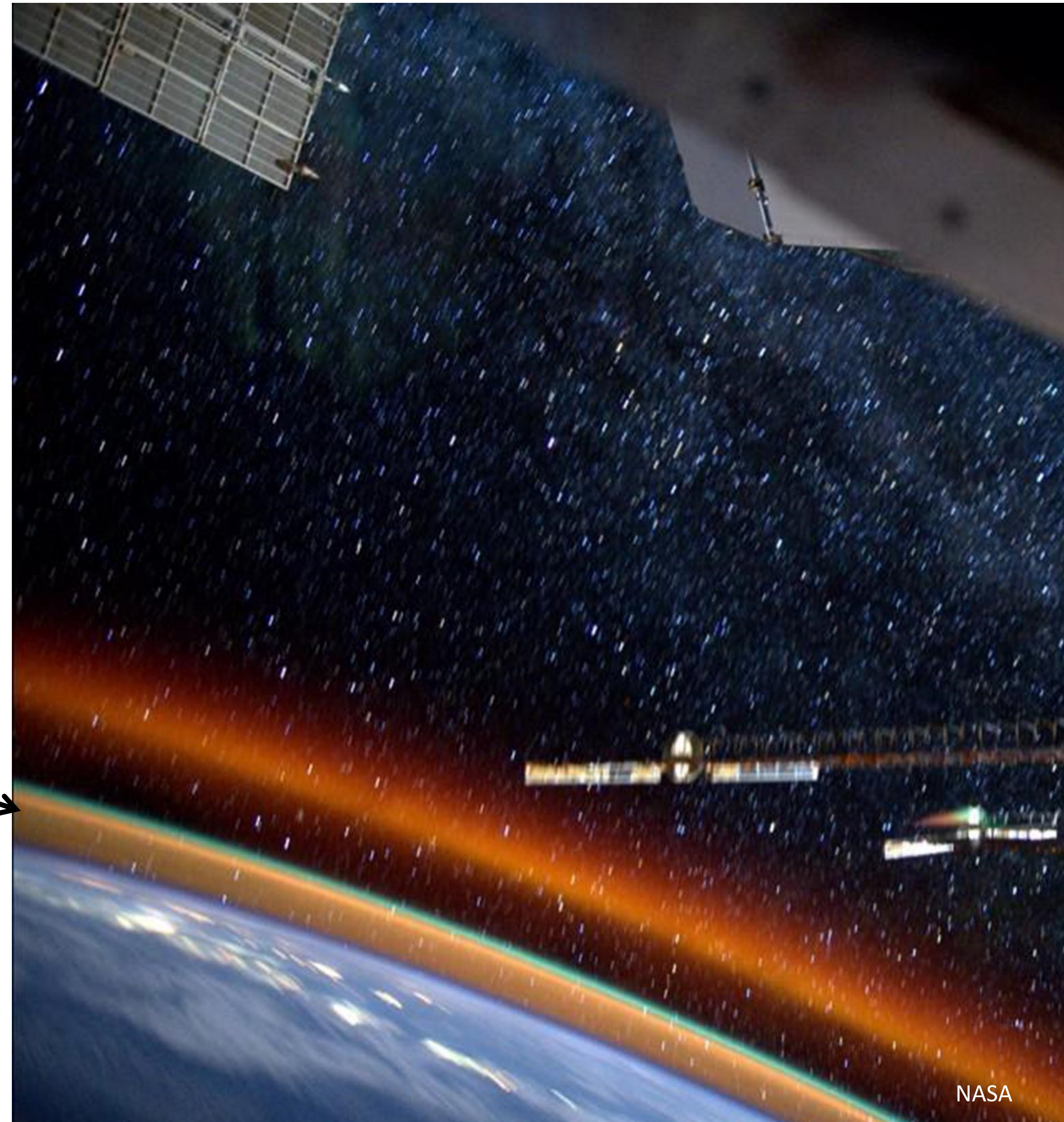
$O + O_2 \rightarrow O_3 + M$

$H + O_3 \rightarrow OH^* + O_2$

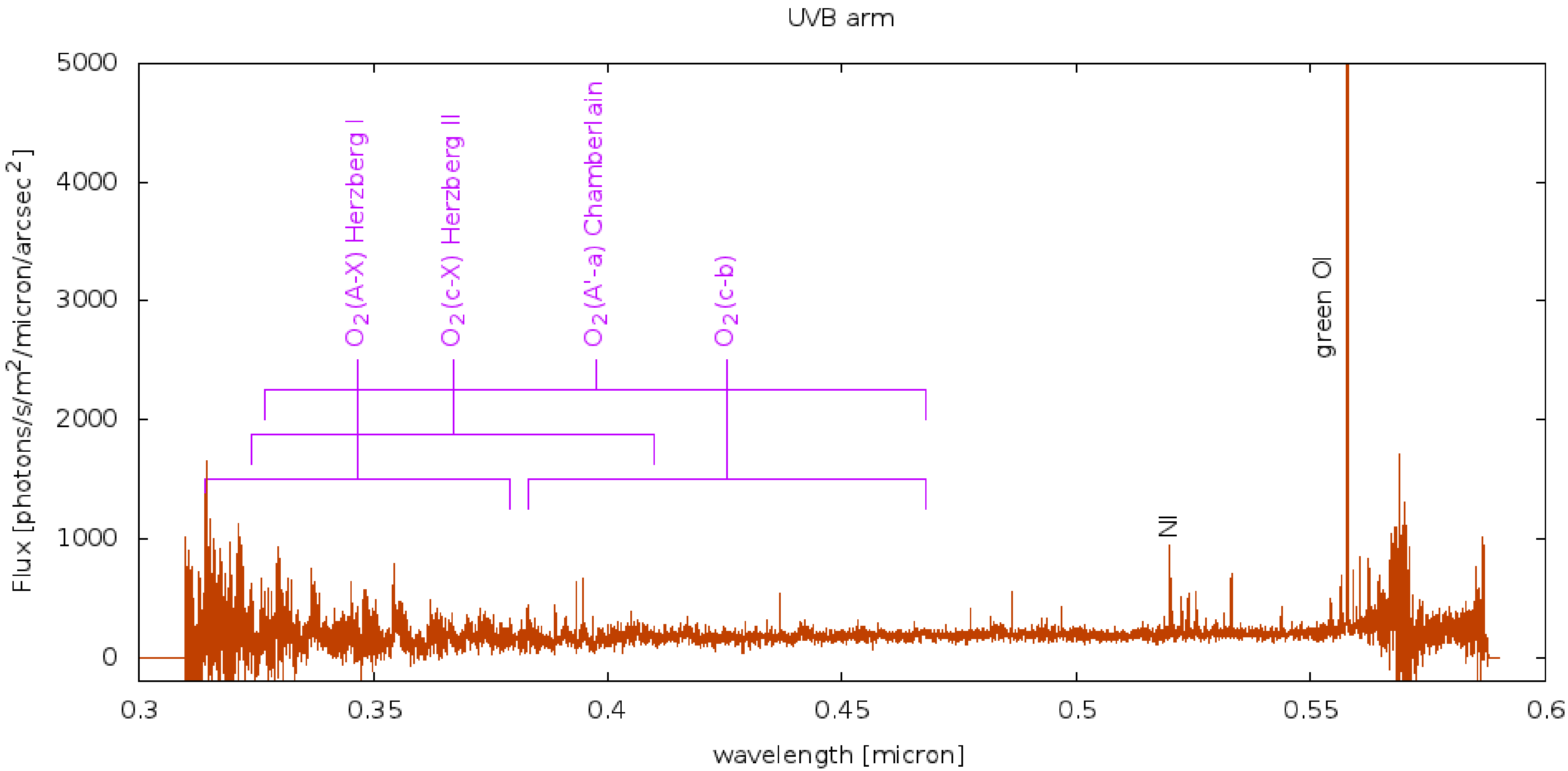
vib-rotational transisions (OH bands)
($0.5\mu m < \lambda < 5\mu m$)

~87km

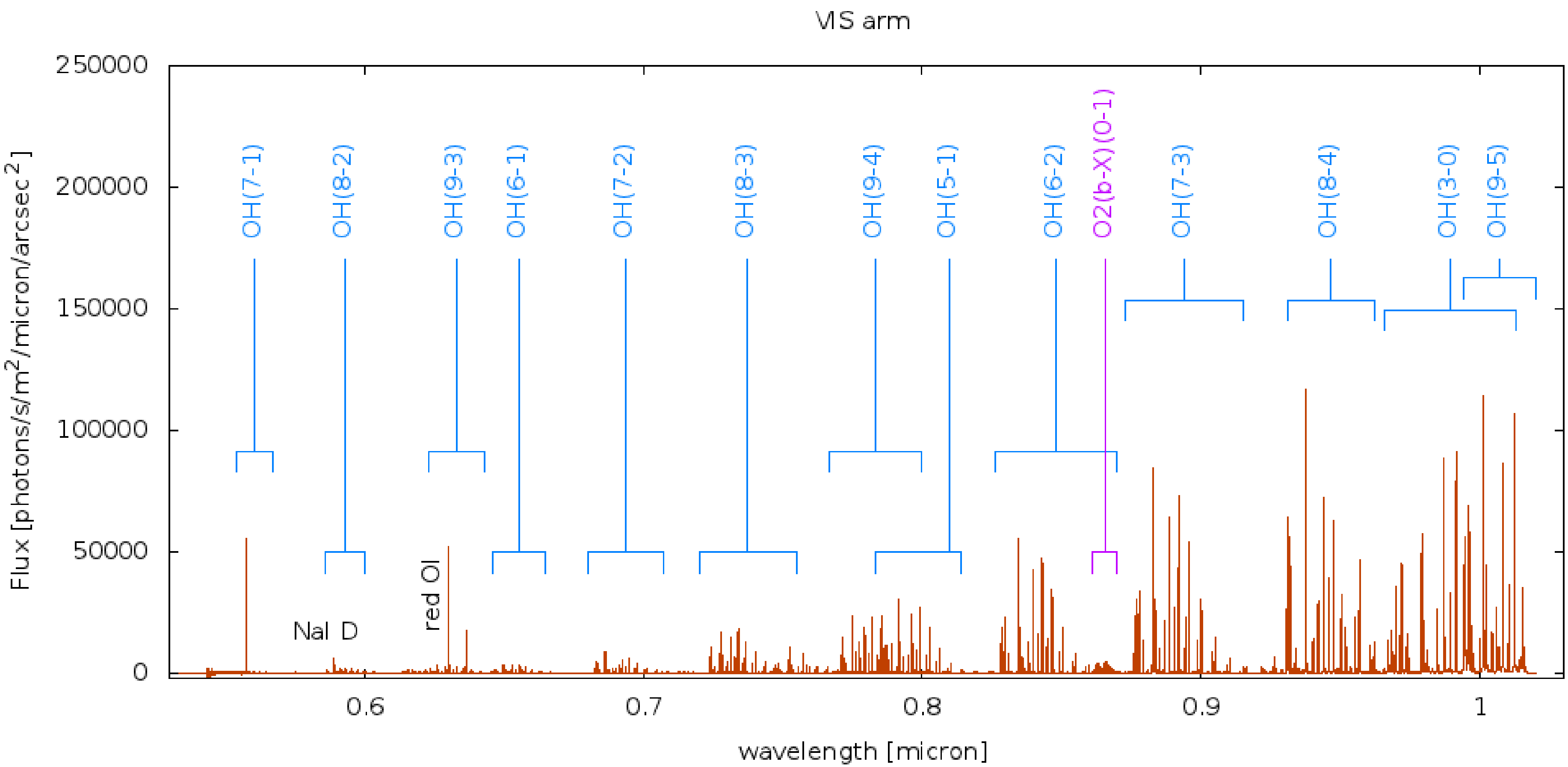
Bates-Nicolet (1961)



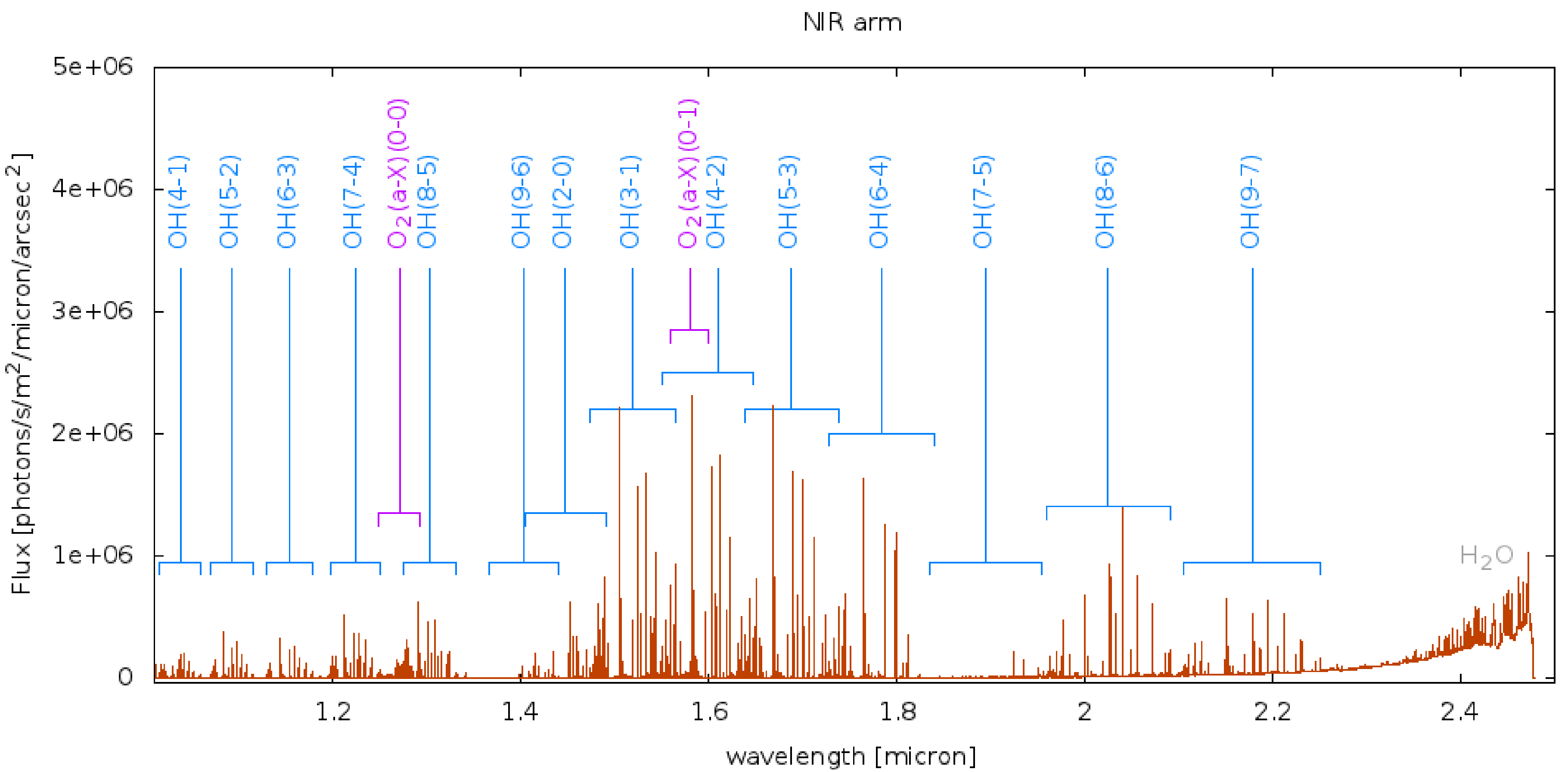
X-Shooter plain sky spectrum



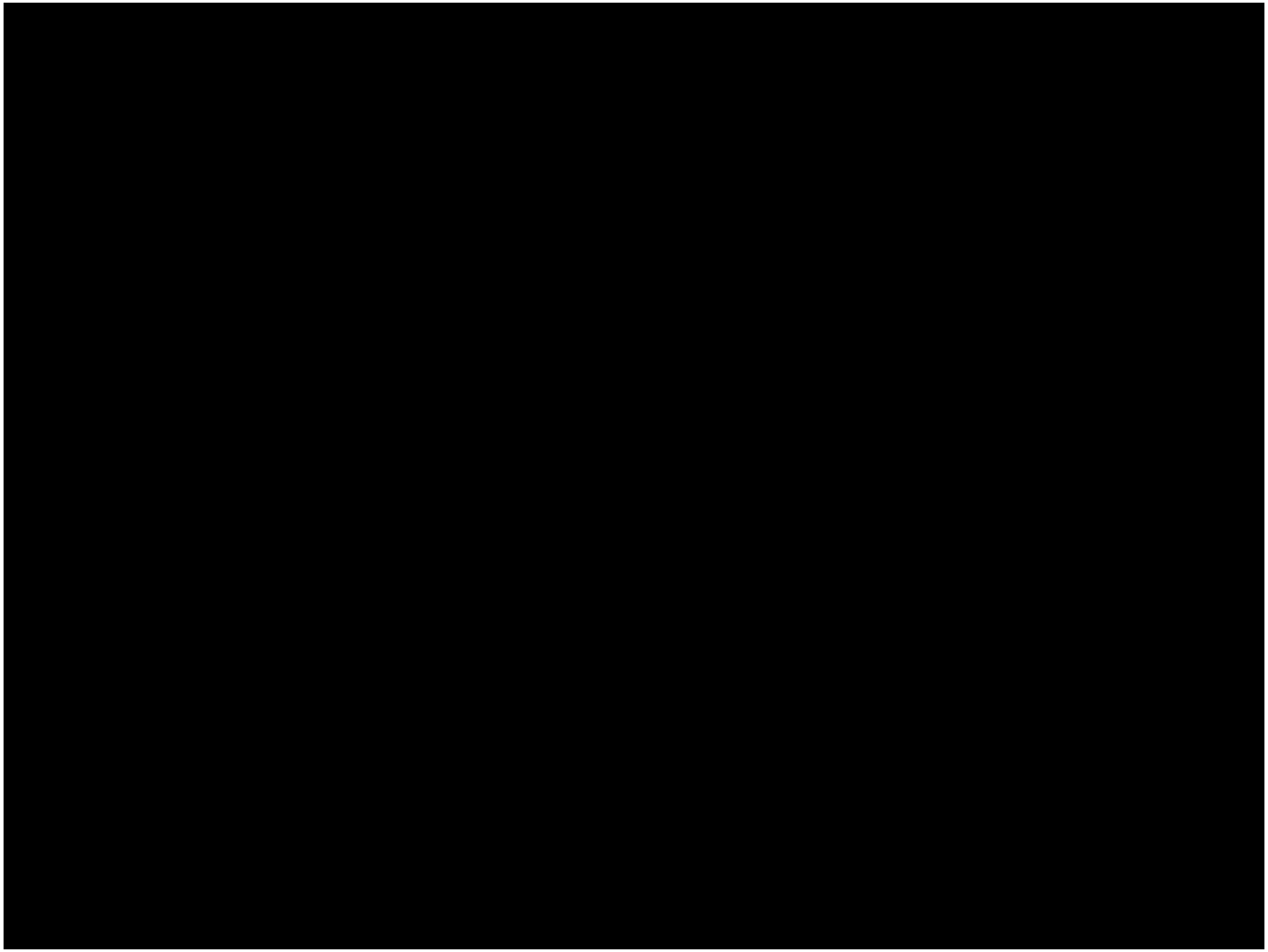
X-Shooter plain sky spectrum



X-Shooter plain sky spectrum



ESO/FORS sky spectra: variability



N. Patat/ESO 2007

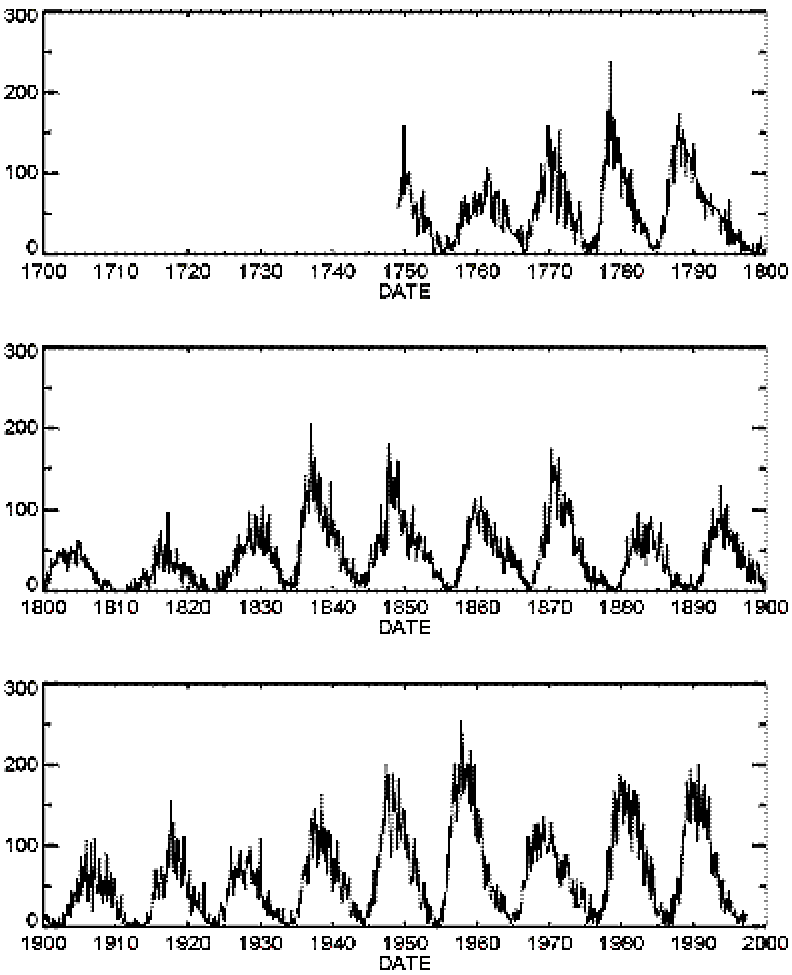
http://www.eso.org/~fpatat/science/skybright/MOVIES/the_dancing_sky_nosound_full.mov

Variability:

- **climate change (decades):**
  it takes a while, until chemical changes in the lower atmosphere reach the mesosphere and above → delay

Variability:

- climate change (decades)
- **solar cycle (11yr)**



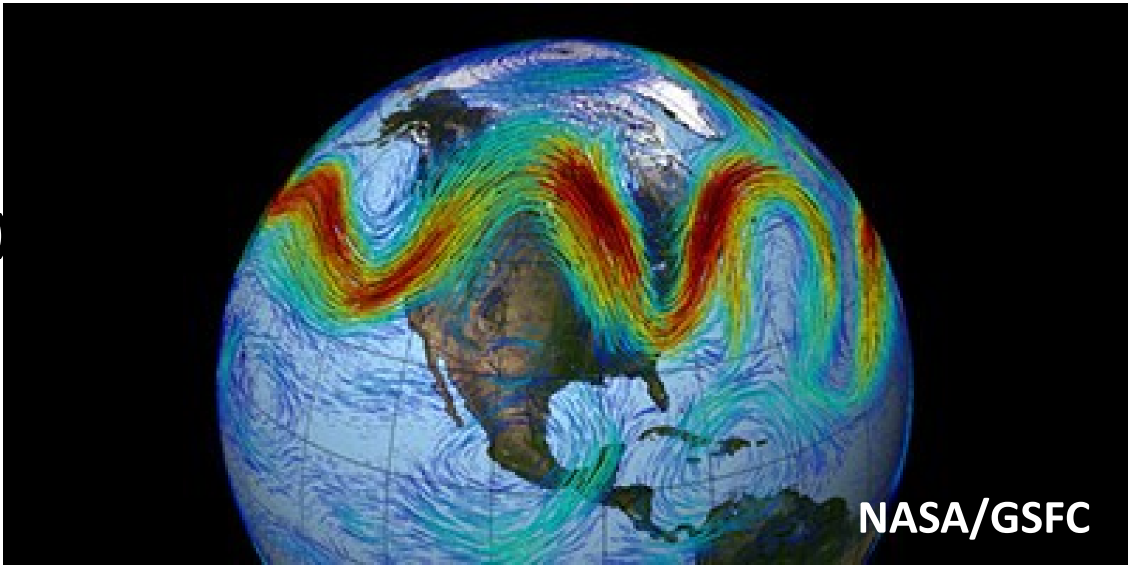
NASA

Variability:

- climate change (decades)
- solar cycle (11yr)
- **seasonal (months):** induced due to seasonal changes (temperature)

Variability:

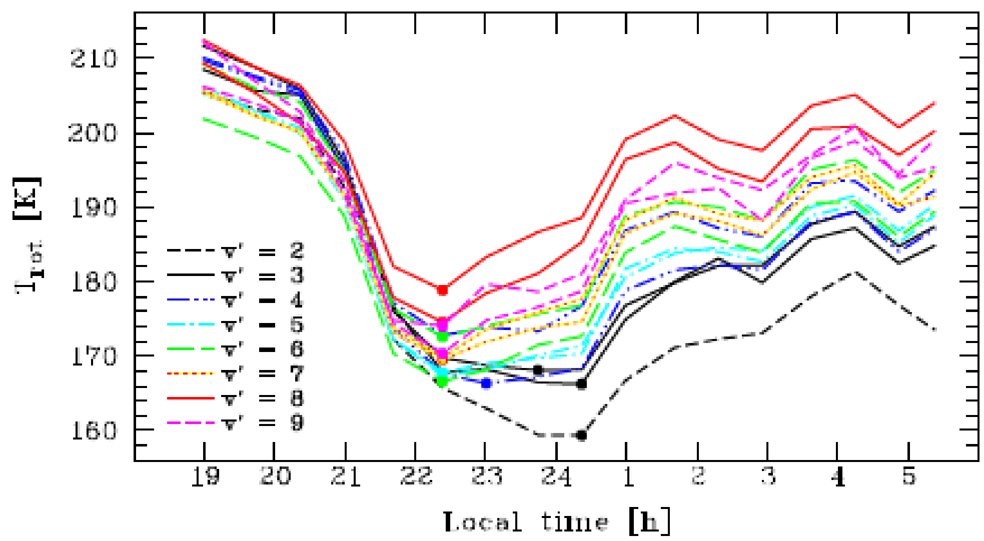
- climate change (decades)
- solar cycle (11yr)
- seasonal (months)
- **planetary waves (few days)**



Variability:

- climate change (decades)
- solar cycle (11yr)
- seasonal (months)
- planetary waves (few days)
- **diurnal (24h)**

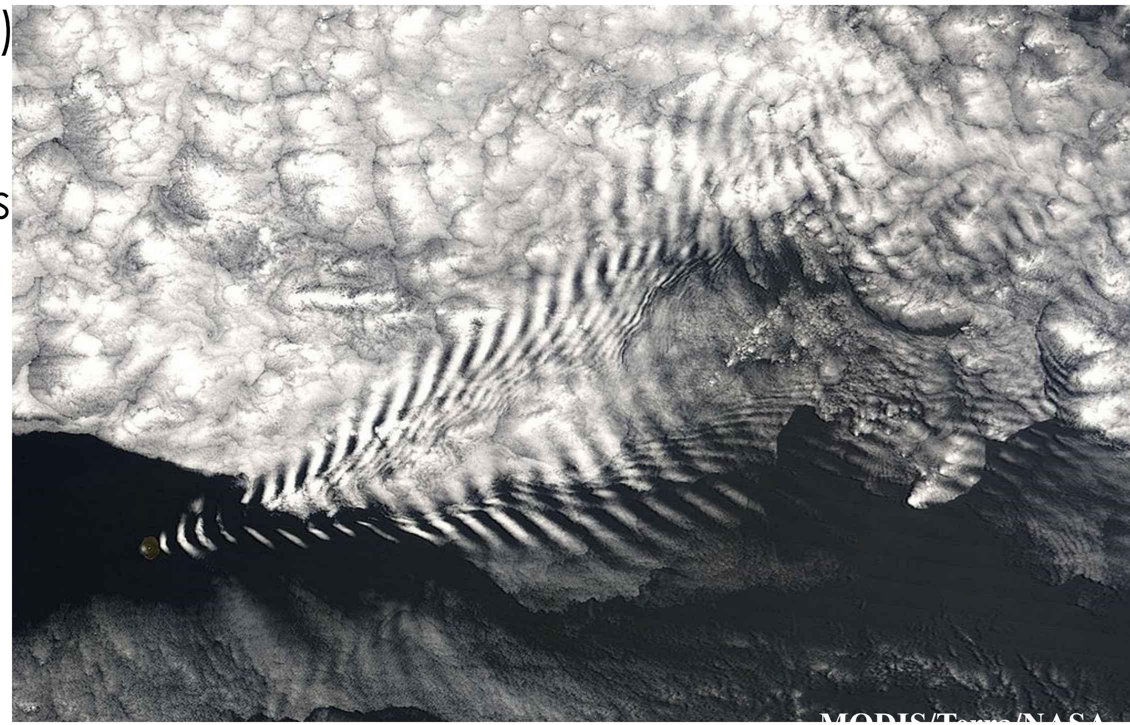
OH



Noll et al, 2015, ACP, 15, 3647

Variability:

- climate change (decades)
- solar cycle (11yr)
- seasonal (months)
- planetary waves (few days
- diurnal (24h)
- **gravity waves (minutes)**



Wikipedia / NASA

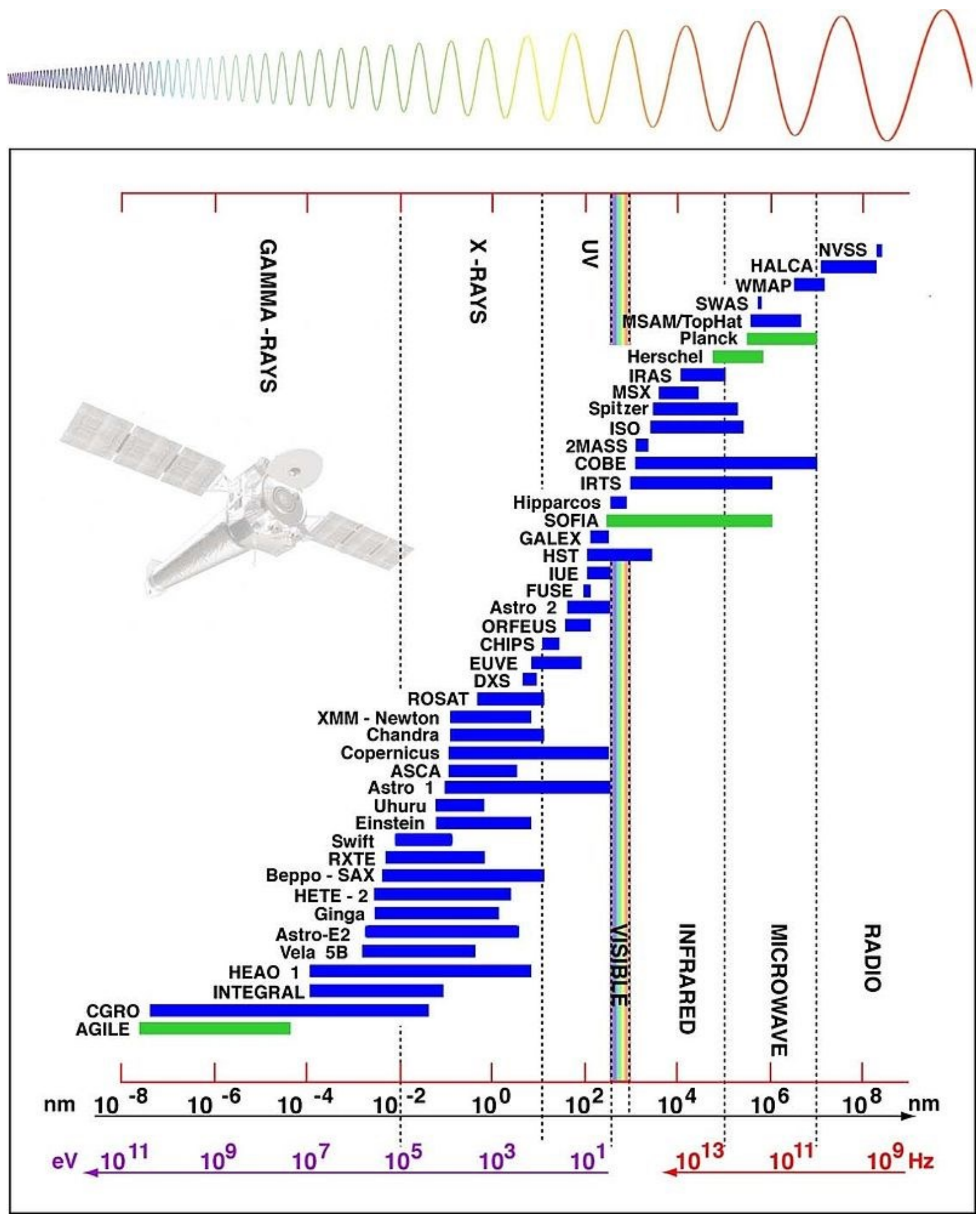
Variability:

- climate change (decades)
- solar cycle (11yr)
- seasonal (months)
- planetary waves (few days)
- diurnal (24h)
- **gravity waves (minutes)**

How can we get rid of this?

Plan #1:
Go to space

Armada of Space Observatories



Wikipedia

Go to Space

Disadvantages

- high risk
- very expensive
- limited payload
- limited lifetime
- no maintainance / upgrades

How can we get rid of this?

Plan A:
Supplementary calibration frames
„Classical method“

Correcting for

absorption

Required: transmission spectrum

Telluric standard stars:

- hot stars without/with few, well known intrinsic spectral features (B-type)
- observation in the vicinity, at least same airmass than science target
- observation directly before/after the science target

emission

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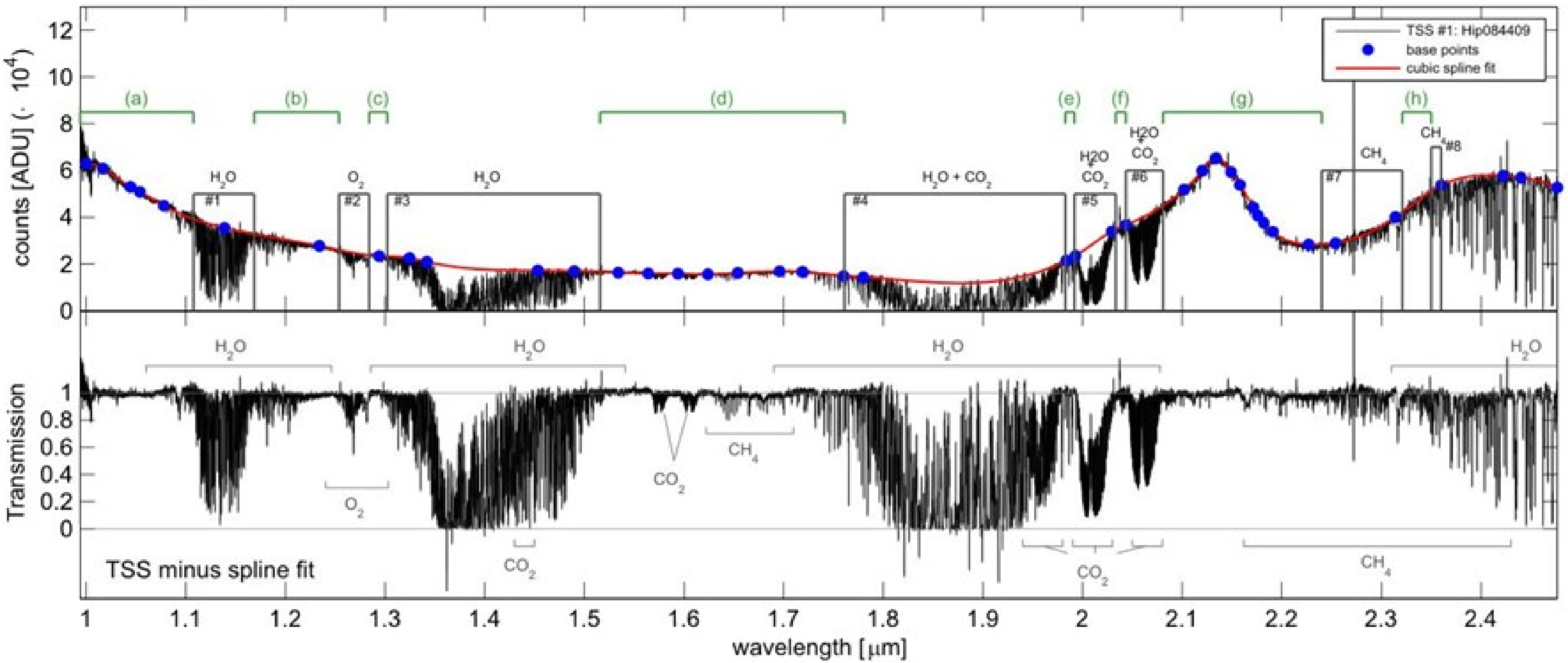

Kausch et al, 2015, A&A, 576, A78

Correcting for

emission

Required: airglow spectrum

Plain sky observations:

- LSS: portion of the slit w/o object
- specific sky spectrum taken before/after the science target and
- taken in the very vicinity of the science target
- same exposure time

Very expensive in terms of telescope time

How can we get rid of this?

Plan α:
Modelling

Correcting for

absorption

Required: transmission spectrum

Telluric standard stars:

- hot stars without/with few, well known intrinsic spectral features (B-type)
- observation in the vicinity, at least same airmass than science target
- observation directly before/after the science target

molecfit

Telluric Absorption Correction with `molecfit`

Basic idea ([1],[2]):

- derive the atmospheric state from its fingerprint in the science spectra
- calculation of synthetic transmission spectra corresponding to this state by means of a radiative transfer code
- iteratively fitting these spectra to absorption features in science spectra
- use the best-fit transmission for the telluric absorption correction

Features:

- comprehensive software suite for telluric absorption correction
- instrument independent
- world-wide use
- based on Ansi-C → high compatibility (Linux+MacOS)
- freely available*

[1] Smette et al. 2015, A&A, 576, A77
[2] Kausch et al. 2015, A&A, 576, A78

*http://www.eso.org/pipelines/skytools

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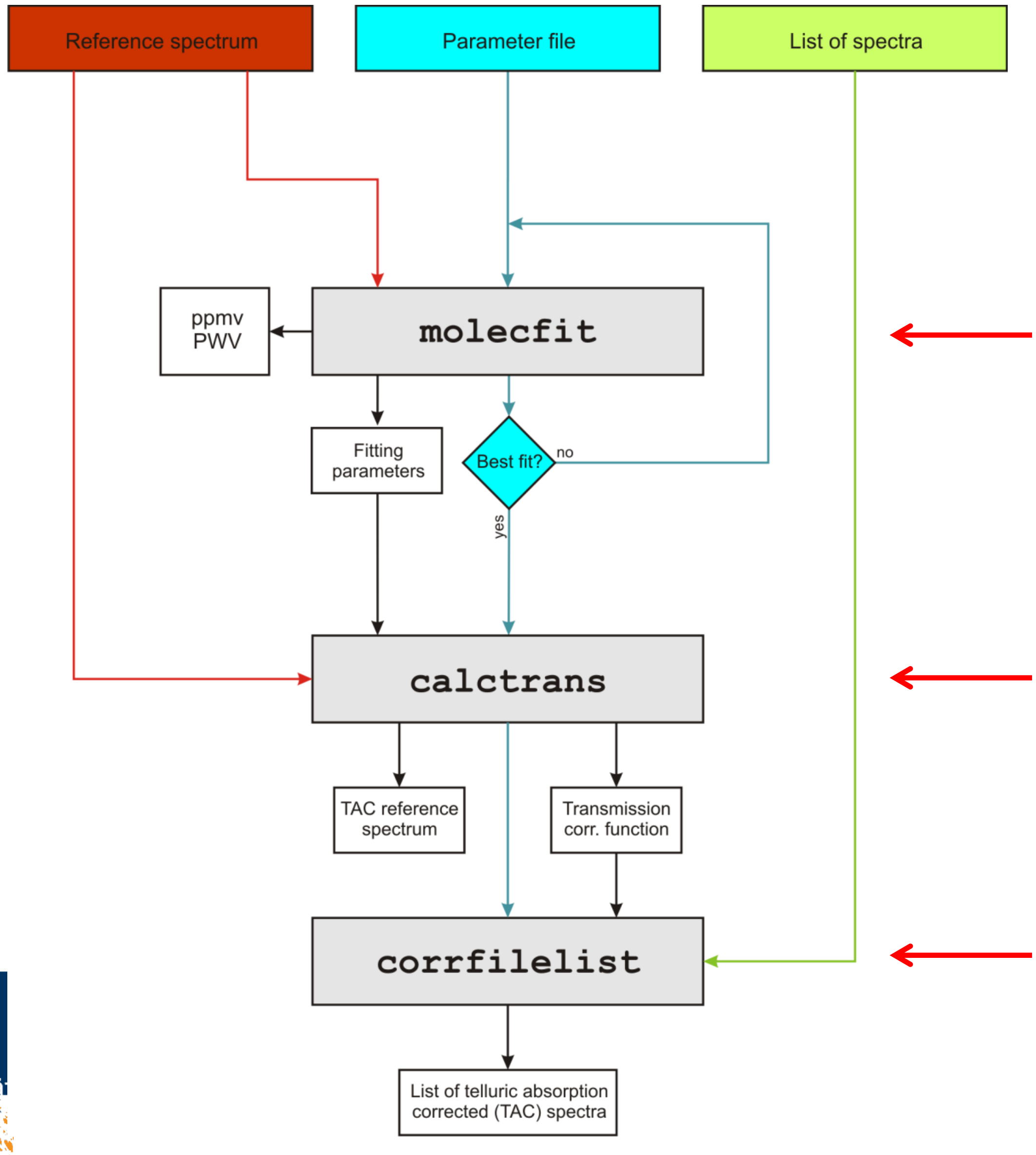
Telluric Absorption Correction with `molecfit`



fitting of spectral features in the fitting ranges → best fit solution

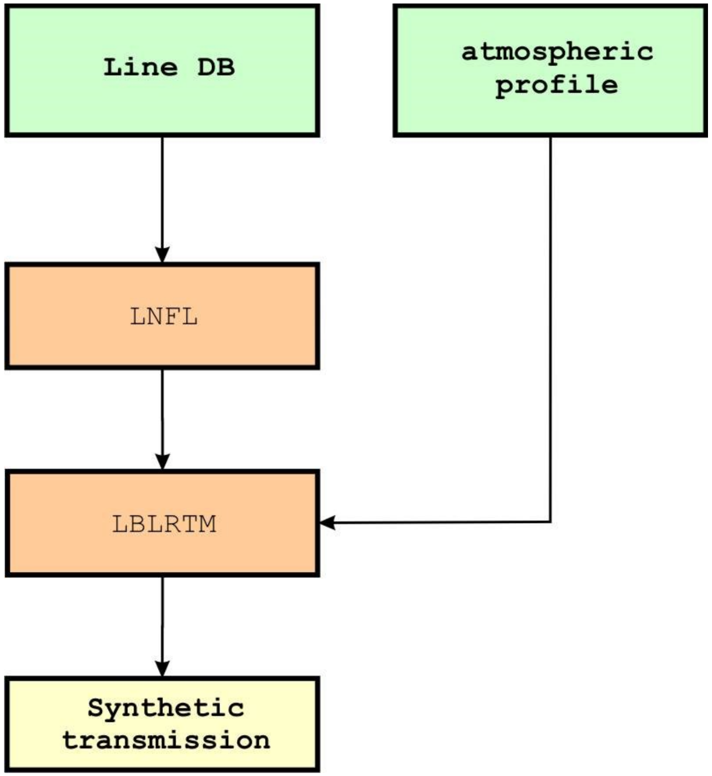
calculation of the transmission based on the fit + application of the telluric abs. correction

application of the correction to other files.

Radiative Transfer Code

LBLRTM ([1],[2]):

- **L**ine-**B**y-**L**ine-**R**adiative-**T**ransfer-**M**odel
- third party code [3]
- V12.2
- widely used in atmospheric research
- still being further developed

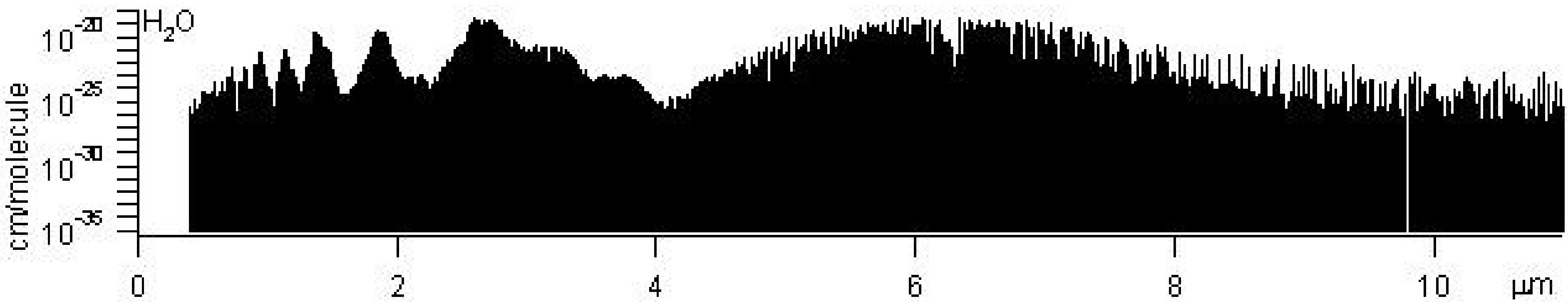


[1] Clough et al., 2005, *J. Quant. Spectrosc. Radiat. Transfer*, **91**, 233-244
[2] Clough et al., 1992, *J. Geophys. Res.*, **97**, 15761-15785
[3] http://rtweb.aer.com/lblrtm_frame.html

Radiative Transfer Code: Line Database

HITRAN database([1],[2],[3]):

- 39 different molecules
- 2,713,968 spectral lines
- calculated & observed data
- V13 (HITRAN 2008)

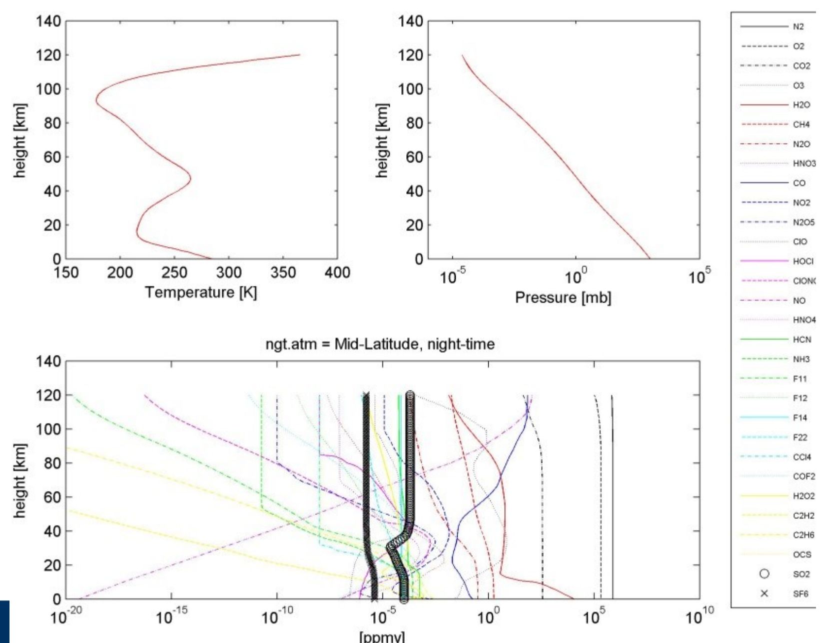


[1] Atomic and Molecular Physics Division, Harvard-Smithsonian Center for Astrophysics
[2] Rothman et al., 2009, Journal of Quantitative Spectroscopy and Radiative Transfer, vol. **110**, pp. 533-572
[3] http://www.cfa.harvard.edu/HITRAN/

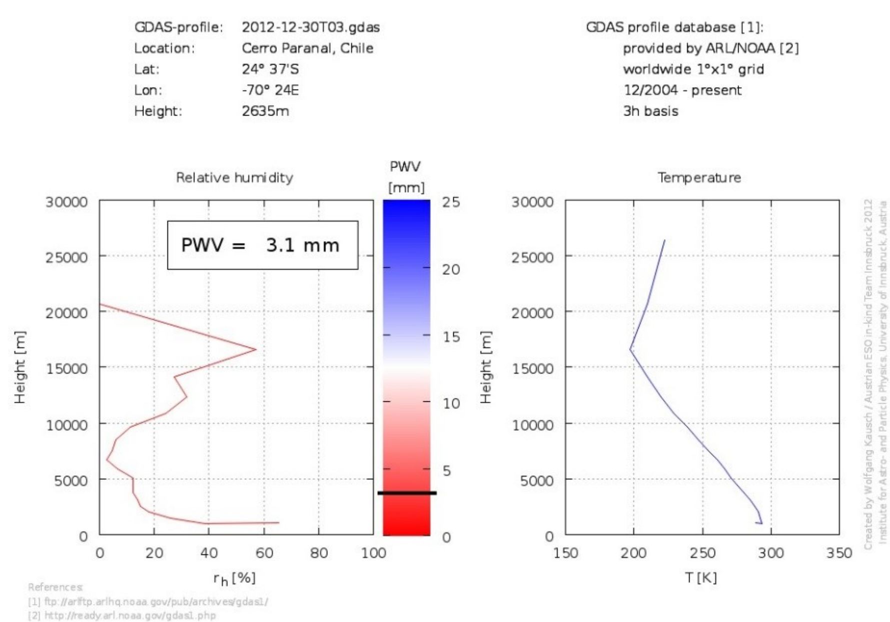
Radiative Transfer Code: Atmospheric Profile

- Static atmospheric standard profile (P, T, mixing ratios for many molecules)
- Global GDAS* weather model: 1° x 1° grid, every 3 h, profiles for P, T, r_H
- Local meteorological data for height of site: P, T, and r_H (taken from FITS header if present) → ESO MeteoMonitor

atmospheric standard profile



GDAS profile: 2012-12-30T03.gdas



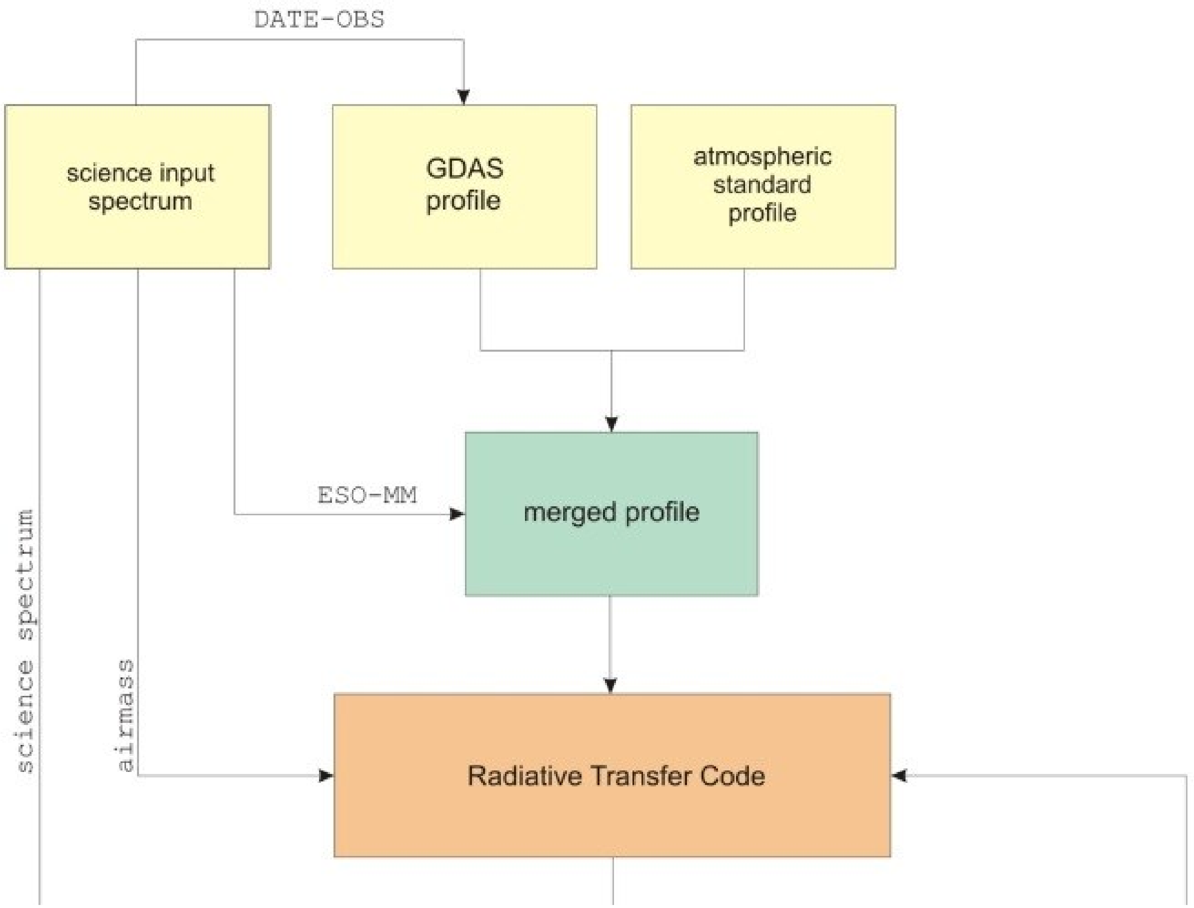
*ftp://ftp.arl.noaa.gov/archives/gdas1/

mpfit Package

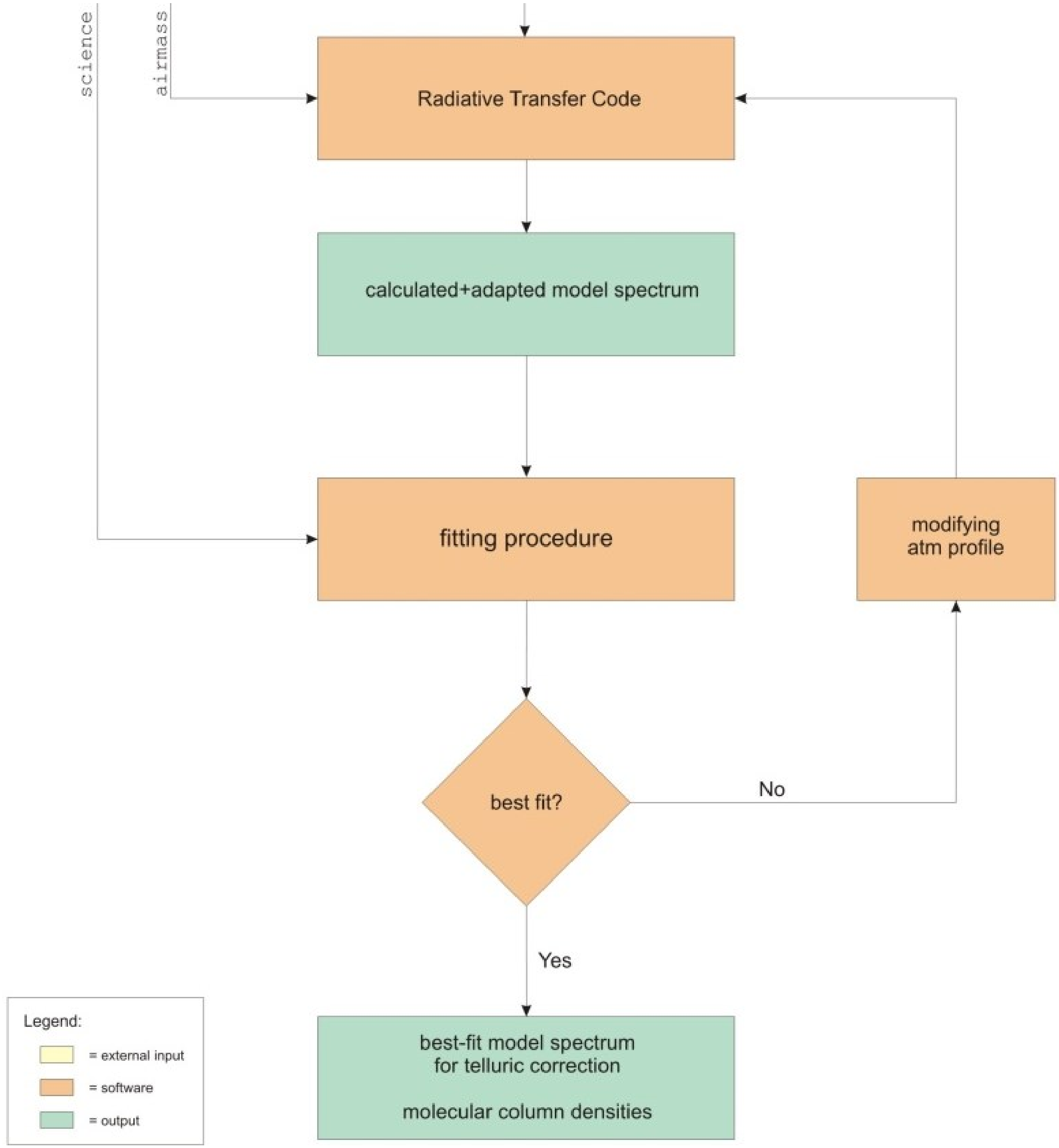
- Software package for fitting issues
- Levenberg-Marquardt technique for solving the least-squares problem
- Fitting core in `molecfit`
- freely available
- very versatile (also used for `skycorr`)
- in ANSI-C and IDL

https://www.physics.wisc.edu/~craigm/idl/cmpfit.html

`molecfit` Workflow



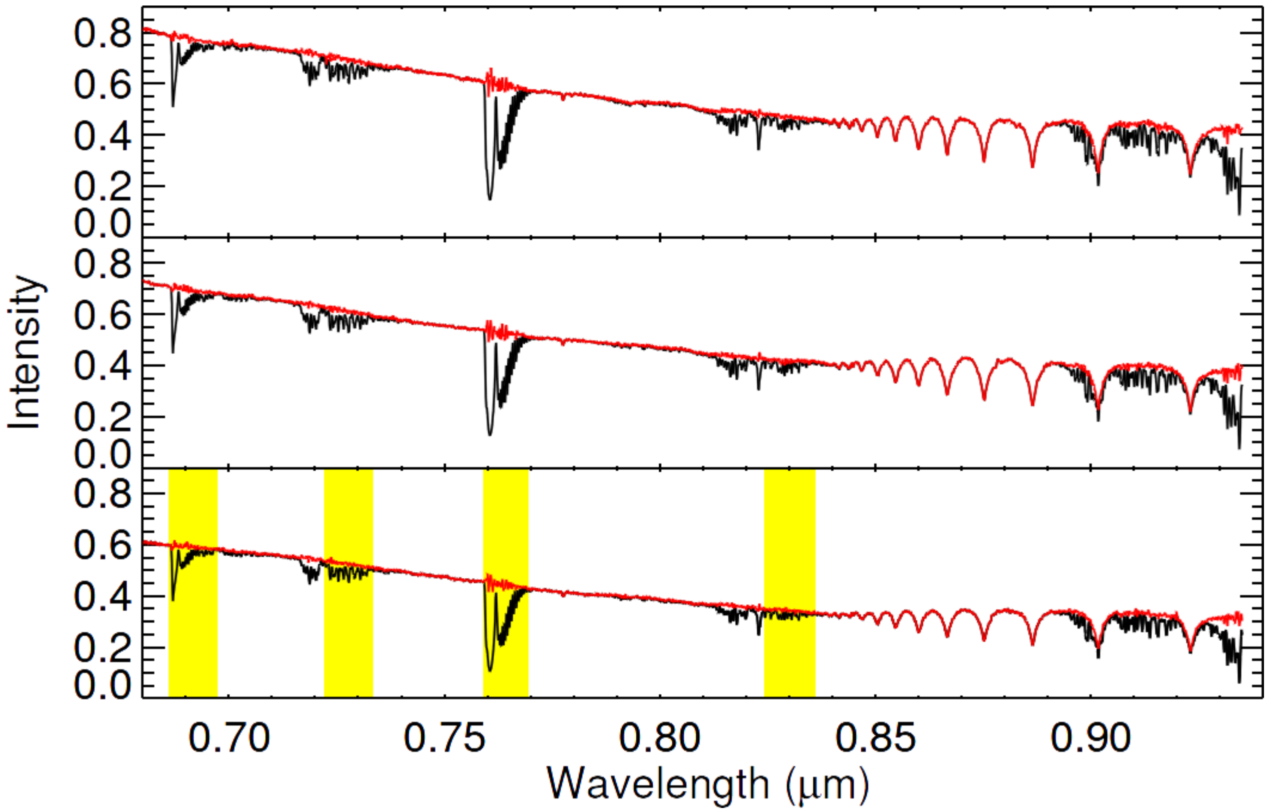
molecfit Workflow



Fitting Procedure

Fitting ranges: lines of intermediate strength; good coverage of wavelength range; as narrow as possible (better continuum fit and shorter code run times)

Exclusion regions: no fitting of bad pixels (or other instrumental defects) and object features



Smette et al. 2015, A&A, 576, A77

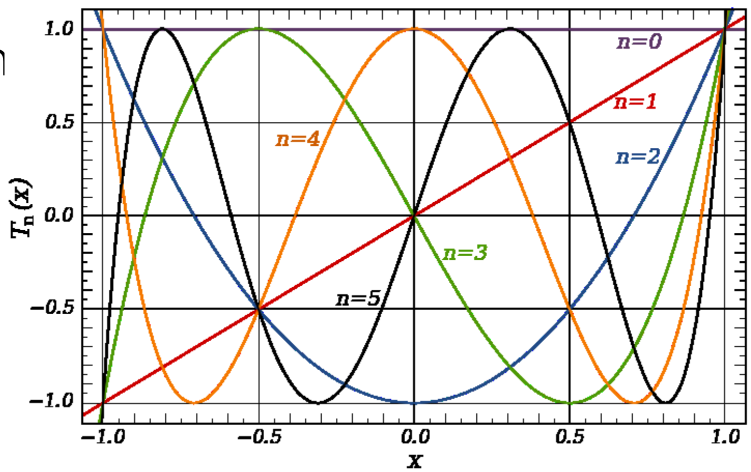
Fitting Procedure

χ^2 minimisation by a Levenberg-Marquardt technique (mpfit[1])

Fitting parameters:

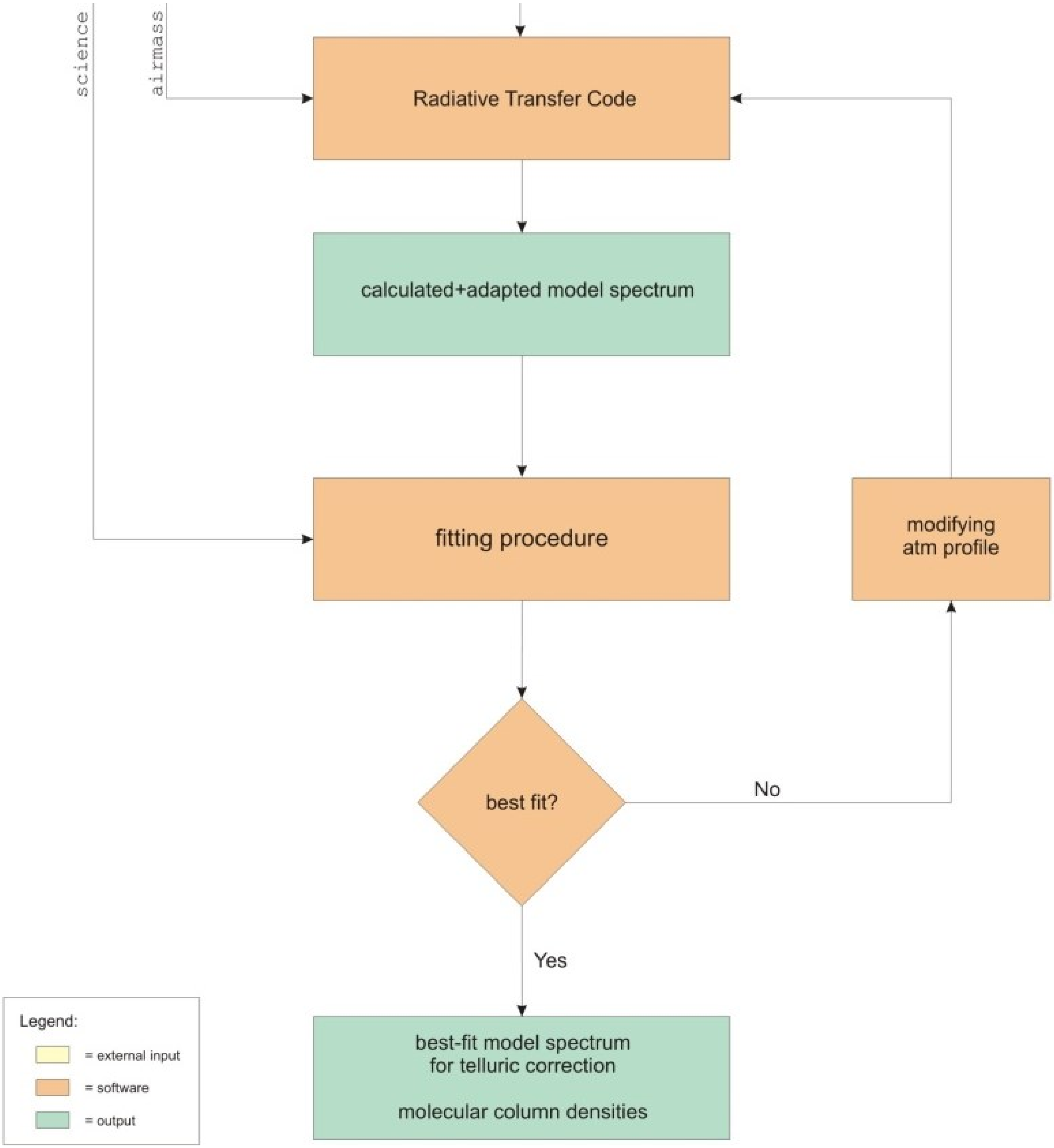
- Scaling factors for molecular profiles
- Coefficients of polynomials for continuum fit
- Coefficients of Chebyshev polynomials for modification of wavelength grid
- Widths of boxcar, Gaussian, and Lorentzian for instrumental profile (alternative: user-provided kernel → no fit)
- Emissivity of greybody (only for fit of sky emission spectra in the thermal IR)

Chebyshev polynomials

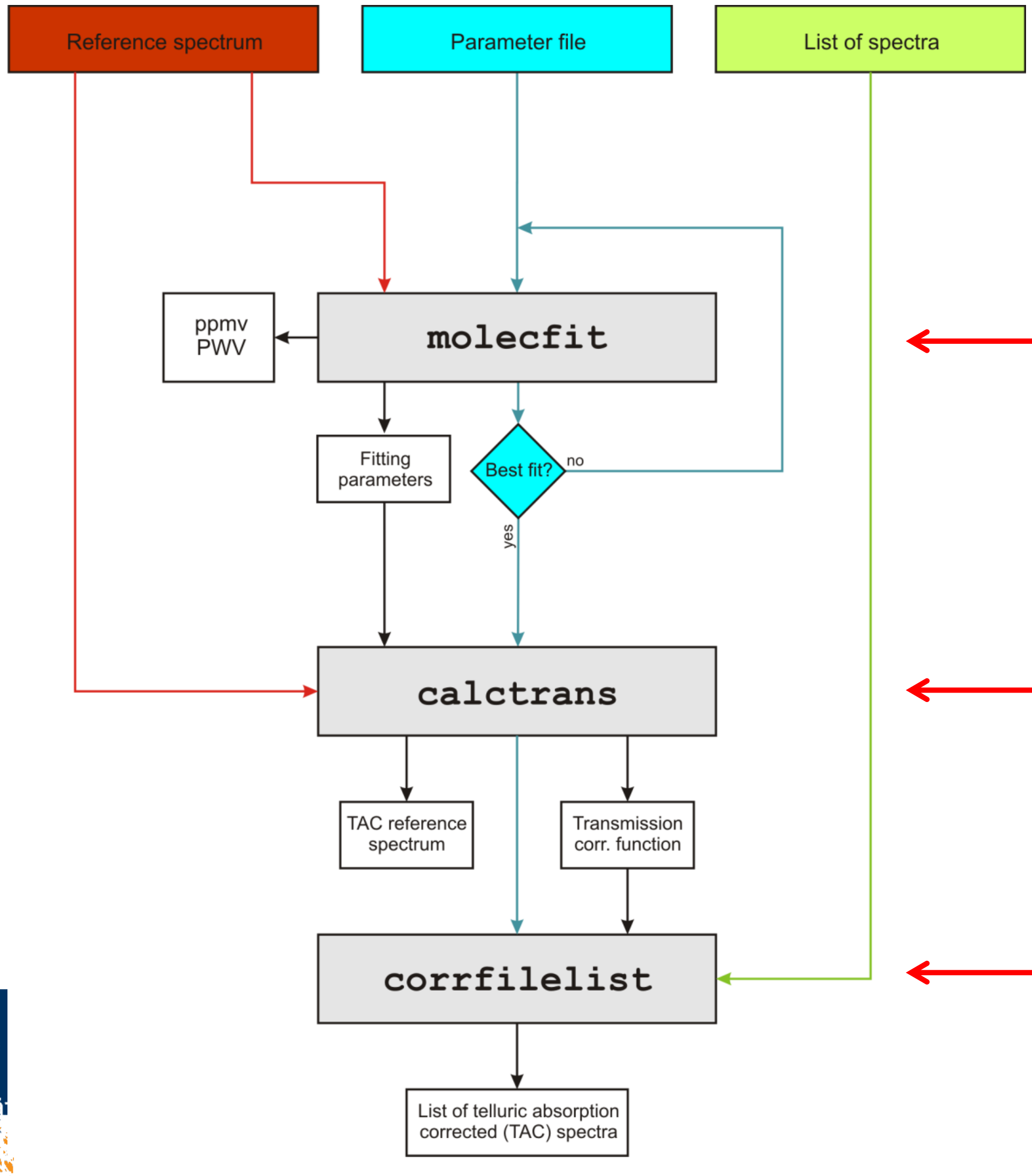


[1] Markwardt, C. B. 2009, in Astronomical Society of the Pacific Conference Series, Vol. 411, Astronomical Data Analysis Software and Systems XVIII, ed. D. A. Bohlender, D. Durand, & P. Dowler, 251

molecfit Workflow



Telluric Absorption Correction with `molecfit`



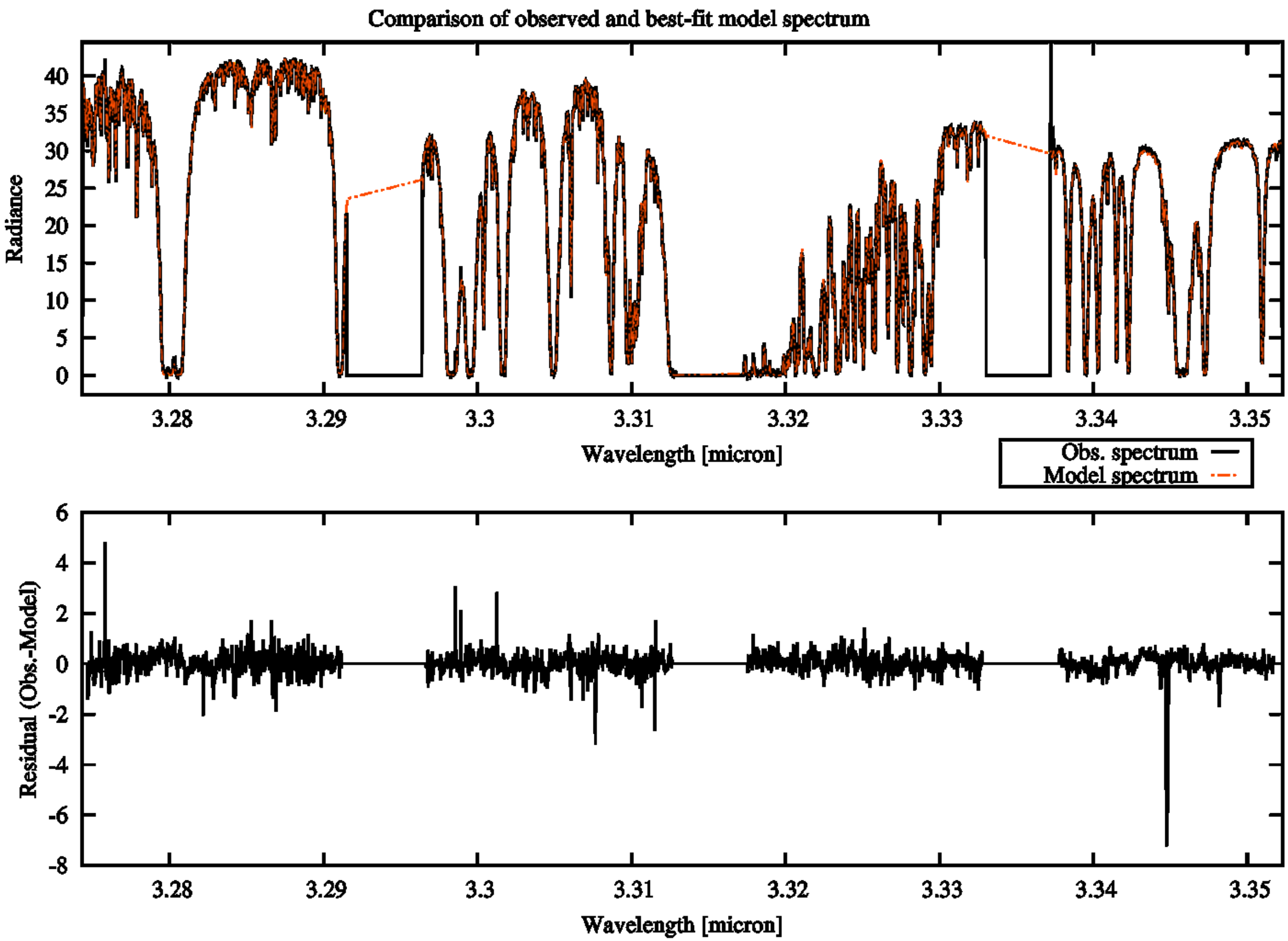
fitting of spectral features in the fitting ranges → best fit solution

calculation of the transmission based on the fit + application of the telluric abs. correction

application of the correction to other files.

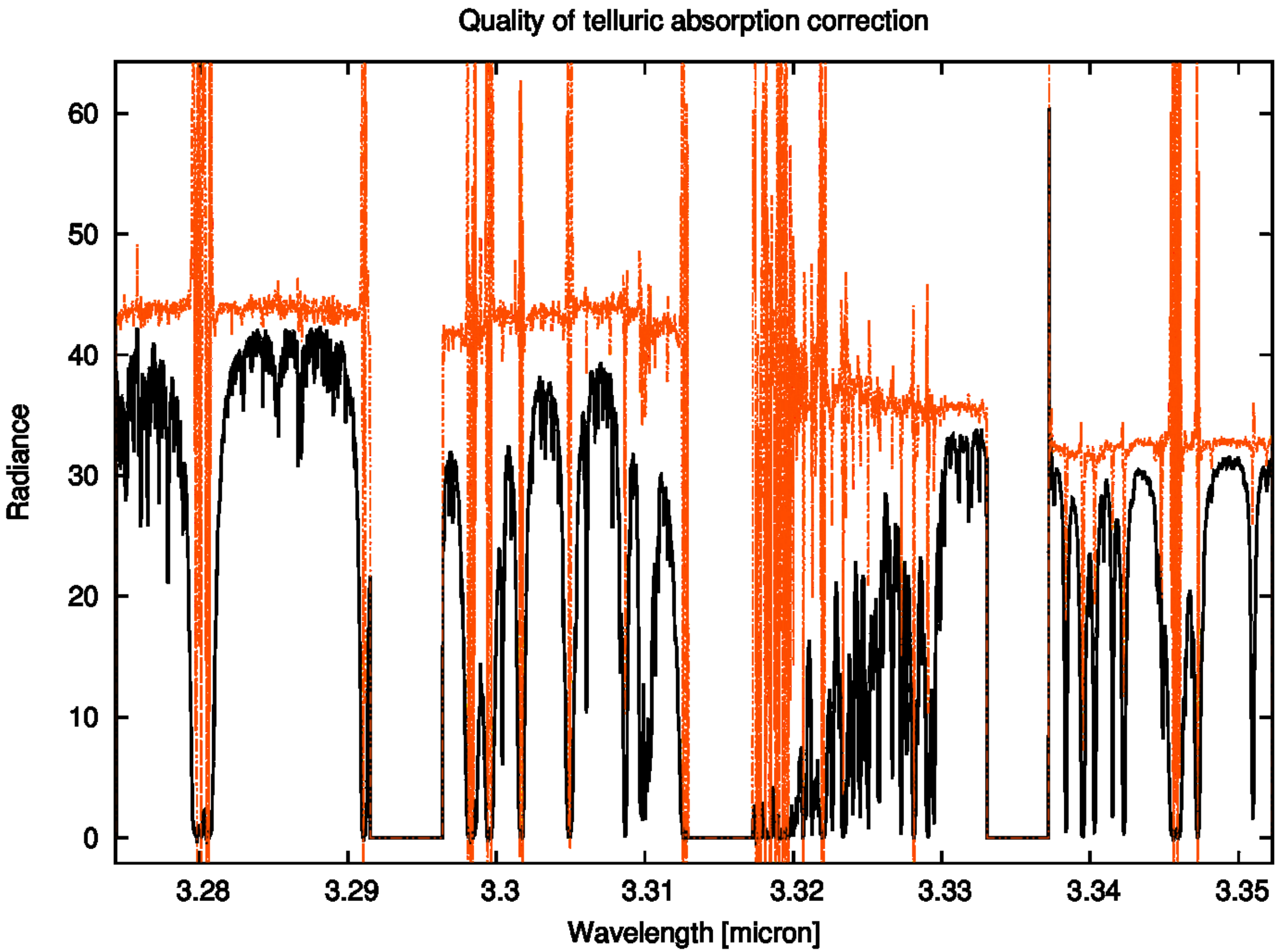
Results/Comparison

CRIRES
- hires IR spectrograph
- 1-5.2µm



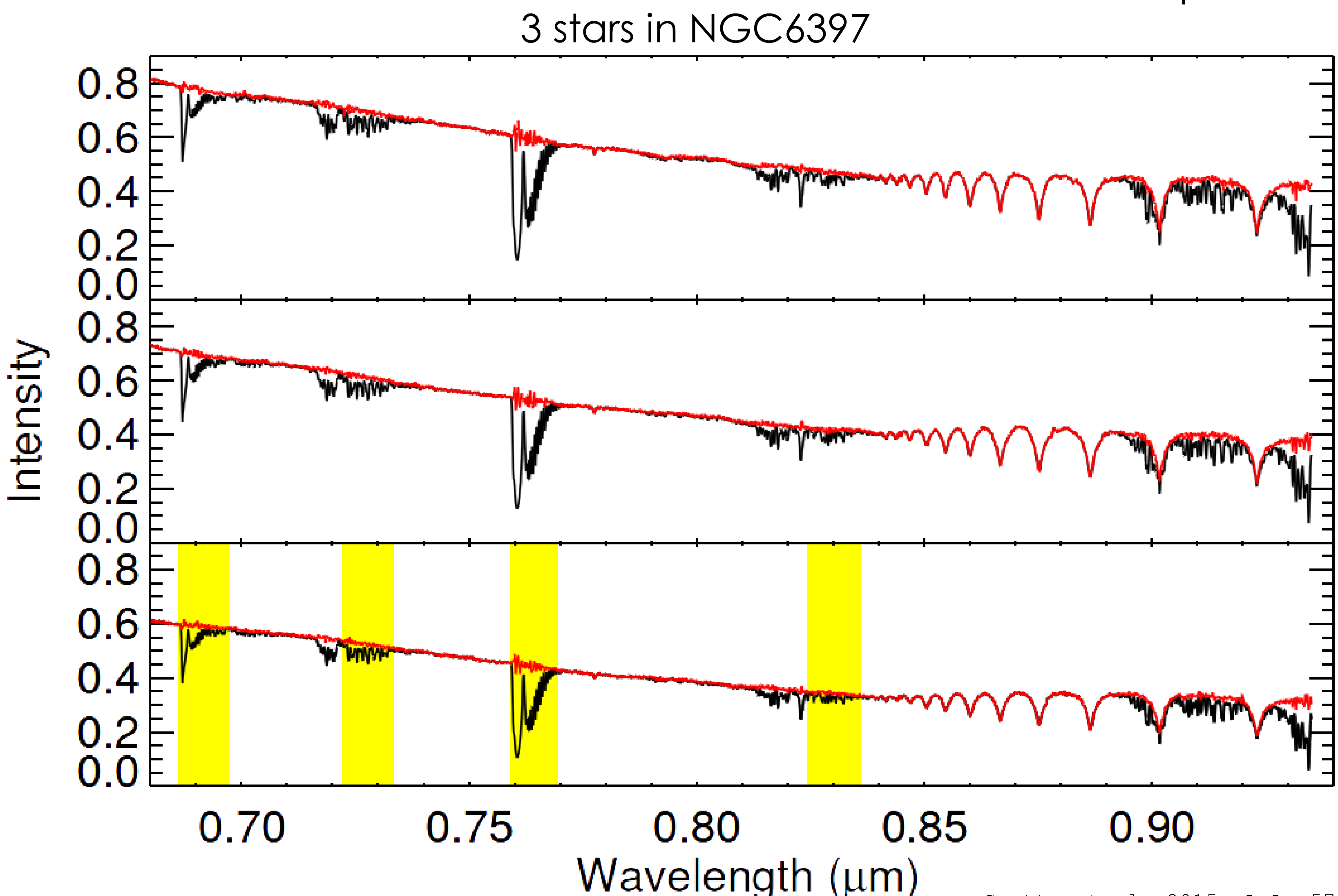
Results/Comparison

CRIRES
- hires IR spectrograph
- 1-5.2µm



Results/Comparison

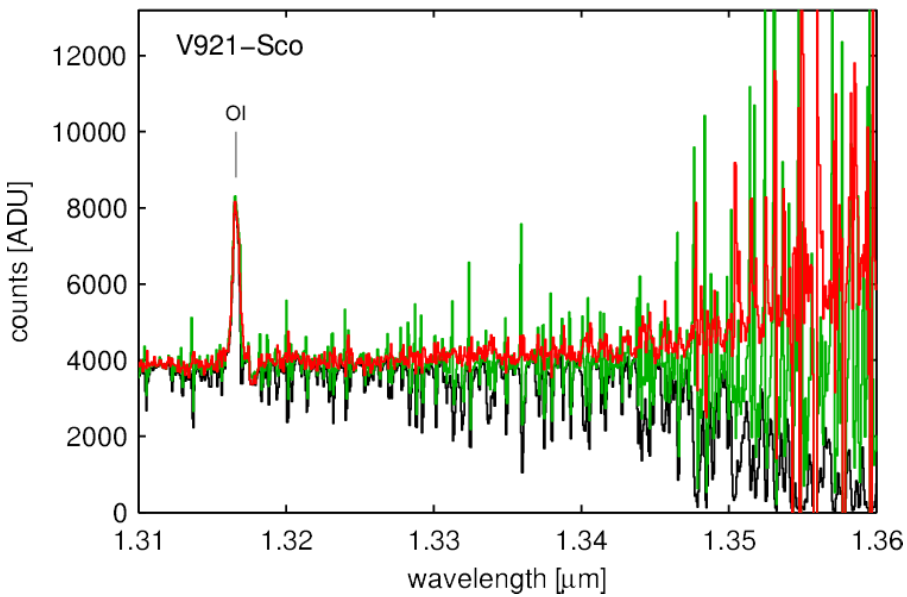
MUSE
- IFU
- optical

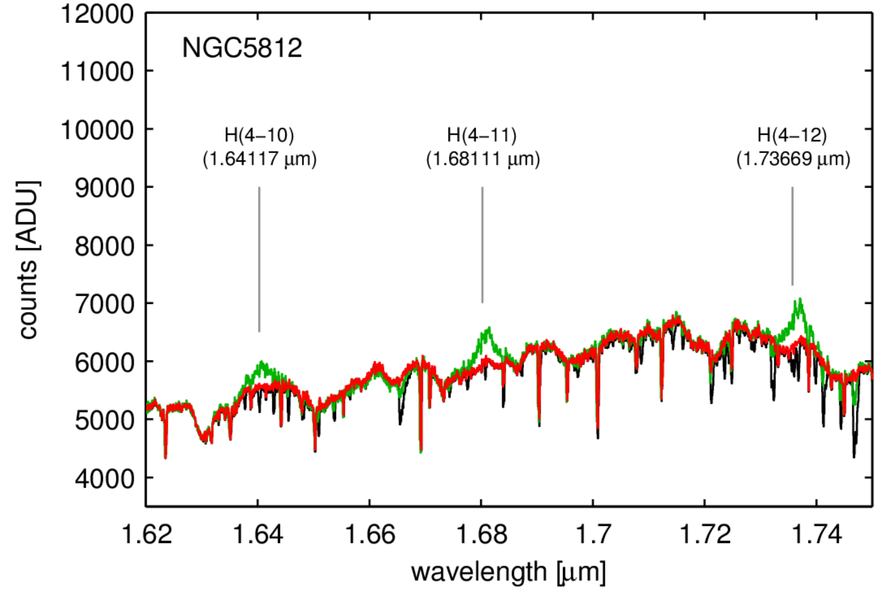


Smette et al. 2015, A&A, 576, A77

Results/Comparison

Comparison with TSS





Object spectrum
molecfit correction
Classical method correction

Kausch et al. 2015, A&A, 576, A78

Limitations

External:

- Accuracy of the line database
- Radiative transfer code accuracy
- Initial atmospheric profile

Internal:

- Low S/N spectra cannot be fitted reliably
- Number of fitting parameters (λ-fit, continuum, LSF,….)
- Intrinsic spectral features of the object
- Resolution

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Correcting for

emission

Required: airglow spectrum

Plain sky observations:

- LSS: portion of the slit w/o object
- specific sky spectrum taken before/after the science target and
- taken in the very vicinity of the science target
- same exposure time

`skycorr`

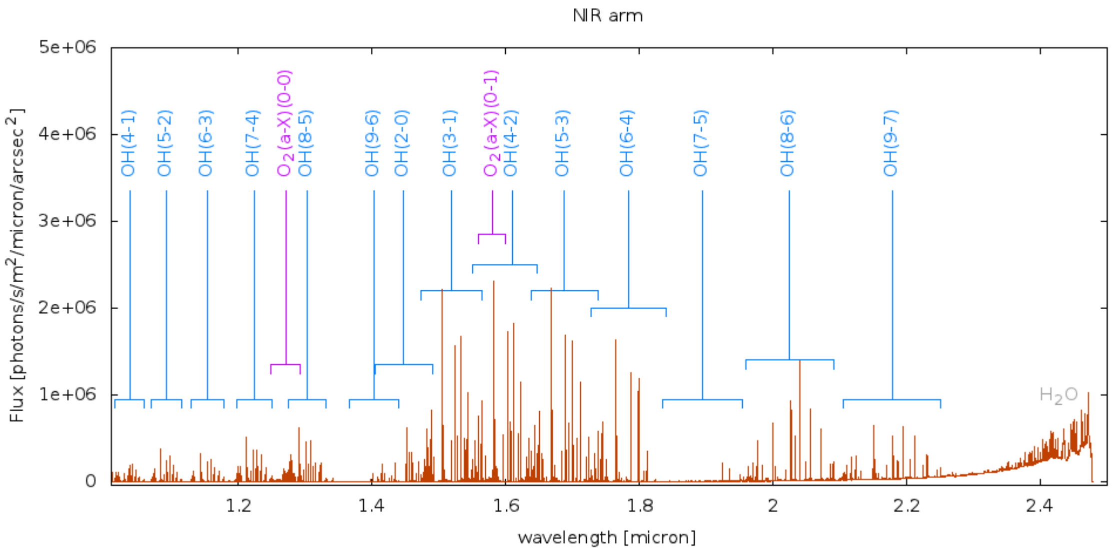
Sky emission removal with `skycorr`

Basic idea ([1], [2]):

- Use an arbitrary plain sky spectrum of the same instrument/setup (archive)
- Iteratively fitting OH line groups individually to corresponding OH emission features in science spectra
- Use the best-fit sky spectrum for the sky emission removal

Features:

- Comprehensive software suite for sky emission removal
- Instrument independent
- world-wide use
- based on Ansi-C
- freely available*

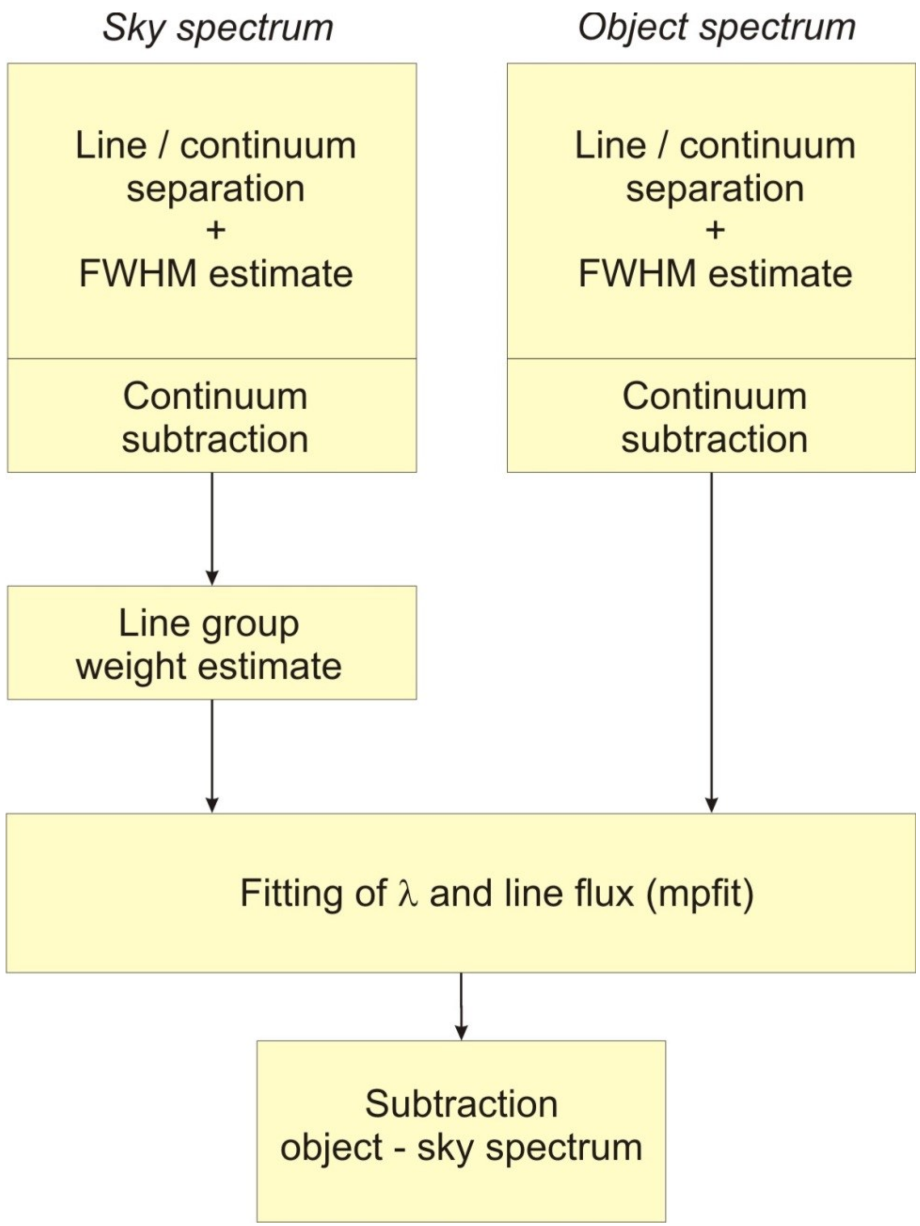


[1] Davies, 2007, MNRAS, 375, 1099
[2] Noll et al., 2014, A&A, 576, 25

*http://www.eso.org/pipelines/skytools

Sky emission removal with `skycorr`

1st step



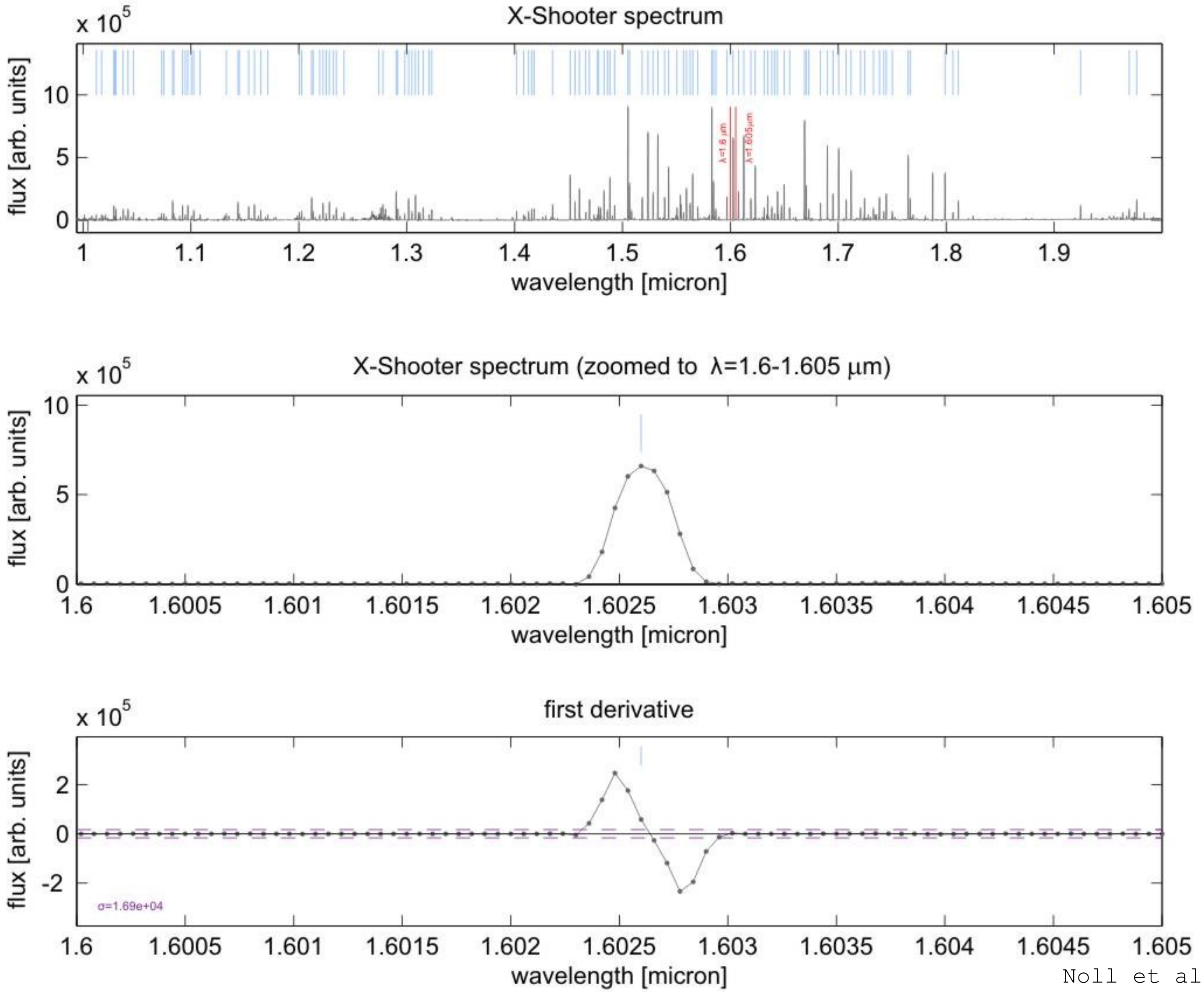
Continuum/Line Separation

- lines:
  sky emission (airglow OH, O_2 [1])
  intrinsic object features

- continuum:
  intrinsic object continuum
  thermal emission (telescope / lower atmosphere)
  airglow continuum (most probably from N_2O [1])
  moonlight [2]
  zodiacal light
  scattered starlight

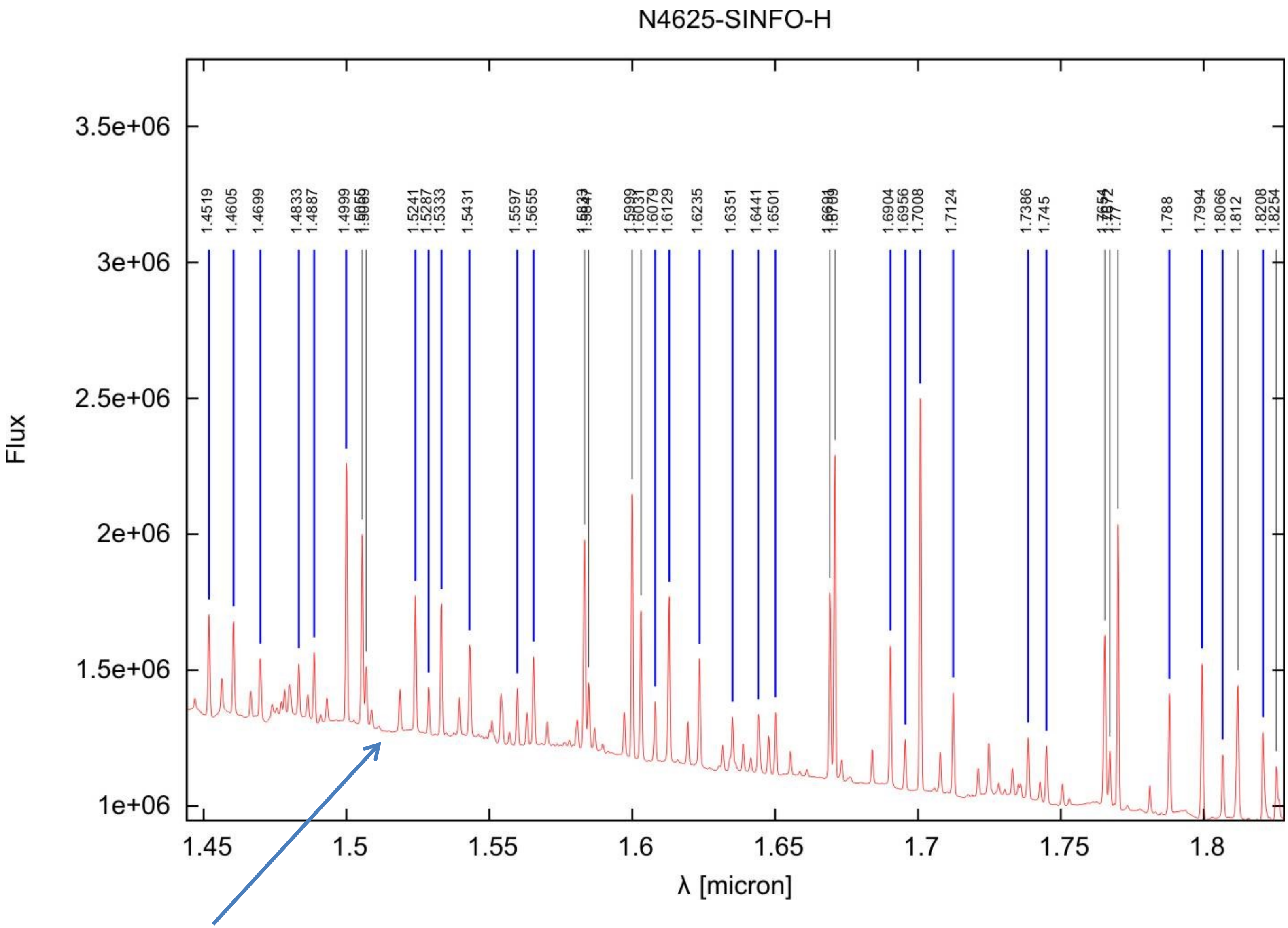
[1] Noll et al. 2012, 2014; Komich et al 2008
[2] Jones et al. 2013, 2015 subm.

Continuum/Line Separation



Noll et al. 2014, A&A, 576, 25

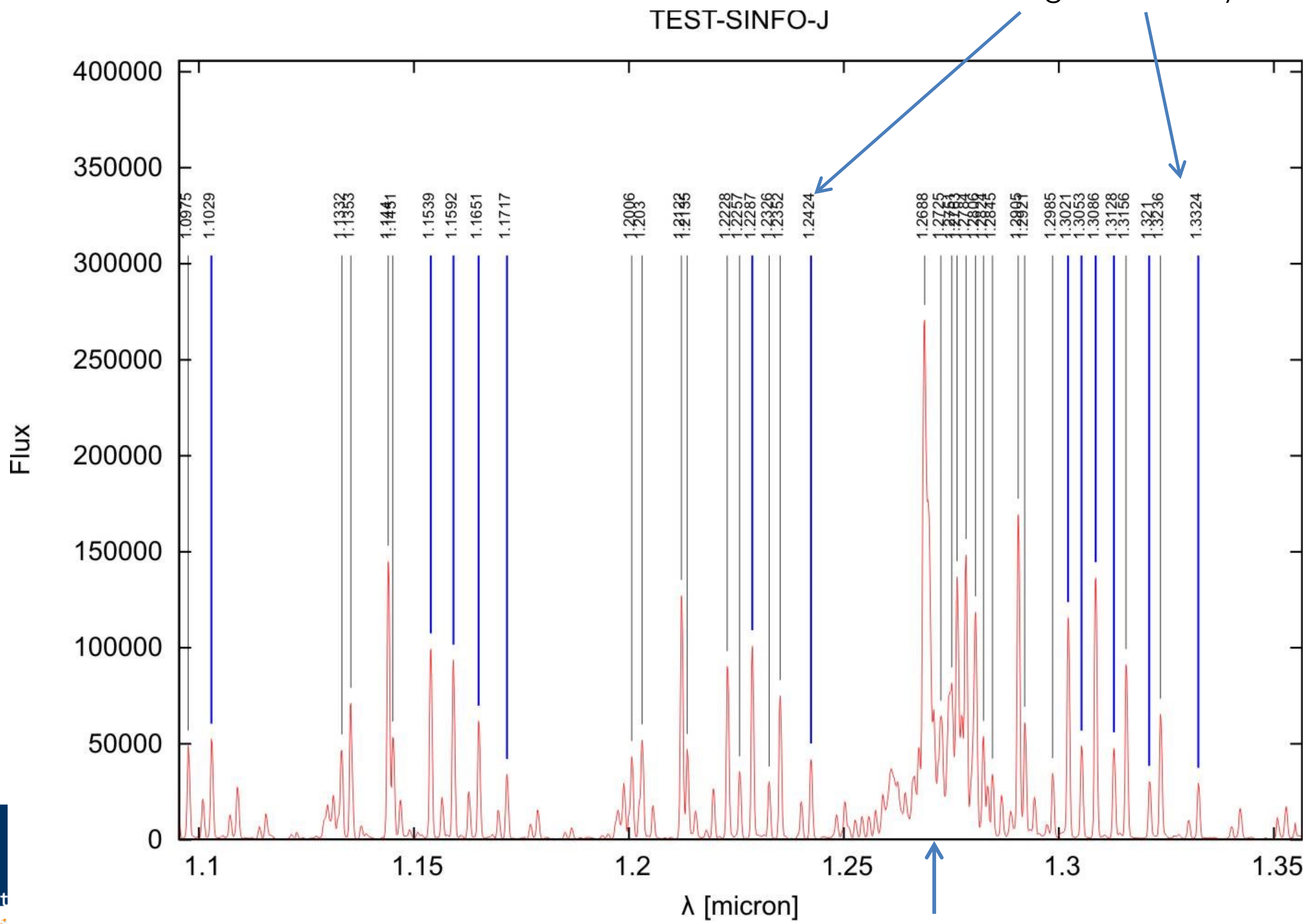
Continuum/Line Separation



continuum slope

Continuum/Line Separation

FWHM determination:
with strong, isolated, symmetric lines



pseudo-continuum (O_2 lines)

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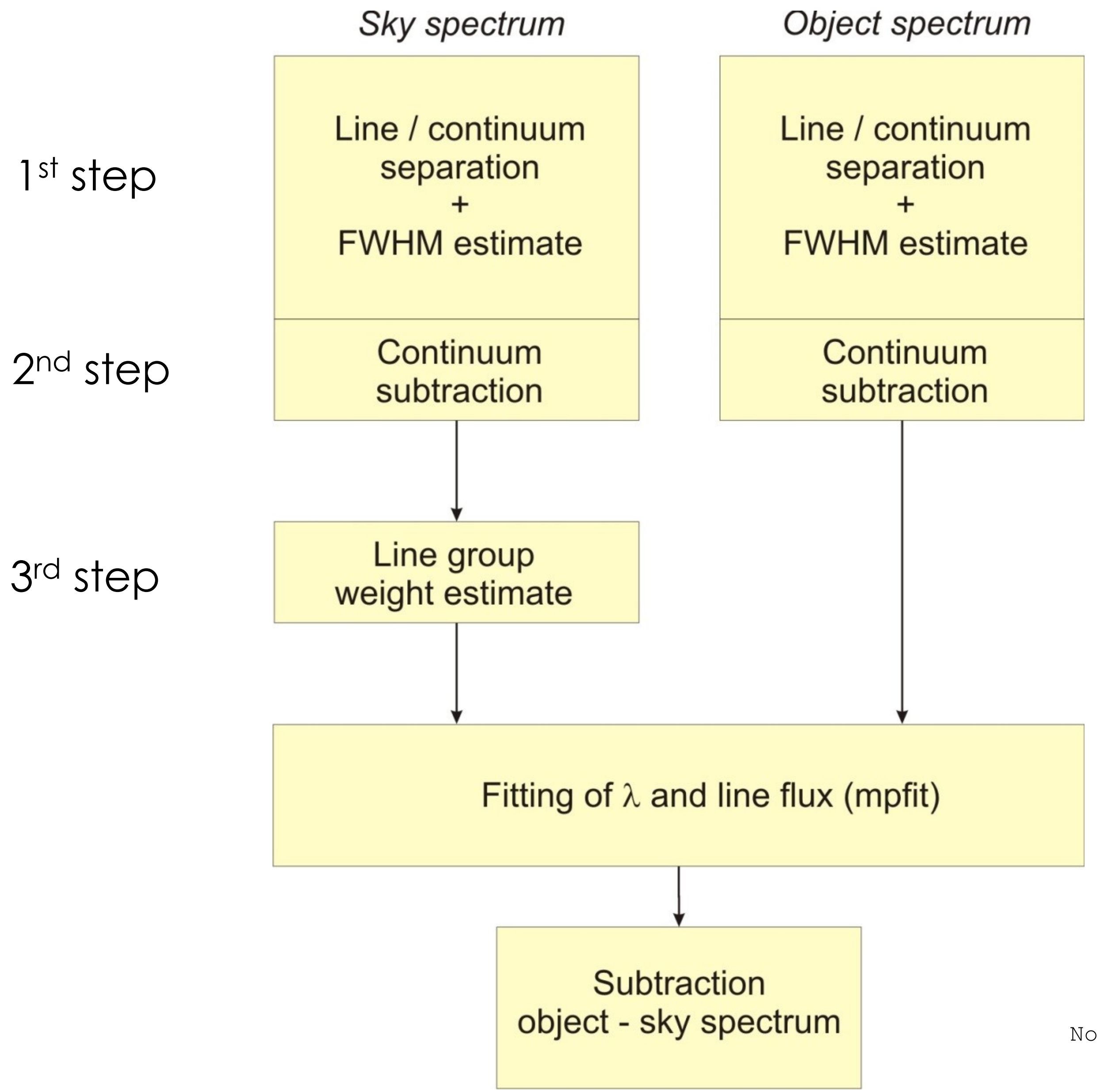
Sky emission removal with `skycorr`

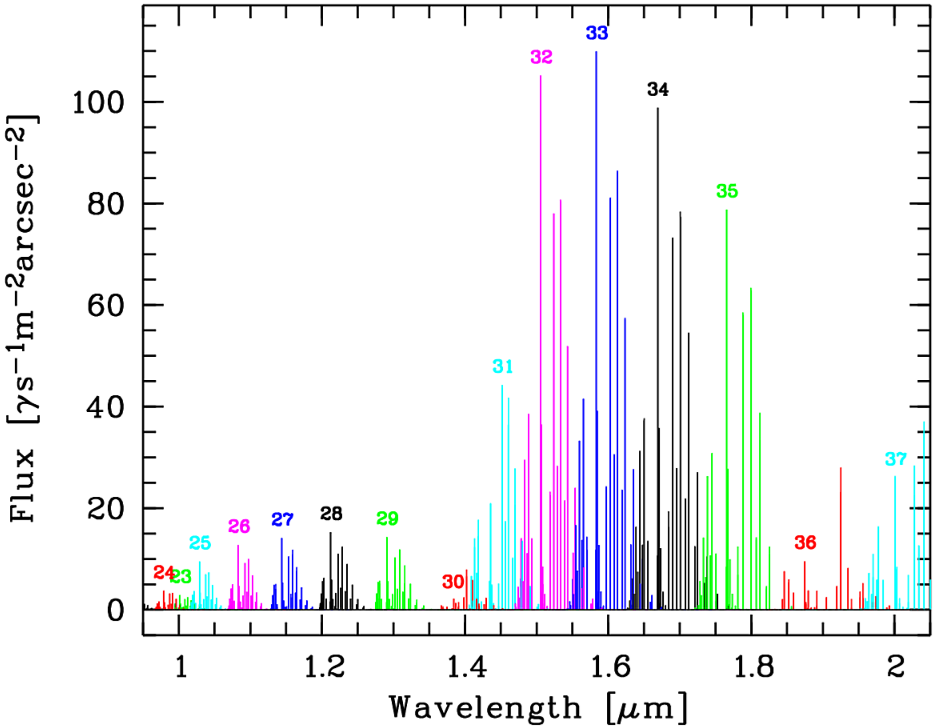


Noll et al. 2014, A&A, 576, A25

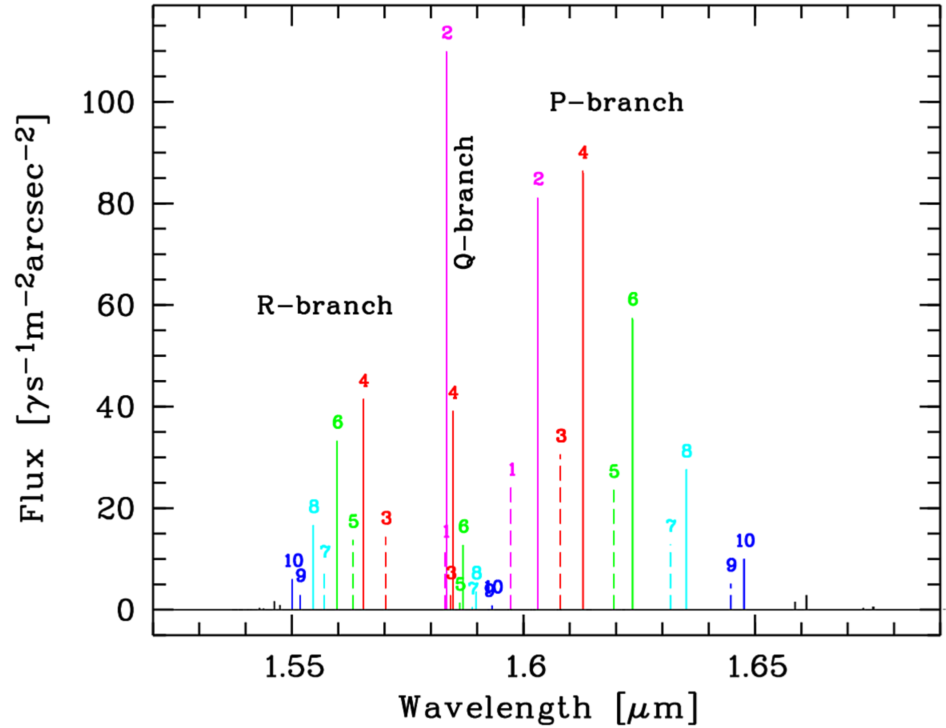
Band Grouping for Line Scaling + Weighting

Grouping by same upper level

Vibrational OH groups (NIR)

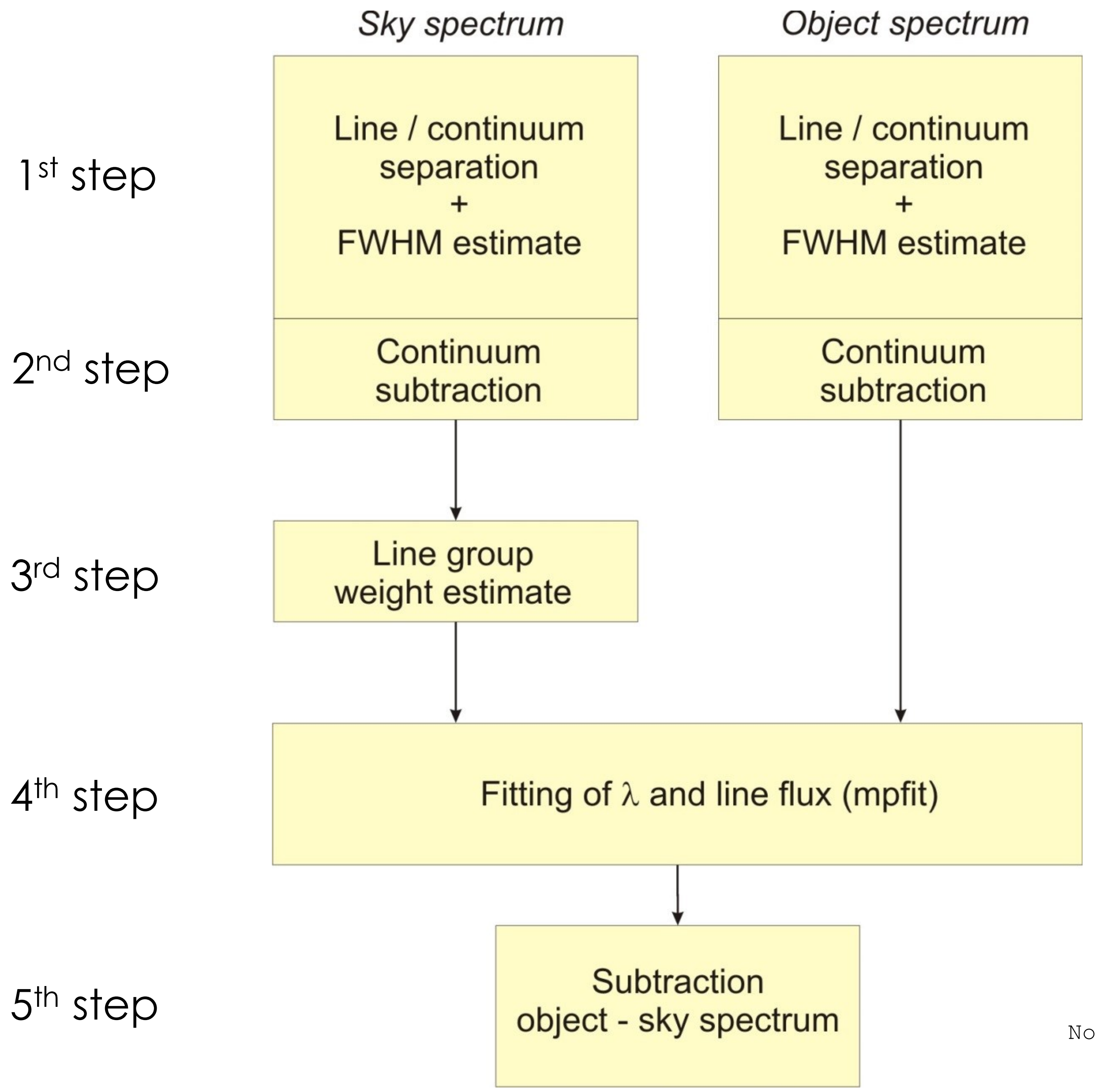


Rotational OH transitions



Noll et al. 2012, A&A, 543, A92
Noll et al. 2014, A&A, 576, A25

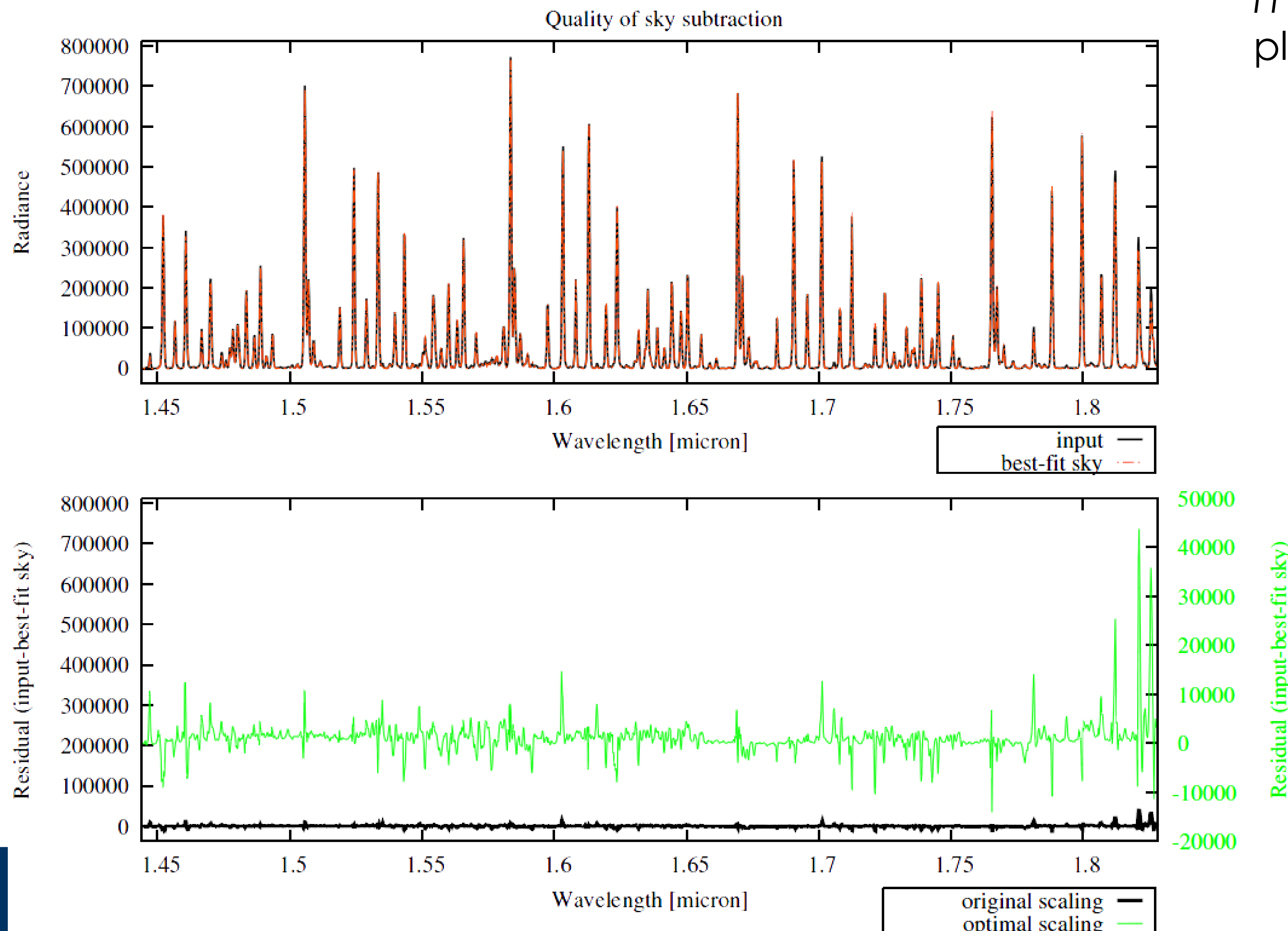
Sky emission removal with `skycorr`



Noll et al. 2014, A&A, 576, A25

Results/Comparison

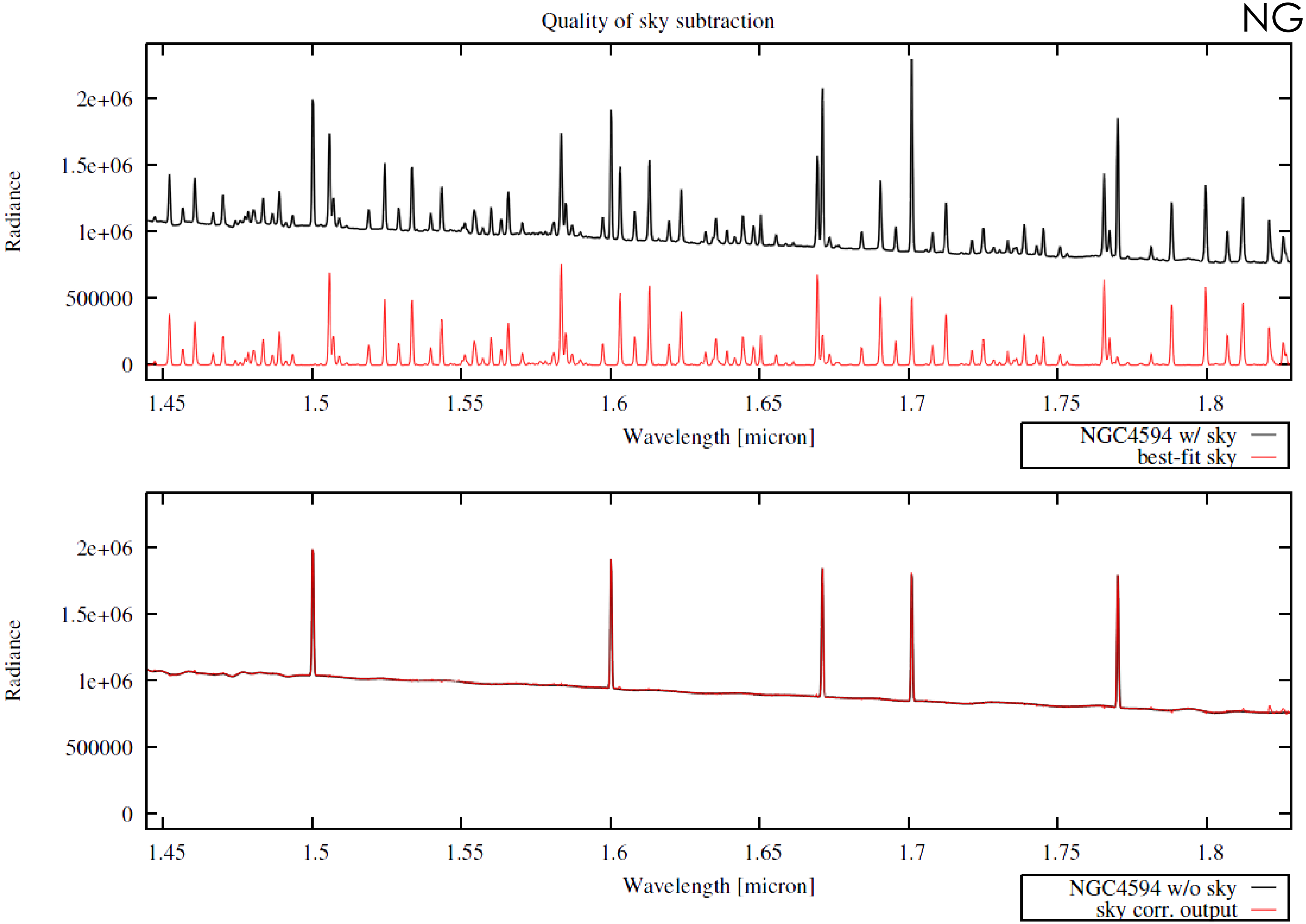
SINFONI
H band
plain sky



Skycorr User Manual, VLT-MAN-ESO-19550-5896

Results/Comparison

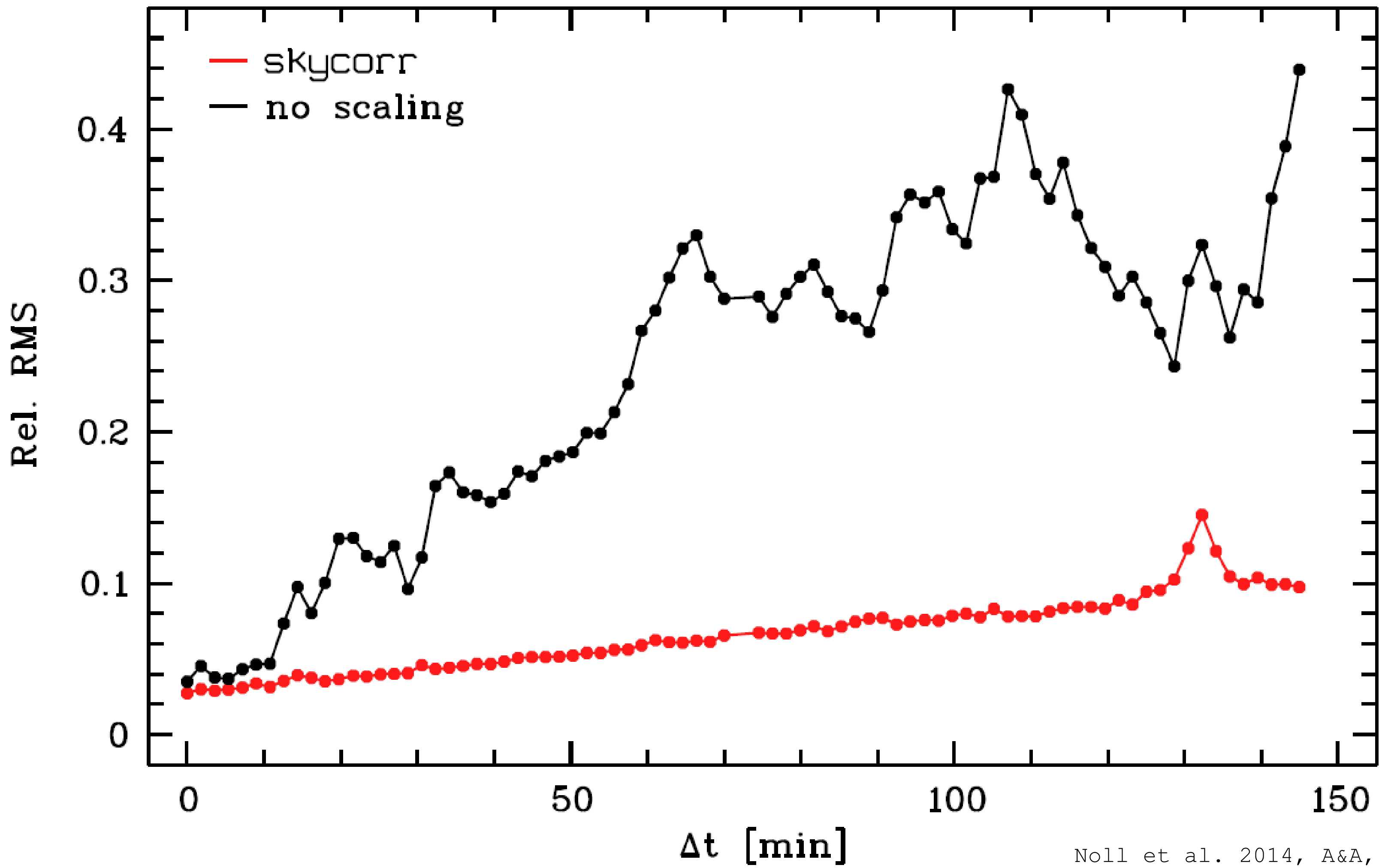
SINFONI
H band
NGC4594



Skycorr User Manual, VLT-MAN-ESO-19550-5896

Results/Comparison: Comparison with Classical Method

RMS of the sky subtraction residuals relative to the mean line peak flux



Noll et al. 2014, A&A, 576, A25

Limitations

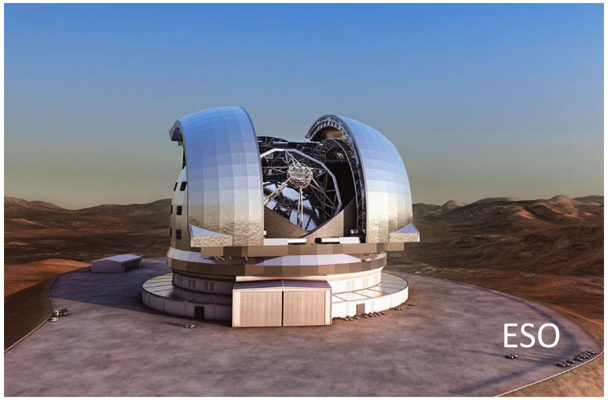
- Accuracy of the incorporated line lists
- Airglow model
- Atmospheric conditions (transparency)
- Instrumental calibration
- Number of fitting parameters (λ-fit, continuum, LSF,….)
- Spectral resolution
- Intrinsic spectral features of the object

Summary & Outlook

Modelling is a good alternative to supplementary observations

`molecfit` and **`skycorr`** are

- Instrument independent
- world-wide use
- based on Ansi-C → high compatibility
- high flexibility
- freely available*



→ Will be implemented in future pipelines

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METIS
Mid-infrared
E-ELT Imager and
Spectrograph

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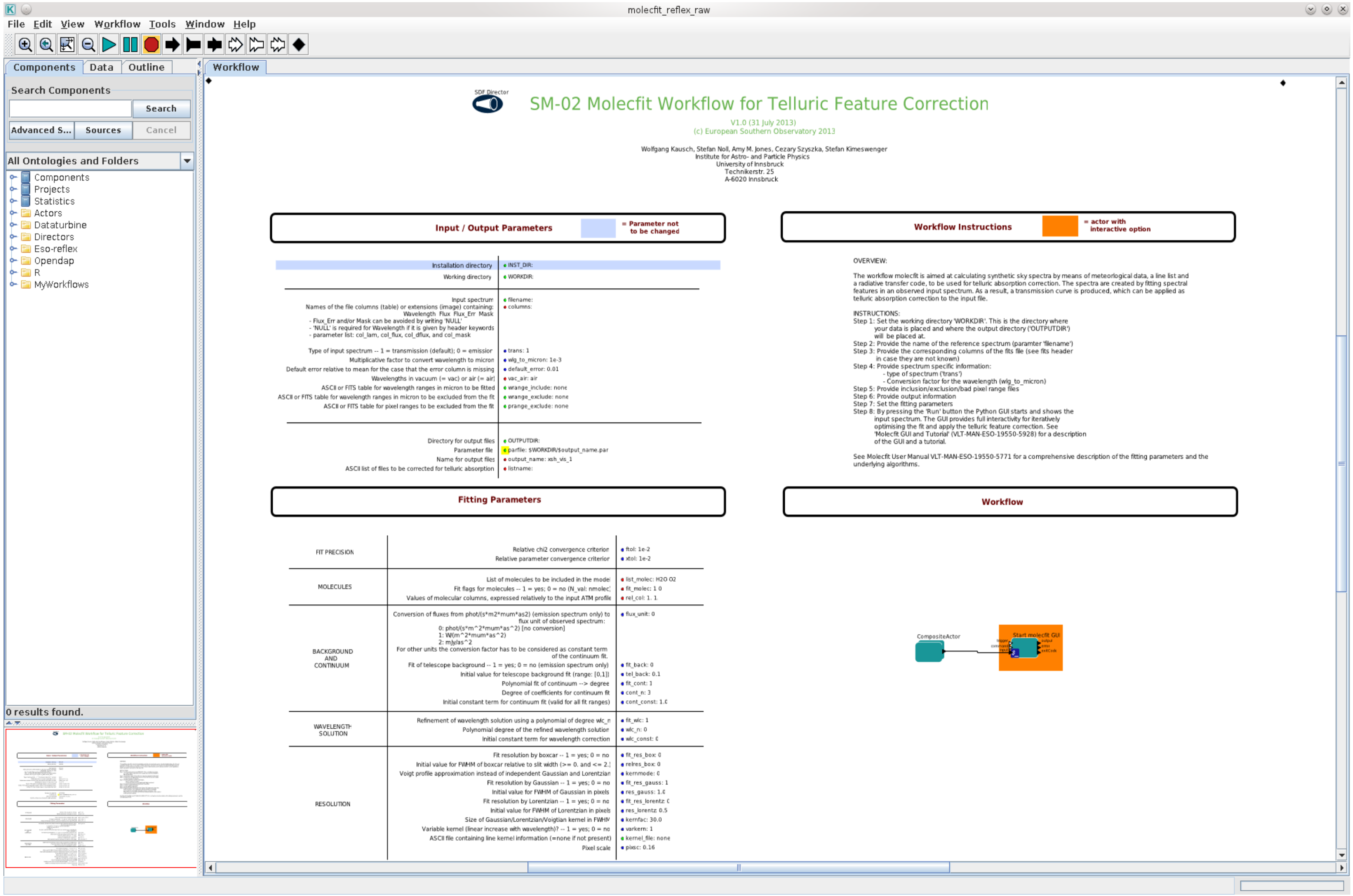
molecfit

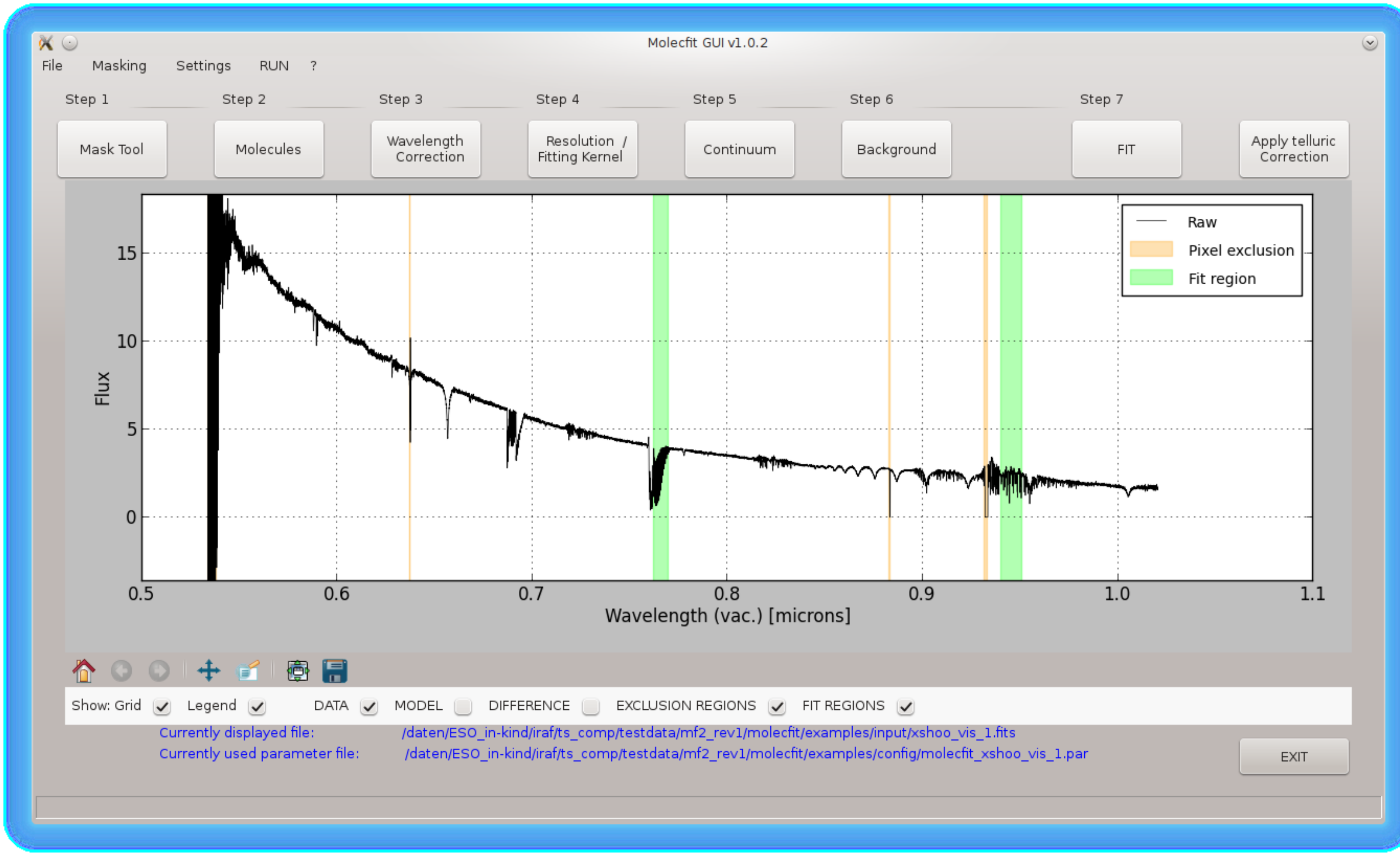
Invoking `molecfit`:

- **Reflex:**



Invoking `molecfit`:

- Reflex
- **GUI:**



Invoking `molecfit`:

- Reflex
- GUI
- **console:**

```
<inst_dir>/bin/molecfit  <parameterfile>
```

`<parameterfile>`:

contains all information required for the telluric absorption correction for a specific file, i.e. filenames, fitting parameters, output,….

Parameter file: plain ASCII file → text editor

```
### Driver for MOLECFIT
## DIRECTORY STRUCTURE
# Base directory (default: ".") for the following folder structure:
#
# |--bin/
# |
# |--config/
# <basedir>----|
# |--data/
# |
# |--output/
#
# A relative or an absolute path can be provided. In the former case MOLECFIT
# has to be started in <basedir>.
basedir: .

## INPUT DATA
# Data file name (path relative to basedir or absolute path)
filename: examples/input/crires_spec_jitter_extracted_0000.fits

# ASCII list of files to be corrected for telluric absorption using the
# transmission curve derived from the input reference file (path of list and
# listed files relative to basedir or absolute path; default: "none")
listname: none

# Type of input spectrum -- 1 = transmission (default); 0 = emission
trans: 1
```

Sections

comments (‚#‘)

parameter:

<parname>: <parvalue>

- or -

<parname>

Parameters: Sections „Directory“ and „Input Data“

```
[…]

# A relative or an absolute path can be provided. In the former case MOLECFIT
# has to be started in <basedir>.
basedir: .

## INPUT DATA
# Data file name (path relative to basedir or absolute path)
filename: examples/input/crires_spec_jitter_extracted_0000.fits

# ASCII list of files to be corrected for telluric absorption using the
# transmission curve derived from the input reference file (path of list and
# listed files relative to basedir or absolute path; default: "none")
listname: none

[…]
```

basedir: In all cases either absolute paths can be given, or paths relative to *basedir*

filename: File, which is to be corrected. This file is the reference, which is usually used for fitting and for the correction

listname: ASCII file containing a list of other spectra, which should be corrected with the same transmission spectrum

Parameters: Sections „Directory“ and „Input Data“

```
[…]

# Type of input spectrum -- 1 = transmission (default); 0 = emission
trans: 1

# Names of the file columns (table) or extensions (image) containing:
# Wavelength Flux Flux_Err Mask
# - Flux_Err and/or Mask can be avoided by writing ’NULL’
# - ’NULL’ is required for Wavelength if it is given by header keywords
# - parameter list: col_lam, col_flux, col_dflux, and col_mask
columns: Wavelength Extracted_OPT Error_OPT NULL

# Default error relative to mean for the case that the error column is missing
default_error: 0.01

[…]
```

trans: molecfit can fit both emission and transmission features;

columns: column names of the input file

default_error: If no error column is present one can give a default error here

Parameters: Sections „Directory“ and „Input Data“

```
[…]

# Multiplicative factor to convert wavelength to micron
# (e.g. nm -> wlgtomicron = 1e-3)
wlgtomicron: 1e-3

# Wavelengths in vacuum (= vac) or air (= air)
vac_air: vac

[…]
```

wlgtomicron: Molecfit calculates internally in [µm]. Thus one needs to specifiy the wavelength unit in the input spectrum

vac_air: Wavelength regime; depends on the pipeline output

Parameters: Sections „Directory“ and „Input Data“

```
[…]

# ASCII or FITS table for wavelength ranges in micron to be fitted
# (path relative to basedir or absolute path; default: "none")
wrange_include: none

# ASCII or FITS table for wavelength ranges in micron to be excluded from the
# fit (path relative to basedir or absolute path; default: "none")
wrange_exclude: none

# ASCII or FITS table for pixel ranges to be excluded from the fit
# (path relative to basedir or absolute path; default: "none")
prange_exclude: examples/config/exclude_crires.dat

[…]
```

Definition of the range files

wrange_include: Path to the file defining the fitting ranges

wrange_exclude: Exclusion range in λ space

prange_exclude: Exclusion range in pixel space

Parameters: Section „Results“

```
[…]

## RESULTS
# Directory for output files (path relative to basedir or absolute path)
output_dir: output

# Name for output files
# (supplemented by "_fit" or "_tac" as well as ".asc", ".atm", ".fits",
# ".par, ".ps", and ".res")
output_name: molecfit_crires

# Plot creation: gnuplot is used to create control plots
# W - screen output only (incorporating wxt terminal in gnuplot)
# X - screen output only (incorporating x11 terminal in gnuplot)
# P - postscript file labelled '<output_name>.ps', stored in <output_dir>
# combinations possible, i.e. WP, WX, XP, WXP (however, keep the order!)

# all other input: no plot creation is performed
plot_creation: XP

# Create plots for individual fit ranges? -- 1 = yes; 0 = no
plot_range: 0

[…]
```

output_dir: directory where all output files are stored in

output_name: Defines name space for output files

plot_creation: Defines type of output plots

plot_range: Defines whether plots for ALL fitting ranges should be created individually

Parameters: Section „Fit Precision“

```
[…]

## FIT PRECISION
# Relative chi2 convergence criterion
ftol: 1e-2

# Relative parameter convergence criterion
xtol: 1e-2

[…]
```

mpfit stops the fitting procedure as soon as either the χ^2-value or the fitting parameters change less than a given certain limit

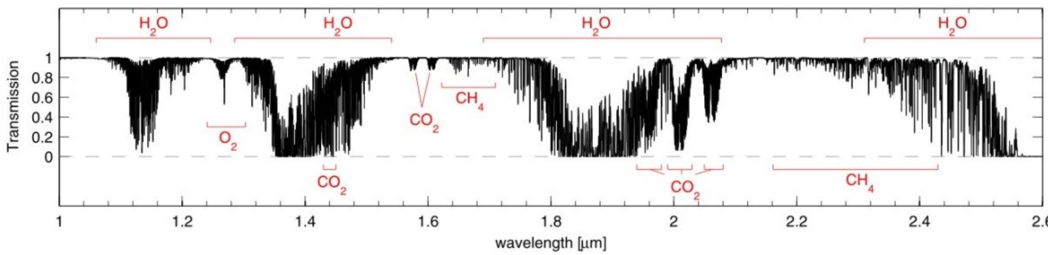
ftol: Convergence criterion for the variation of the χ^2-value

xtol: Convergence criterion for the variation of the fitting parameters

Note: Use with care!

Parameters: Section „Molecular column“

```
[…]

# List of molecules to be included in the model
# (default: 'H2O', N_val: nmolec)
list_molec: H2O CH4 O3

# Fit flags for molecules -- 1 = yes; 0 = no (N_val: nmolec)
fit_molec: 1 1 1

# Values of molecular columns, expressed relatively to the input ATM profile
# columns (N_val: nmolec)
relcol: 1. 1. 1.

[…]
```



list_molec: List of molecules to be considered by the radiative transfer code; Depends on the chosen fitting range

fit_molec: Defines, whether a molecular column should be fitted or assumed to be constant

relcol: Scaling factor for the molecular column (starting value);

NOTE: # of values in *fit_molec* and *relcol* must be equal to number of molecules (order!);

Parameters: Section „Background and continuum“

```
[…]

## BACKGROUND AND CONTINUUM
# Conversion of fluxes from phot/(s*m2*mum*as2) (emission spectrum only) to
# flux unit of observed spectrum:
# 0: phot/(s*m^2*mum*as^2) [no conversion]
# 1: W/(m^2*mum*as^2)
# 2: erg/(s*cm^2*A*as^2)
# 3: mJy/as^2
# For other units, the conversion factor has to be considered as constant term
# of the continuum fit.
flux_unit: 0

# Fit of telescope background -- 1 = yes; 0 = no (emission spectrum only)
fit_back: 0

# Initial value for telescope background fit (range: [0,1])
telback: 0.1

[…]
```

flux_unit: Same as wlgtomicron, but for the flux (internal units: photons/(s*m^2*µm*as^2))

fit_back: Defines, whether the telescope background should be fitted (greybody). Only important for emission spectra (parameter: *trans*: 0)

telback: Initial value for the telescope background (greybody factor)

Parameters: Section „Background and continuum“

```
[…]

# Polynomial fit of continuum --> degree: cont_n
fit_cont: 1

# Degree of coefficients for continuum fit
cont_n: 3

# Initial constant term for continuum fit (valid for all fit ranges)
# (emission spectrum: about 1 for correct flux_unit)
cont_const: 1.

[…]
```

fit_cont: Defines whether the continuum should be fitted as poynomial

cont_n: degree of continuum polynomial

cont_const: Initial constant continuum value; Can be only roughly in the order of the continuum level

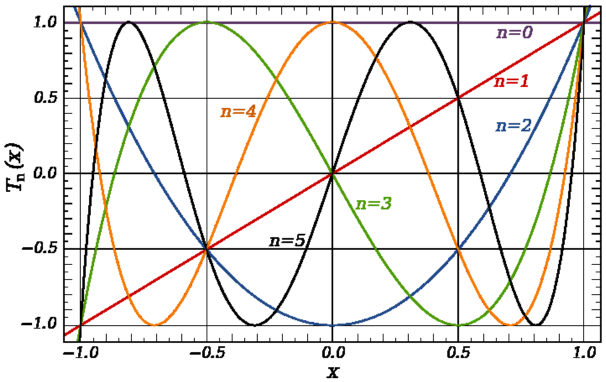
Parameters: Section „Wavelength solution“

```
[…]

## WAVELENGTH SOLUTION
# Refinement of wavelength solution using a polynomial of degree wlc_n
fit_wlc: 1

# Polynomial degree of the refined wavelength solution
wlc_n: 3

# Initial constant term for wavelength correction (shift relative to half
# wavelength range)
wlc_const: 0.

[…]
```

fit_wlc: Defines whether the wavelegth grid should be fitted with a Chebyshev polynome

wlc_n: degree of Chebyshev polynomial

wlc_const: Initial constant term for the wavelength correctopm



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Parameters: Section „Resolution“

```
[…]

## RESOLUTION
# Fit resolution by boxcar -- 1 = yes; 0 = no
fit_res_box: 0

# Initial value for FWHM of boxcar relative to slit width (>= 0. and <= 2.)
relres_box: 0.

# Voigt profile approximation instead of independent Gaussian and Lorentzian
# kernels? -- 1 = yes; 0 = no
kernmode: 0

[…]
```

fit_res_box: Defines whether the Line Spread Function (LSF) kernel should contain a boxcar component

relres_box: Initial value for the BOXCAR component relative to the slit width

kernmode: molecfit can fit the line profile by either a Voigt profile, or by independent Gaussian/Lorentzian kernel

Parameters: Section „Resolution“

```
[…]

# Fit resolution by Gaussian -- 1 = yes; 0 = no
fit_res_gauss: 1

# Initial value for FWHM of Gaussian in pixels
res_gauss: 1.

# Fit resolution by Lorentzian -- 1 = yes; 0 = no
fit_res_lorentz: 0

# Initial value for FWHM of Lorentzian in pixels
res_lorentz: 0.5

[…]
```

fit_res_gauss:

rel_gauss: Initial value for FWHM of the GAUSSIAN component

fit_res_lorentz:

res_lorentz: Initial value for FWHM of the LORENTZIAN component

Parameters: Section „Instrumental parameters“

```
[…]

## INSTRUMENTAL PARAMETERS
# Slit width in arcsec (taken from FITS header if present)
slitw: 0.4
slitw_key: ESO INS SLIT1 WID

# Pixel scale in arcsec (taken from this file only)
pixsc: 0.086
pixsc_key: NONE

[…]
```

slitw: Slit width in arcsec (taken from FITS header if present)

slitw_key: fitsheader keyword describing the slit width

pixsc: Pixel scale in arcsec

pixsc_key: fitsheader keyword describing the pixel scale

Parameters: Sections „Ambient parameters“ and „Atmospheric profiles“

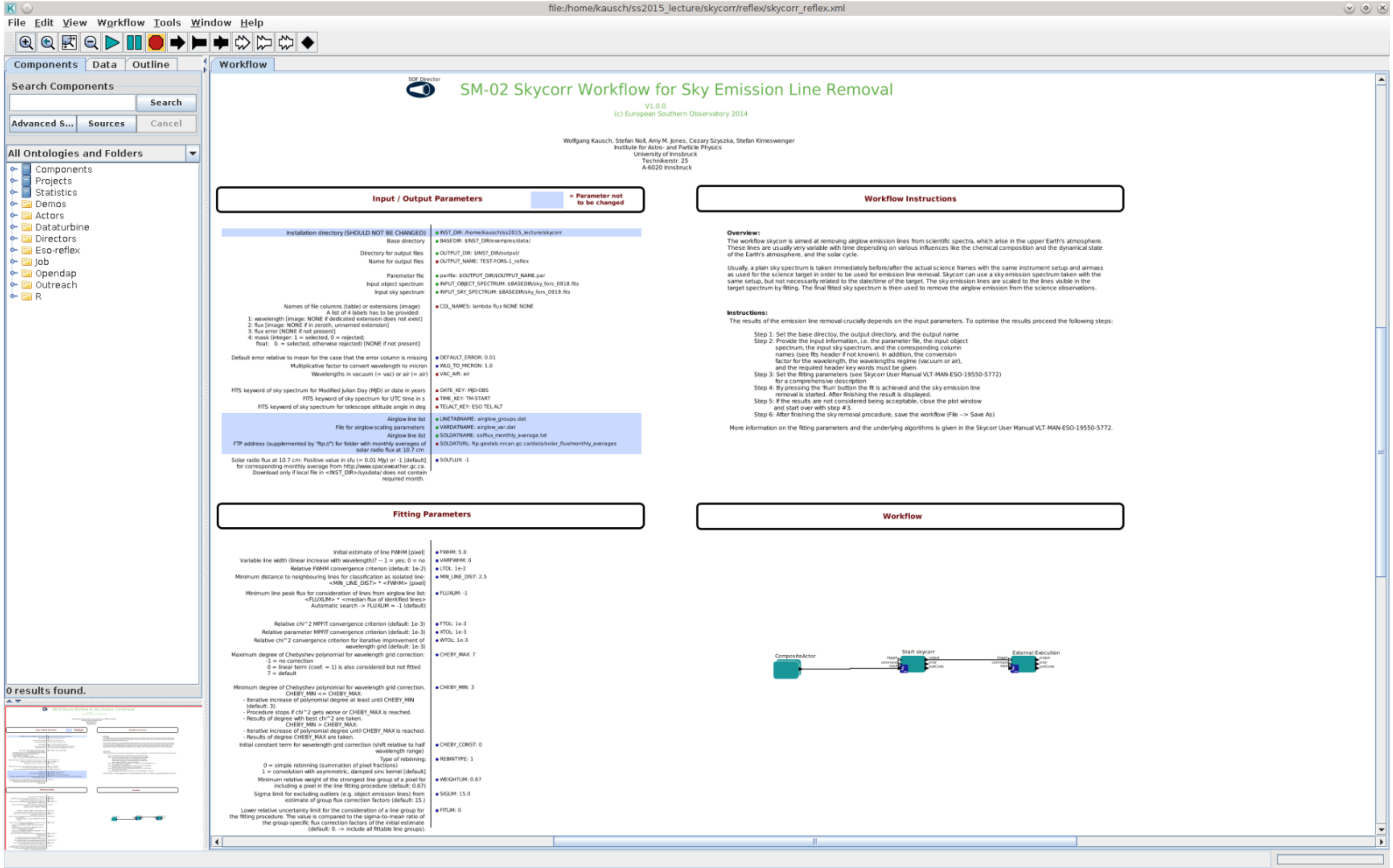
These sections incorporate parameters describing the date/time of the observations, the airmass, atmopsheric state during the time of the observations (r_H, P, T, M1 temperature,…), longitude/latitude of observatory, ….

Mostly taken from fits header keyword („<parameter>_key“), or should not be modified.

skycorr

Invoking `skycorr`:

- **Reflex:**



Invoking `skycorr`:

- Reflex
- **console:**

```
<inst_dir>/bin/skycorr  <parameterfile>
```

`<parameterfile>`:

contains all information required for the removal of sky emission lines for a specific file, i.e. filenames, fitting parameters, output,….

Parameter file: plain ASCII file → text editor (as `molecfit`)

```
# ----------------------------------------------------------------------------
# -------------------- INPUT PARAMETER FILE FOR SKYCORR ----------------------
# ----------------------------------------------------------------------------

# ---------------------------DIRECTORIES + FILES-------------------------------
# Absolute path of skycorr installation directory
INST_DIR=../../

# Absolute or relative (with respect to INST_DIR) path and filename of input
# object spectrum
INPUT_OBJECT_SPECTRUM=src/test/data/sky_sinfo_1.fits

# Absolute or relative (with respect to INST_DIR) path and filename of input
# sky spectrum
INPUT_SKY_SPECTRUM=src/test/data/sky_sinfo_2.fits

# Absolute or relative (with respect to INST_DIR) path and filename of output
# directory (will be created if not present; default: <INST_DIR>/output/)
OUTPUT_DIR=output

# Main name of diagnostic output files, extensions will be added
OUTPUT_NAME=TEST-SINFO-H

.
.
.
```

comments (‚#‘)

Sections

parameter:

<parname>: <parvalue>

- or -

<parname>

Parameter file: plain ASCII file → text editor (as `molecfit`)

```
[…]

# ---------------------------DIRECTORIES + FILES-----------------------------
# Absolute path of skycorr installation directory
INST_DIR=../../

# Absolute or relative (with respect to INST_DIR) path and filename of input
# object spectrum
INPUT_OBJECT_SPECTRUM=src/test/data/sky_sinfo_1.fits

# Absolute or relative (with respect to INST_DIR) path and filename of input
# sky spectrum
INPUT_SKY_SPECTRUM=src/test/data/sky_sinfo_2.fits

# Absolute or relative (with respect to INST_DIR) path and filename of output
# directory (will be created if not present; default: <INST_DIR>/output/)
OUTPUT_DIR=output

# Main name of diagnostic output files, extensions will be added
OUTPUT_NAME=TEST-SINFO-H

[…]
```

Section for FILES and DIRECTORIES […]

Parameter file: plain ASCII file → text editor (as `molecfit`)

```
[…]

#------------------------------INPUT STRUCTURE--------------------------------
# Names of file columns (table) or extensions (image)
# A list of 4 labels has to be provided:
# 1: wavelength [image: NONE if dedicated extension does not exist]
# 2: flux [image: NONE if in zeroth, unnamed extension]
# 3: flux error [NONE if not present]
# 4: mask (integer: 1 = selected, 0 = rejected;
# float: 0. = selected, otherwise rejected) [NONE if not present]
COL_NAMES=lambda flux NONE NONE

# Error relative to mean if no error column is provided (default: 0.01)
DEFAULT_ERROR=0.01

# Multiplicative factor to convert wavelength to micron
# e.g.: wavelength unit = A -> WLG_TO_MICRON = 1e-4
WLG_TO_MICRON=1.

# Wavelengths in vacuum (= vac) or air (= air)
VAC_AIR=vac
[…]
```

Section for INPUT structure `[…]` : as for `molecfit`

Parameter file: plain ASCII file → text editor (as `molecfit`)

```
[…]

# ------------------------------------------------------------------------------
# ------------------------- EXPERT MODE PARAMETERS ----------------------------
# ------------------------------------------------------------------------------

[…]
```

Section for EXPERT MODE: Should be used with care!

FITS keywords, line lists, scaling parameters for airglow, solar radio flux database, etc….

Parameter file: plain ASCII file → text editor (as `molecfit`)

```
[…]

# ---------------------------LINE IDENTIFICATION------------------------------
# Initial estimate of line FWHM [pixel]
FWHM=5.0

# Variable line width (linear increase with wavelength)? -- 1 = yes; 0 = no
VARFWHM=0

# Relative FWHM convergence criterion (default: 1e-2)
LTOL=1e-2

# Minimum distance to neighbouring lines for classification as isolated line:
# <MIN_LINE_DIST> * <FWHM> [pixel]
MIN_LINE_DIST=2.5

# Minimum line peak flux for consideration of lines from airglow line list:
# <FLUXLIM> * <median flux of identified lines>
# Automatic search -> FLUXLIM = -1 (default)
FLUXLIM=-1

[…]
```

FWHM: Estimate of the FWHM for the line identification

VARFWHM: Switch whether the FWHM should be assumed to be variable

LTOL: convergence criterion for the FWHM fit

MIN_LINE_DIST: min. distance between two lines to be assumed as being separated ([FWHM])

FLUXLIM: minimum line peak flux to be considered from the airglow line list

Parameter file: plain ASCII file → text editor (as `molecfit`)

```
[…]

# ---------------------------FITTING OF SKY LINES-----------------------------
# Relative chi^2 MPFIT convergence criterion (default: 1e-3)
FTOL=1e-3

# Relative parameter MPFIT convergence criterion (default: 1e-3)
XTOL=1e-3

# Relative chi^2 convergence criterion for iterative improvement of
# wavelength grid (default: 1e-3)
WTOL=1e-3

[…]
```

Parameters for fitting the sky emission lines: same as `molecfit`

WTOL: convergence criterion for the wavelength fit

Parameter file: plain ASCII file → text editor (as `molecfit`)

```
[…]

# Maximum degree of Chebyshev polynomial for wavelength grid correction:
# -1 = no correction
# 0 = linear term (coef. = 1) is also considered but not fitted
# 7 = default
CHEBY_MAX=7

# Minimum degree of Chebyshev polynomial for wavelength grid correction.
# CHEBY_MIN <= CHEBY_MAX:
# - Iterative increase of polynomial degree at least until CHEBY_MIN
# (default: 3).
# - Procedure stops if chi^2 gets worse or CHEBY_MAX is reached.
# - Results of degree with best chi^2 are taken.
# CHEBY_MIN > CHEBY_MAX:
# - Iterative increase of polynomial degree until CHEBY_MAX is reached.
# - Results of degree CHEBY_MAX are taken.
CHEBY_MIN=3

# Initial constant term for wavelength grid correction (shift relative to half
# wavelength range)
CHEBY_CONST=0.

[…]
```

Parameters for fitting the wavelength grid with Chebyshev polynomials

Parameter file: plain ASCII file → text editor (as `molecfit`)

```
[…]

# Type of rebinning:
# 0 = simple rebinning (summation of pixel fractions)
# 1 = convolution with asymmetric, damped sinc kernel [default]
REBINTYPE=1

# Minimum relative weight of the strongest line group of a pixel for
# including a pixel in the line fitting procedure (default: 0.67)
WEIGHTLIM=0.67

# Sigma limit for excluding outliers (e.g. object emission lines) from
# estimate of group flux correction factors (default: 15.)
SIGLIM=15.

# Lower relative uncertainty limit for the consideration of a line group for
# the fitting procedure. The value is compared to the sigma-to-mean ratio of
# the group-specific flux correction factors of the initial estimate
# (default: 0. -> include all fittable line groups).
FITLIM=0.

[…]
```

REBINTYPE: Output can be rebinned, defines simple/kernel convolution rebinning
WEIGHTLIM: minimum relative weight for the strongest line group of a pixel
SIGLIM: Exclusion criterion for outliers
FITLIM:

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