Retrievals of vertical profiles of temperature from NOMAD on-board ESA's TGO

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and the ROADMAP team

1. Why are we interested into atmospheric temperature ?

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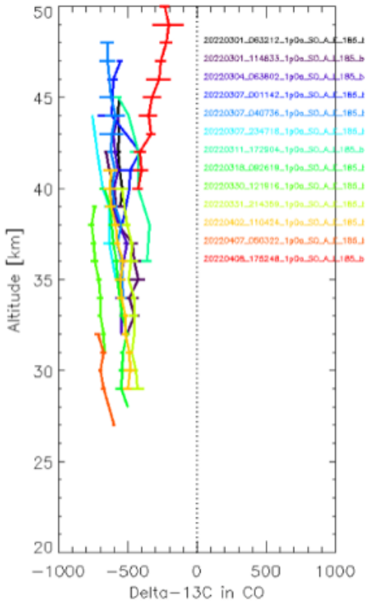
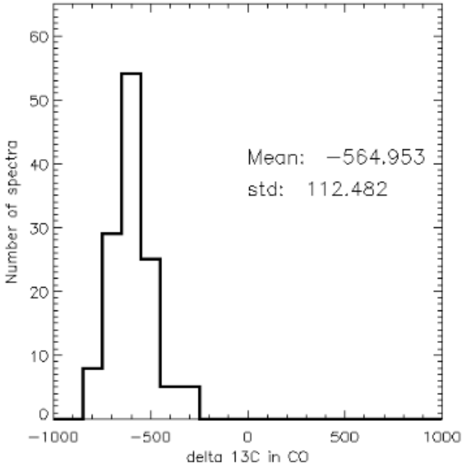
Depletion of ^{13}C in CO in the Atmosphere of Mars Suggested by ExoMars-TGO/NOMAD Observations

S. Aoki[1,2], K. Shiobara[3], N. Yoshida[3], L. Trompet[2], T. Yoshida[3], N. Terada[3], H. Nakagawa[3], G. Liuzzi[4], A. C. Vandaele[2], I. R. Thomas[2], G. L. Villanueva[5], M. A. Lopez-Valverde[6], A. Brines[6], M. R. Patel[7], S. Faggi[5,8], F. Daerden[2], J. T. Erwin[2], B. Ristic[2], G. Bellucci[9], J. J. Lopez-Moreno[6], H. Kurokawa[10,11], and Y. Ueno[11]

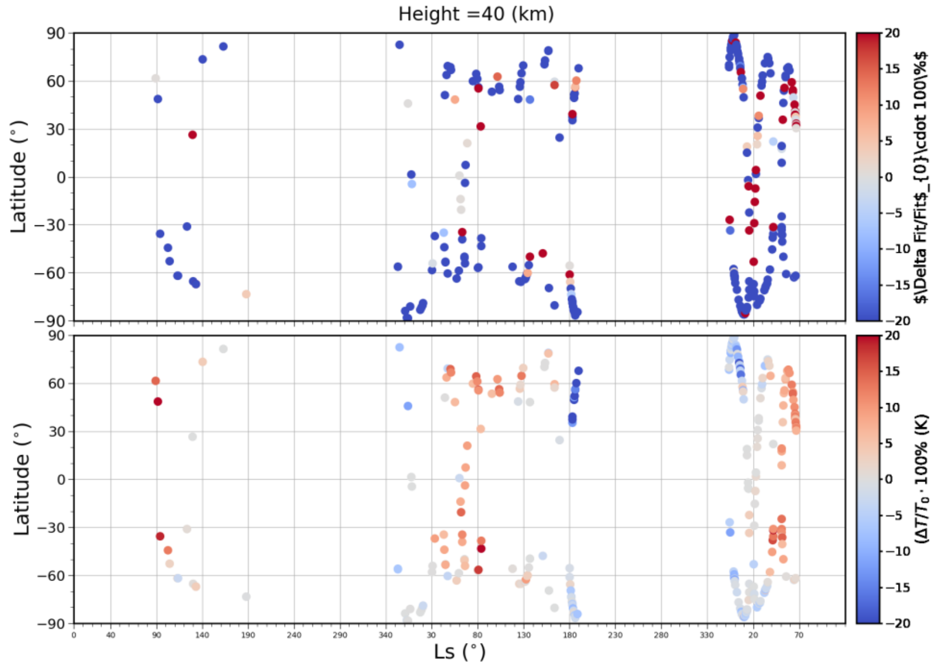


with retrieved T



S. Aoki et al. (2023)

Sensitivity of O_3 retrievals to temperature

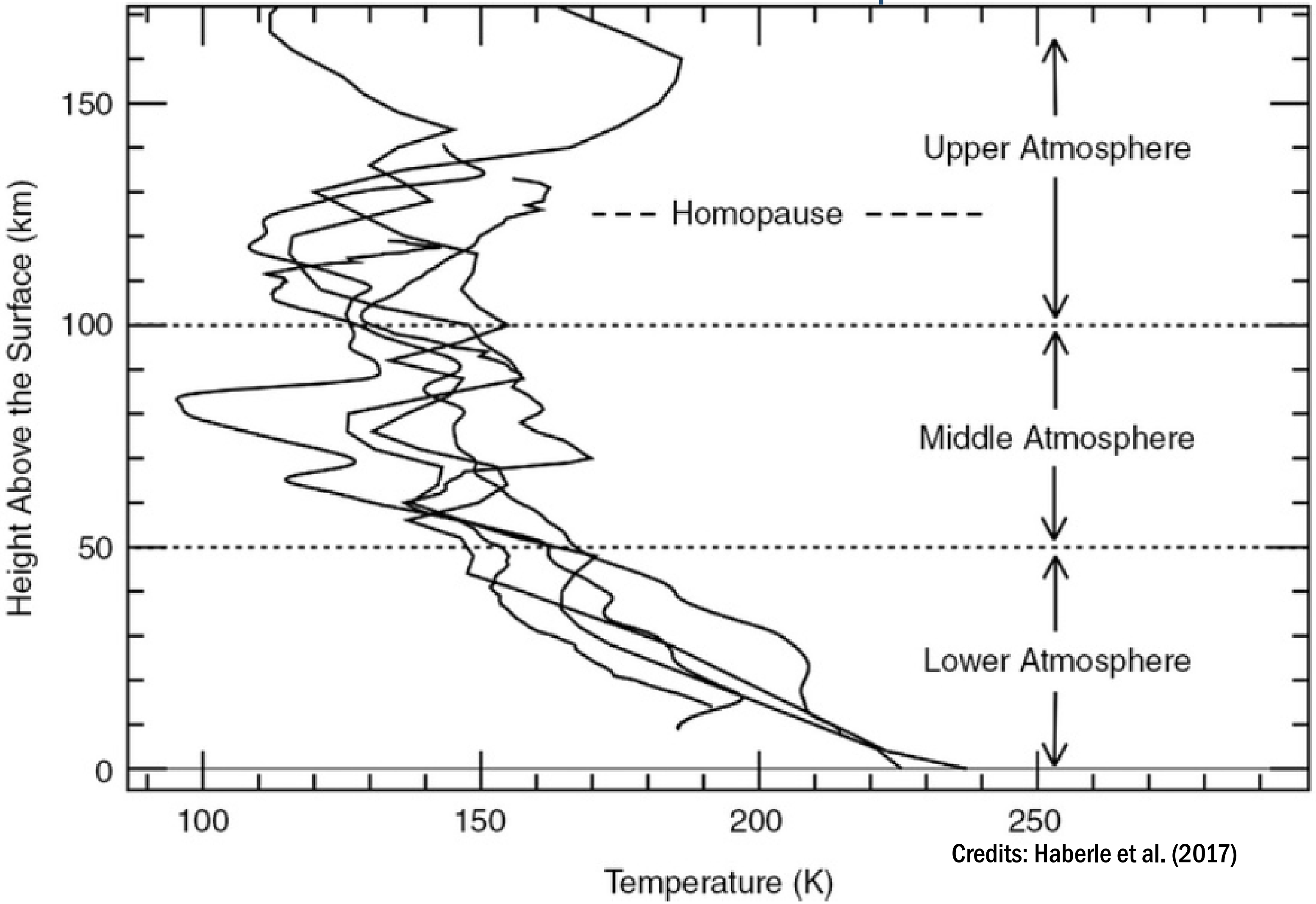


More than 25% of variability

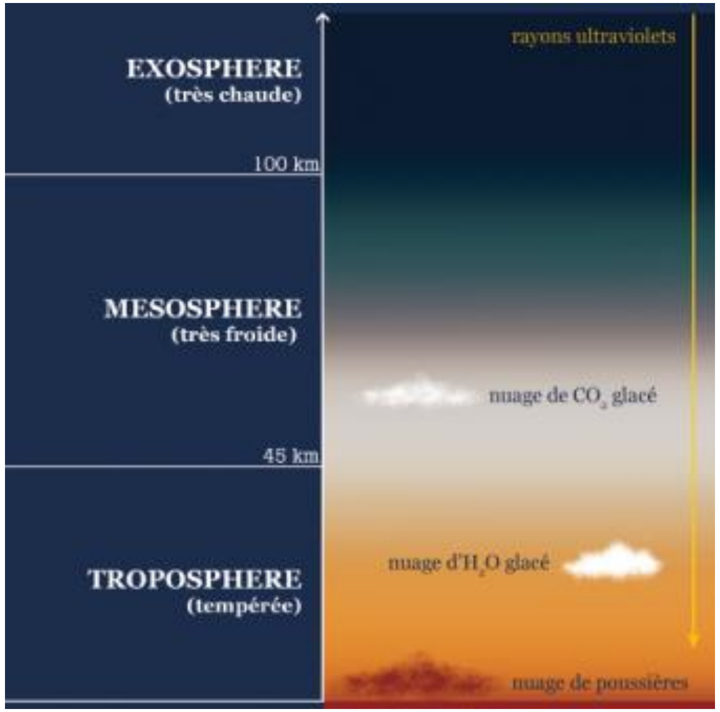
A. Piccialli et al., in prep

1. Why are we interested into atmospheric temperature ?

In situ measurements of temperature

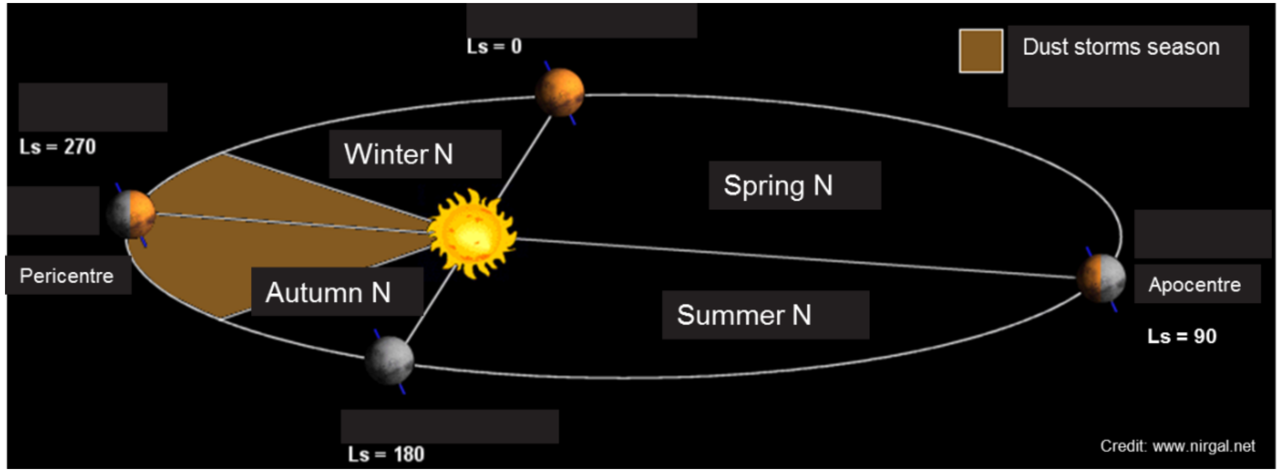


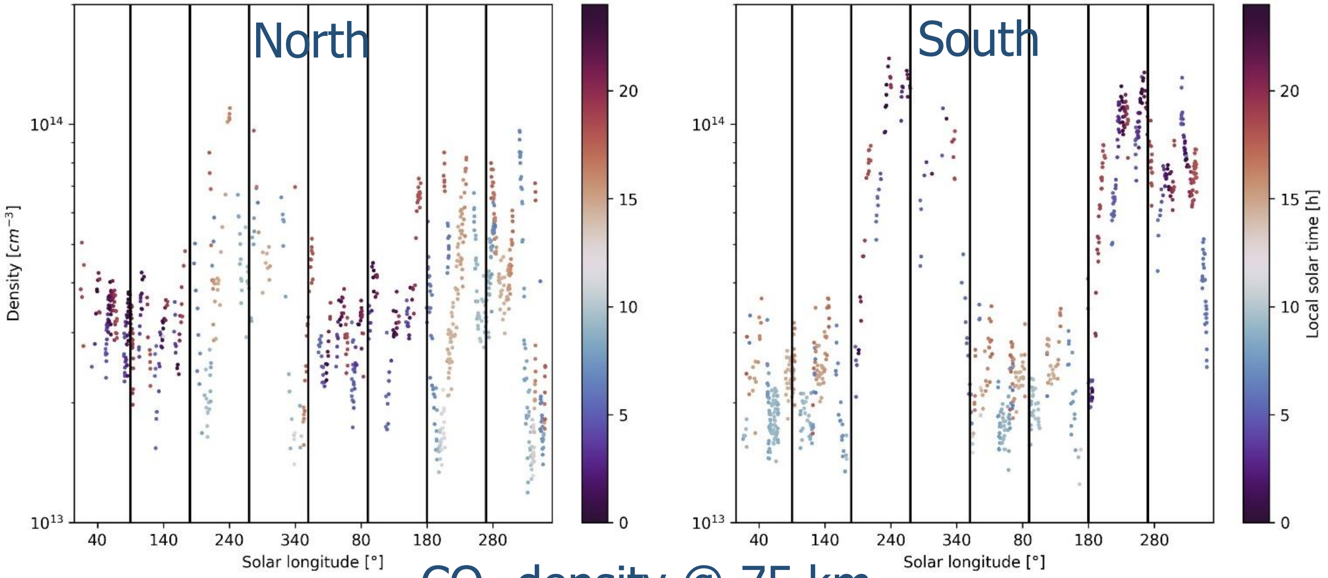
Credits: Haberle et al. (2017)



Credit: Laurine Moreau

1. Why are we interested into atmospheric temperature ?



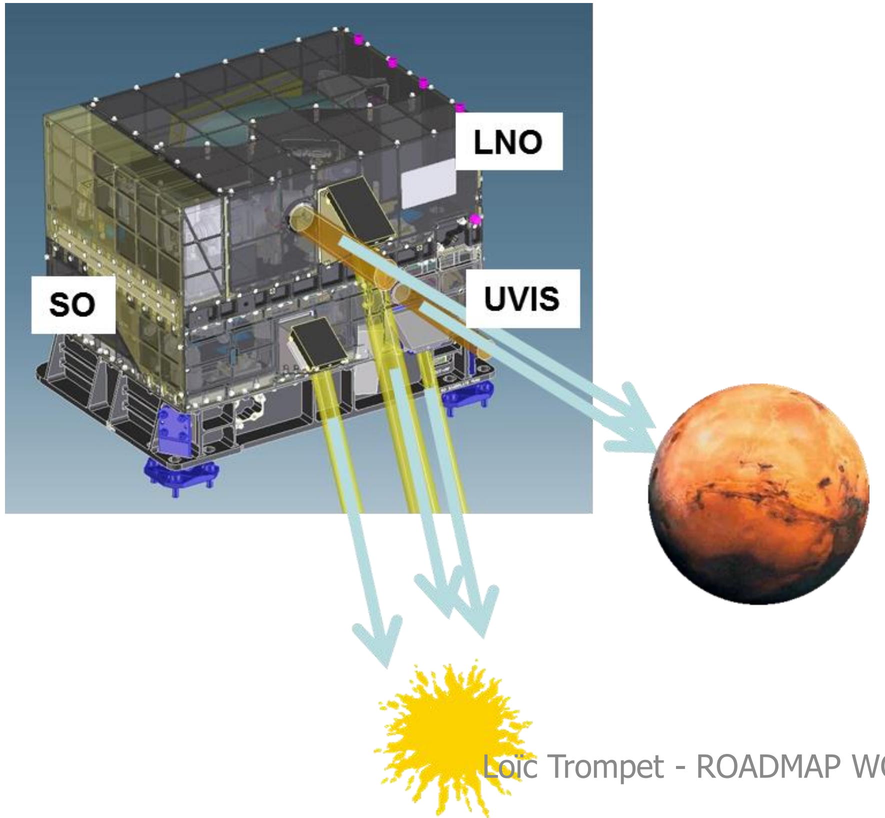


CO_2 density @ 75 km

2. How to retrieve atmospheric temperature ?

The NOMAD Instrument

On-board ESA's Trace Gas Orbiter
- Circular orbit @ 400 km altitude (2 h period)
- Science operations started 21/04/2018



PI: Ann Carine Vandaele (BIRA-IASB)

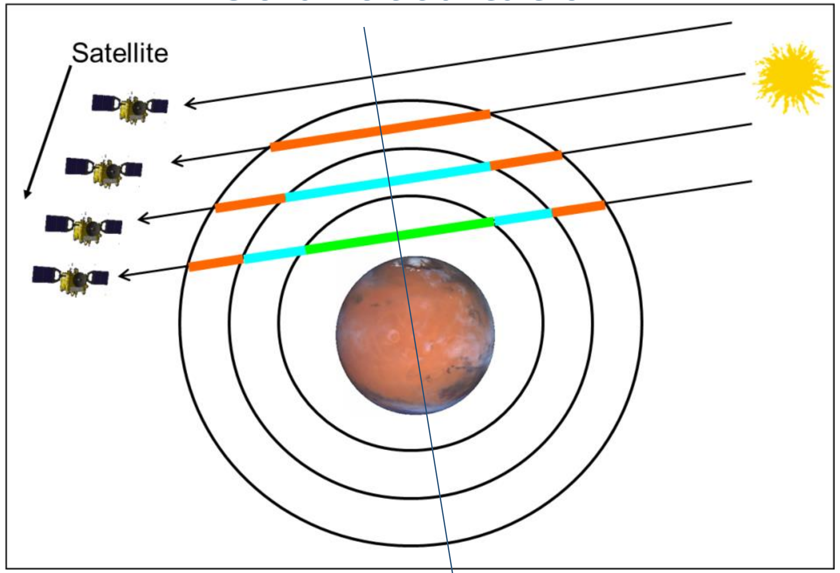
NOMAD

High resolution occultation and nadir spectrometers

Atmospheric composition (CH_4, O_3, trace species, isotopes) dust, clouds, P&T profiles

UVIS: (0.20 – 0.65 μm) λ/Δλ ~ 250	SO	Limb	Nadir
LNO: IR (2.3 – 3.8 μm) λ/Δλ ~ 11,000	SO	Limb	Nadir
SO: IR (2.3 – 4.3 μm) λ/Δλ ~ 22,000	SO		

Solar occultation



Terminator

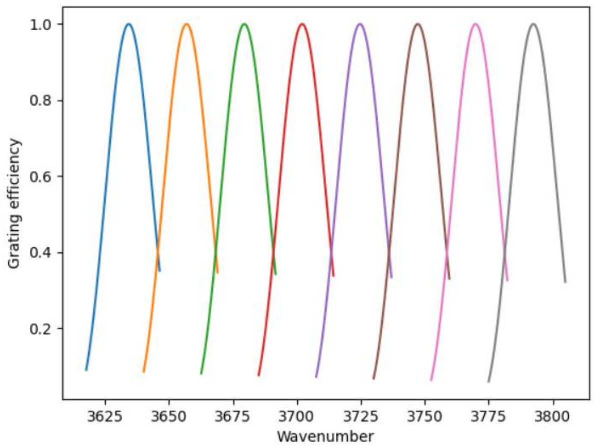
2. How to retrieve atmospheric temperature ?

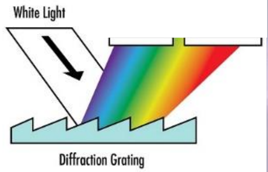
The NOMAD-SO channel

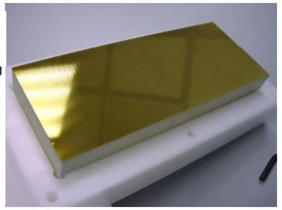
Main optical components:

- **Echelle grating:** diffraction orders 110 to 210: 2400 to 4800 cm^{-1} (4.2 to 2.1 µm)
  - 1 order = 20 to 35 cm^{-1}
- **Acousto-optic tunable filter** (AOTF)
- **Slit:** ~0.15 cm^{-1} spectral resolution

Blaze function for diffraction orders 161 to 168

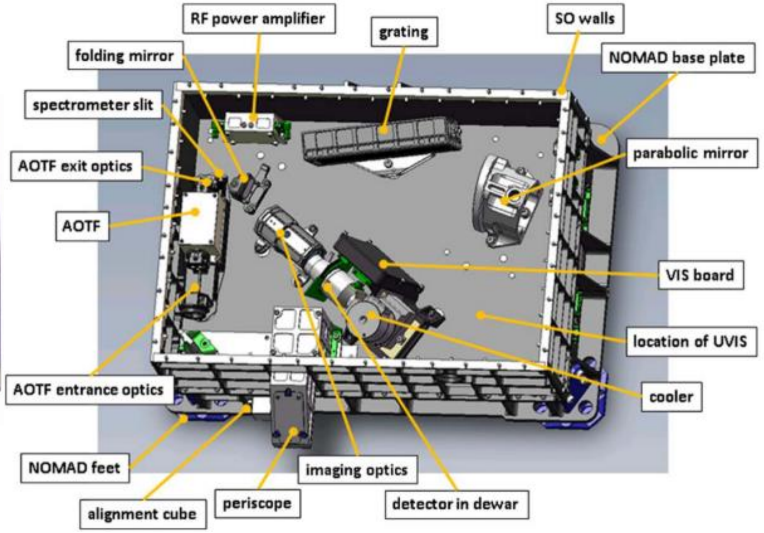




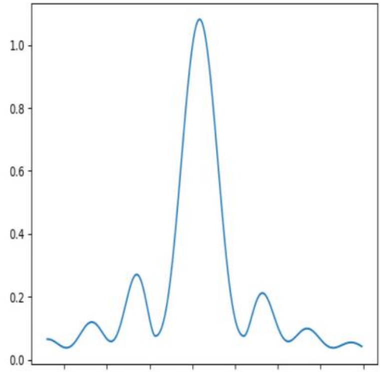


Echelle grating

AOTF



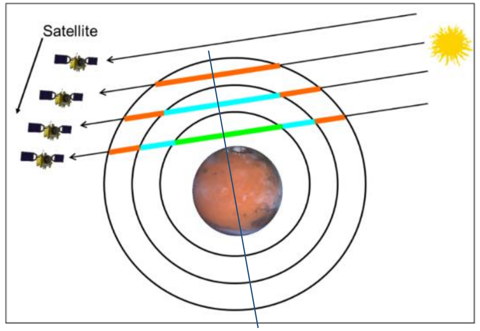
AOTF transfer function



Credits: Neefs et al. (2015)

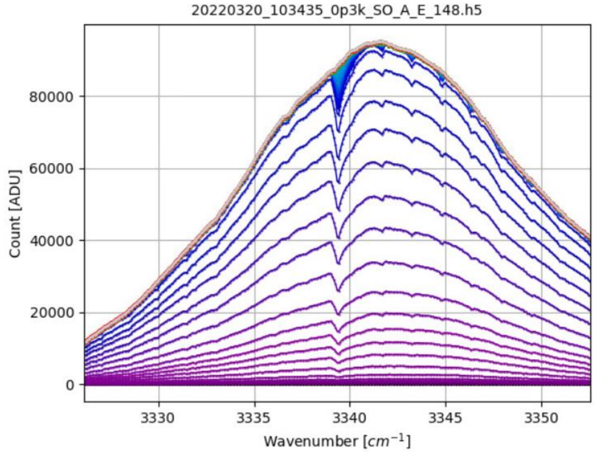
Transmittance calibration

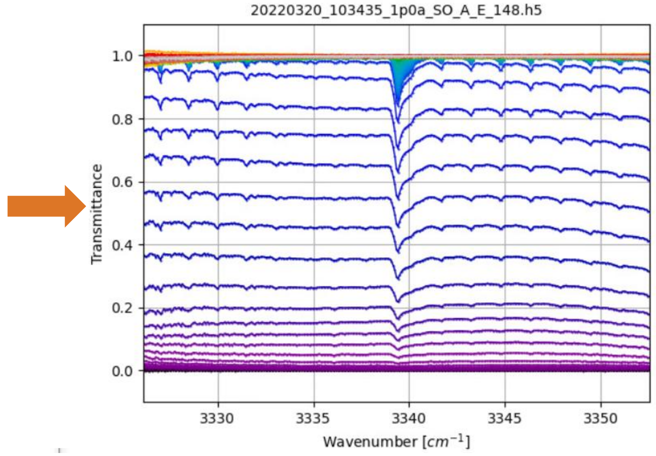
Solar occultation



Terminator

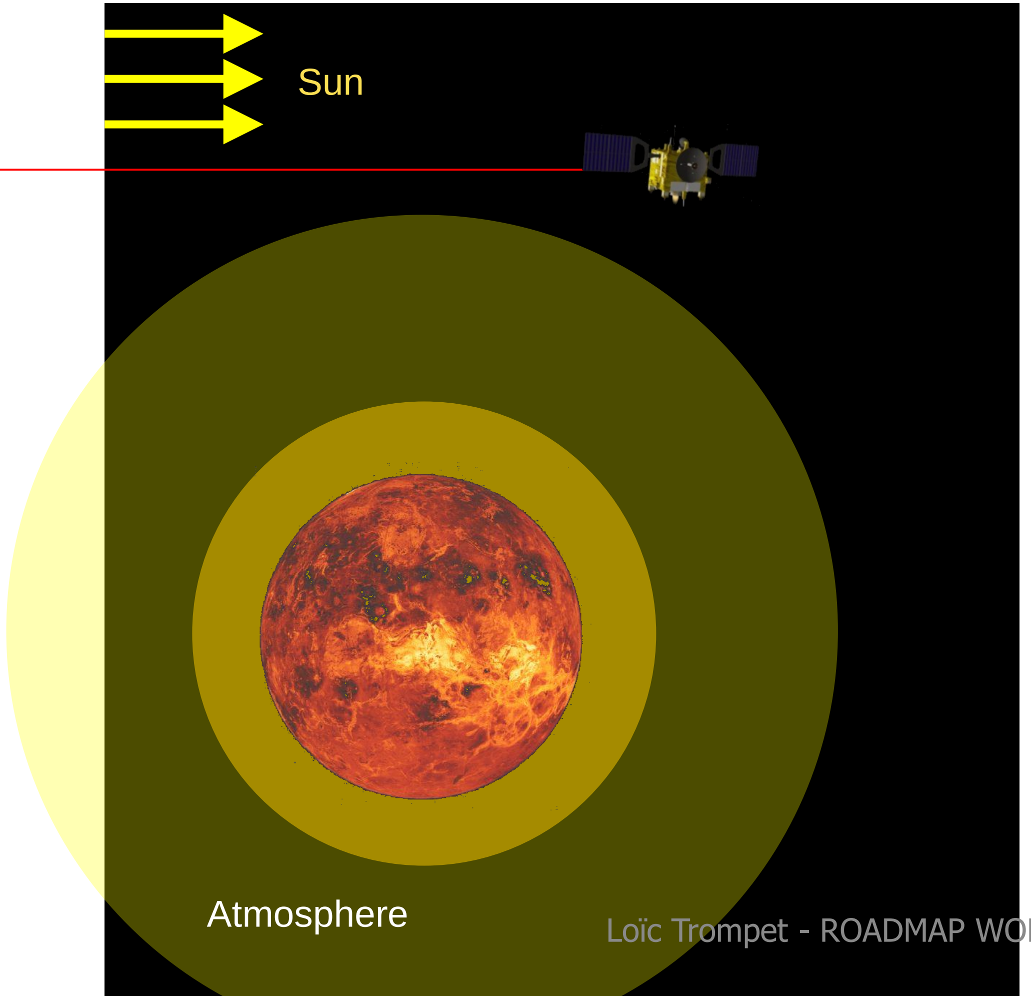
Diffraction order 148



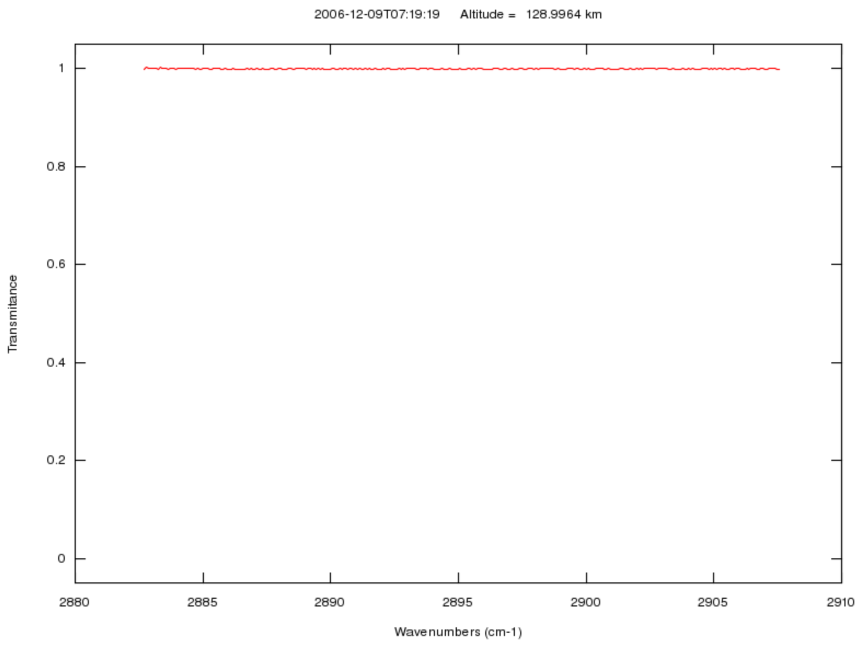


2. How to retrieve atmospheric temperature ?

Solar occultations (here SOIR/VEx)

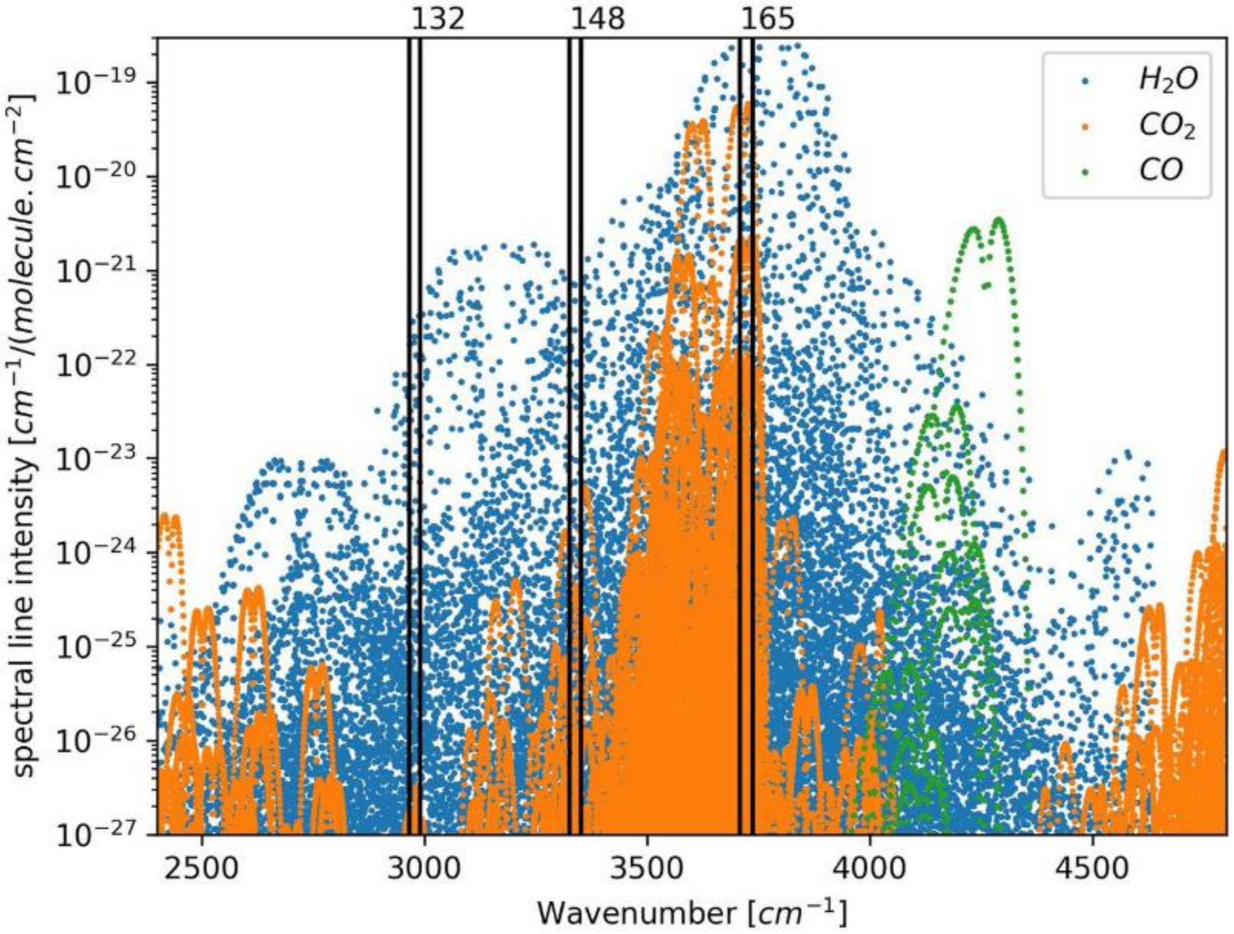


Orbit 232 – Order 129



2. How to retrieve atmospheric temperature ?

Main lines in NOMAD-SO spectral range

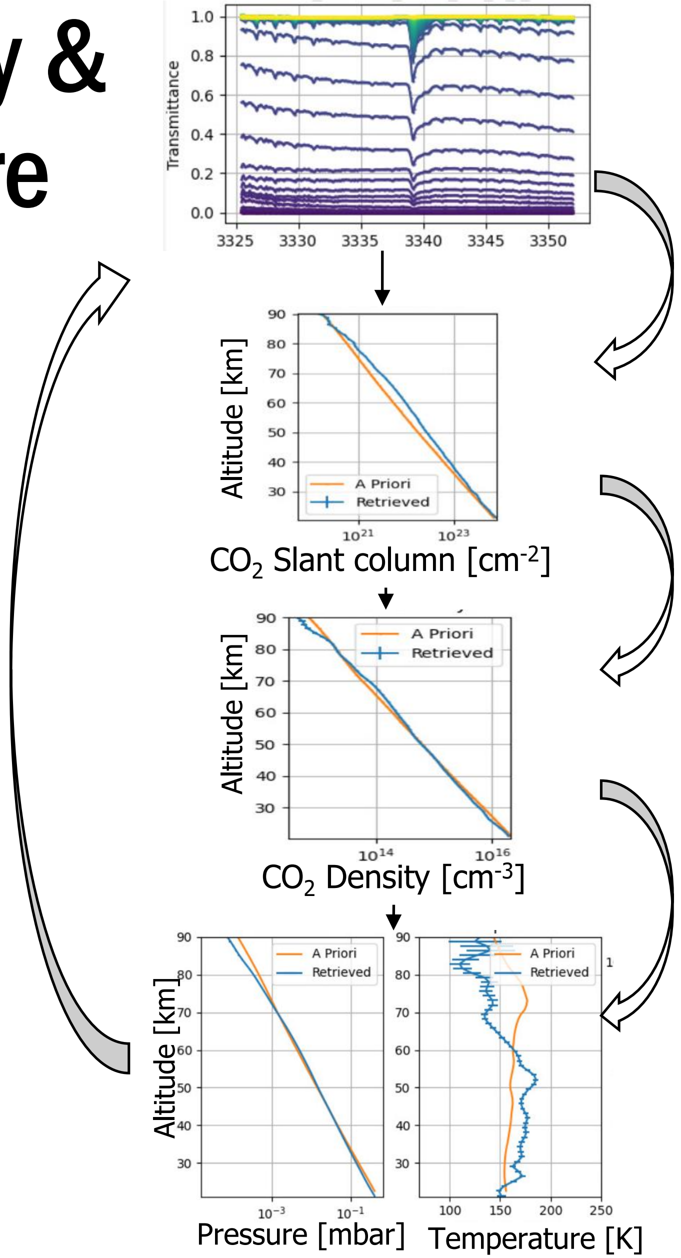


$\nu_2 + \nu_3$ $2\nu_1 + \nu_2$ $\nu_1 + \nu_3$

- SO scans 6 orders / occultation
- Main diffraction orders for CO_2 :
  - 132, 148, 155, and 165
- S/N: 2500
- FOV at terminator: 1.6 to 1.9 km

2. How to retrieve atmospheric temperature ?

CO_2 Density & Temperature Retrieval



Loop on T
Convergence
in 1 to 3 loops

Step 1: Spectral inversion

- Slant columns retrieved from spectra (independently)
- Radiative transfer code: ASIMUT (Vandaele et al. 2006)
- Initial temperature, pressure from GEM-Mars (Daerden et al., 2019, Neary and Daerden, 2018)
- Instrument model (Villanueva et al., 2022)

Step 2: Vertical inversion

- Regularization with iterated Tikhonov method (Quémerais et al., 2006)
- No a priori
- Regularization fine-tuned with the Expected Error Estimation (Steck 2002, Xu et al., 2016)

Step 3: Integration

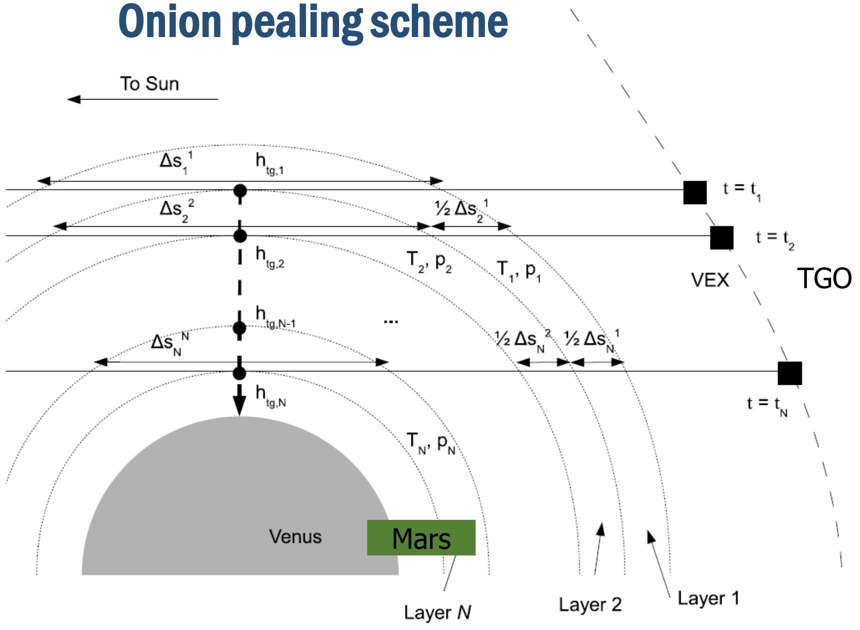
Hydrostatic equilibrium equation $\delta p = \rho \; g \; \delta z$

Vertical resolution: ~1.6 - 3 km
Uncertainties: ~2.5% (5% at top, 2% at bottom)

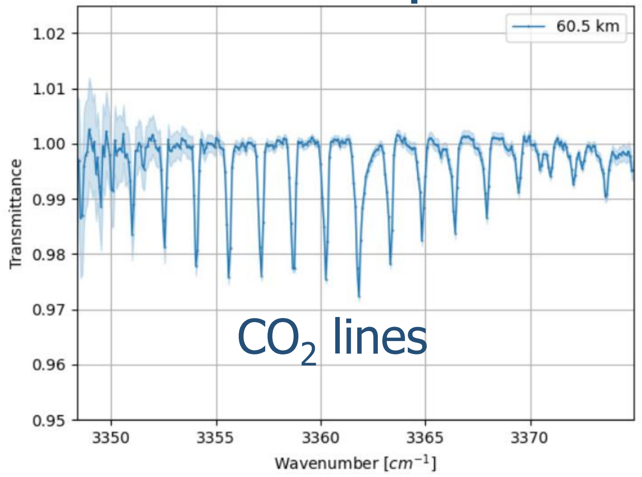
2. How to retrieve atmospheric temperature ?

Step 1: Spectral inversion

Onion pealing scheme



Transmittance spectrum



$c(h)$ is fitted with the ASIMUT radiative transfer code

Beer-Lamber law:

$$Tr(h,\nu) = IF * e^{-\int \sigma(\nu, p(s),\ t(s))\, n(s)\, ds}$$

$$c(h) = \int n(s)\, ds$$

$$c = Kn$$

$$K_{ij} = 2\int_{h_j}^{h_{j-1}} f(s)\frac{s}{\sqrt{s^2 - h_i^2}}ds$$

Tr: Transmittance
IF: Instrument function
ν: wavenumber
h: height above surface
n: number density

c: slant column
s: slant path
p: pressure
t: temperature

2. How to retrieve atmospheric temperature ?

Step2: Vertical inversion - Regularization

$c = Kn$

where K is the Abel transform,

c is the slant column density and n is the unknown density,

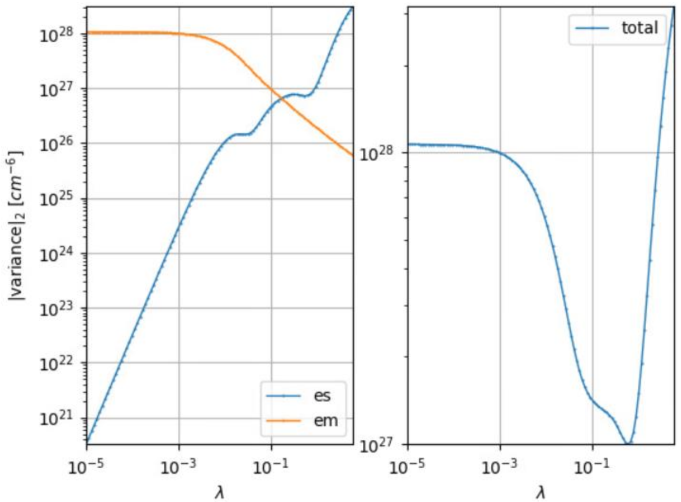
$n = Gc$

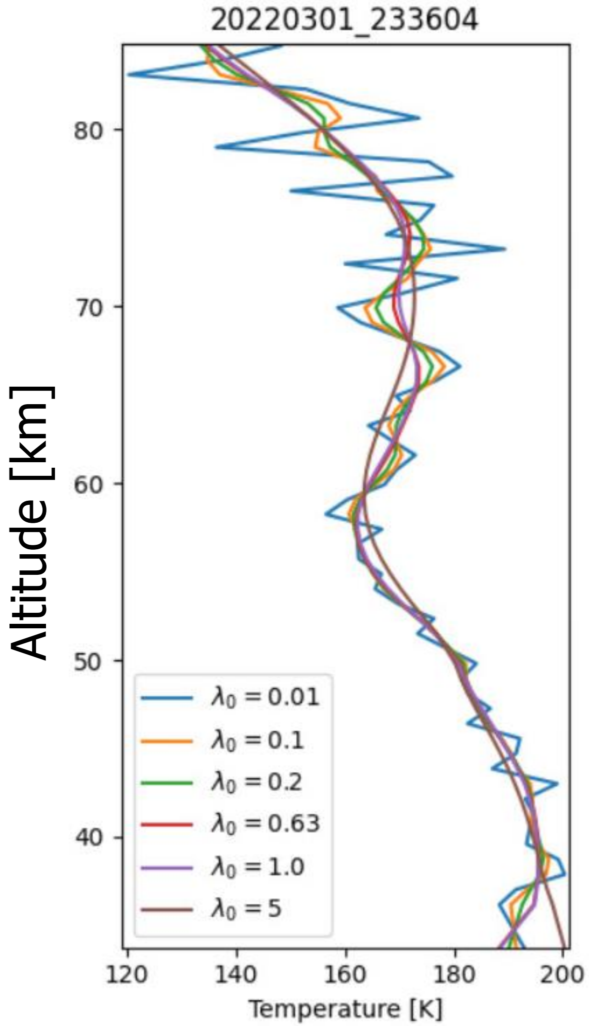
where $G = (K^T S_c^{-1} K + \lambda L^T S_n^{-1} L)^{-1} K^T S_c^{-1}$

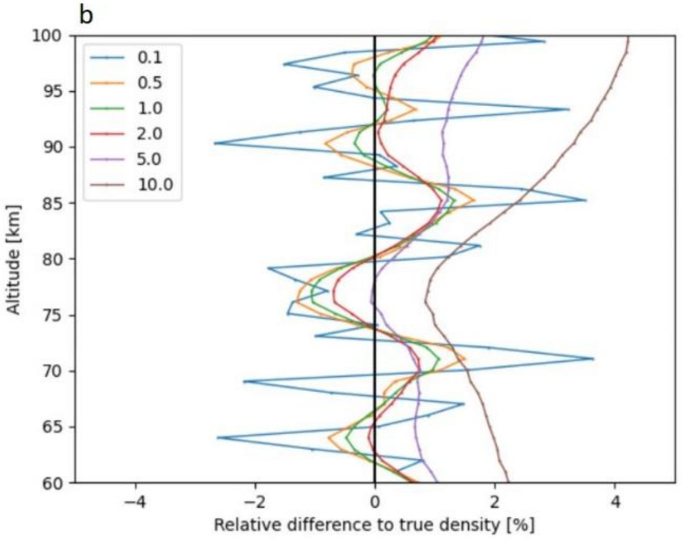
where S_c and S_n are the covariance matrices over c and n, and L is the second derivative operator

$A = GK$

Find $\min_{\lambda} [\|(A - I)n\|^2 + \|S_c\|^2 tr(GG^T)]$

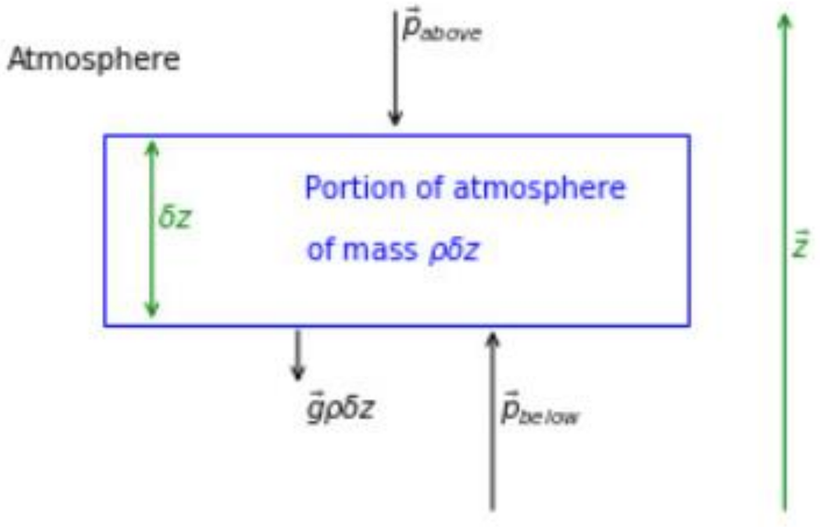






Step 3: Hydrostatic equilibrium

First find the pressure:



$$\delta p = m\ g\ n\ \delta z$$

$$\Delta p_i = \frac{m\, g_0\, r_M^2\, n_i}{h_i} \exp(a_i) \left[\frac{E_2(a_i)}{a_i} - \frac{E_2(b_i)}{b_i} \right]$$

where $E_n(x) = x^{n-1} \int_x^\infty \frac{\exp(-z)}{z^n} dz$

$$a_i = \frac{r_M + z_i}{h_i}$$

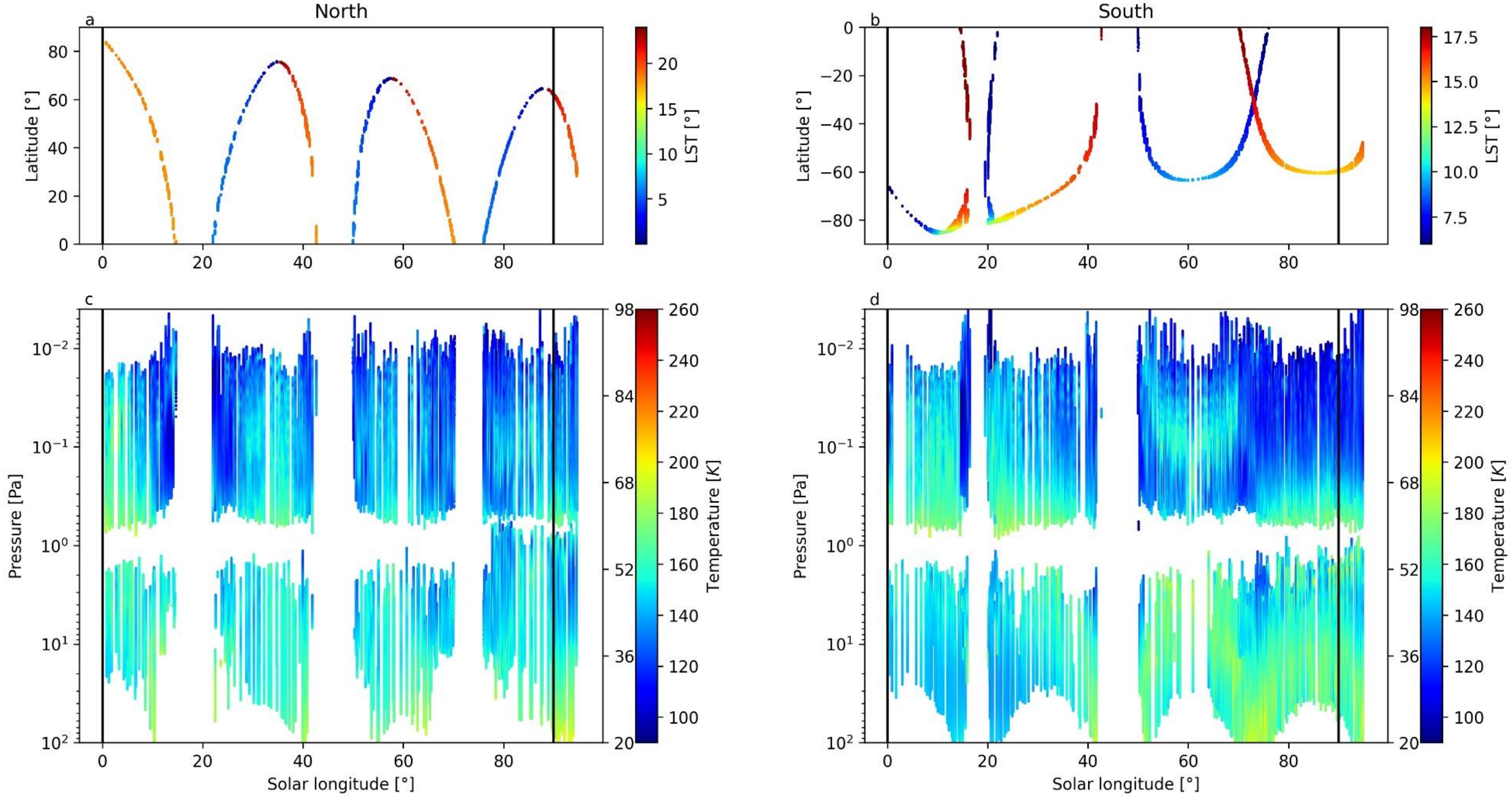
$$b_i = \frac{r_M + z_{i+1}}{h_i}$$

m: atomic mass
g: gravity
n: number density
r_M: Mars radius
h: scale height
k_B: Boltzmann constant

Then find the temperature with the ideal gas law $\Delta t_i = \frac{\Delta p_i}{k_B n_i}$

2. How to retrieve atmospheric temperature ?

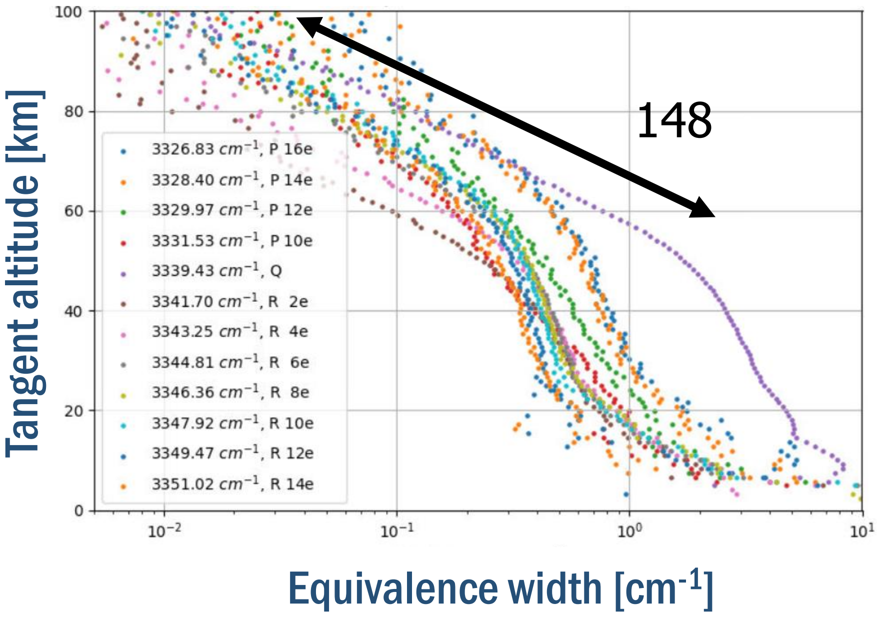
Some examples of NOMAD-SO temperature profiles in MY 37



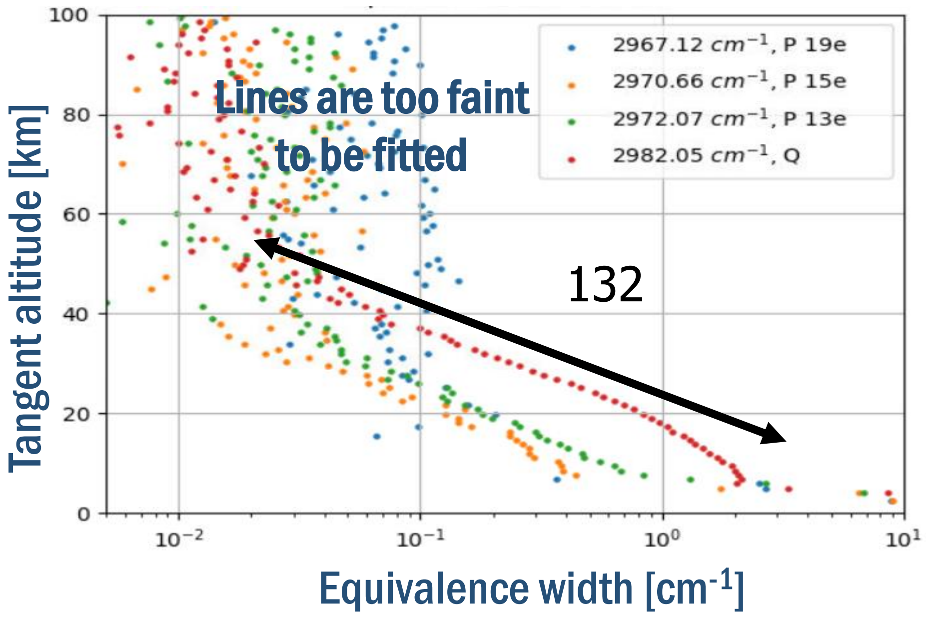
Combination of diffraction order 148 and 132

Only the linear part of the curve of growth of the equivalence width of the molecular lines are used for the retrieval.

Diffraction order 148



Diffraction order 132



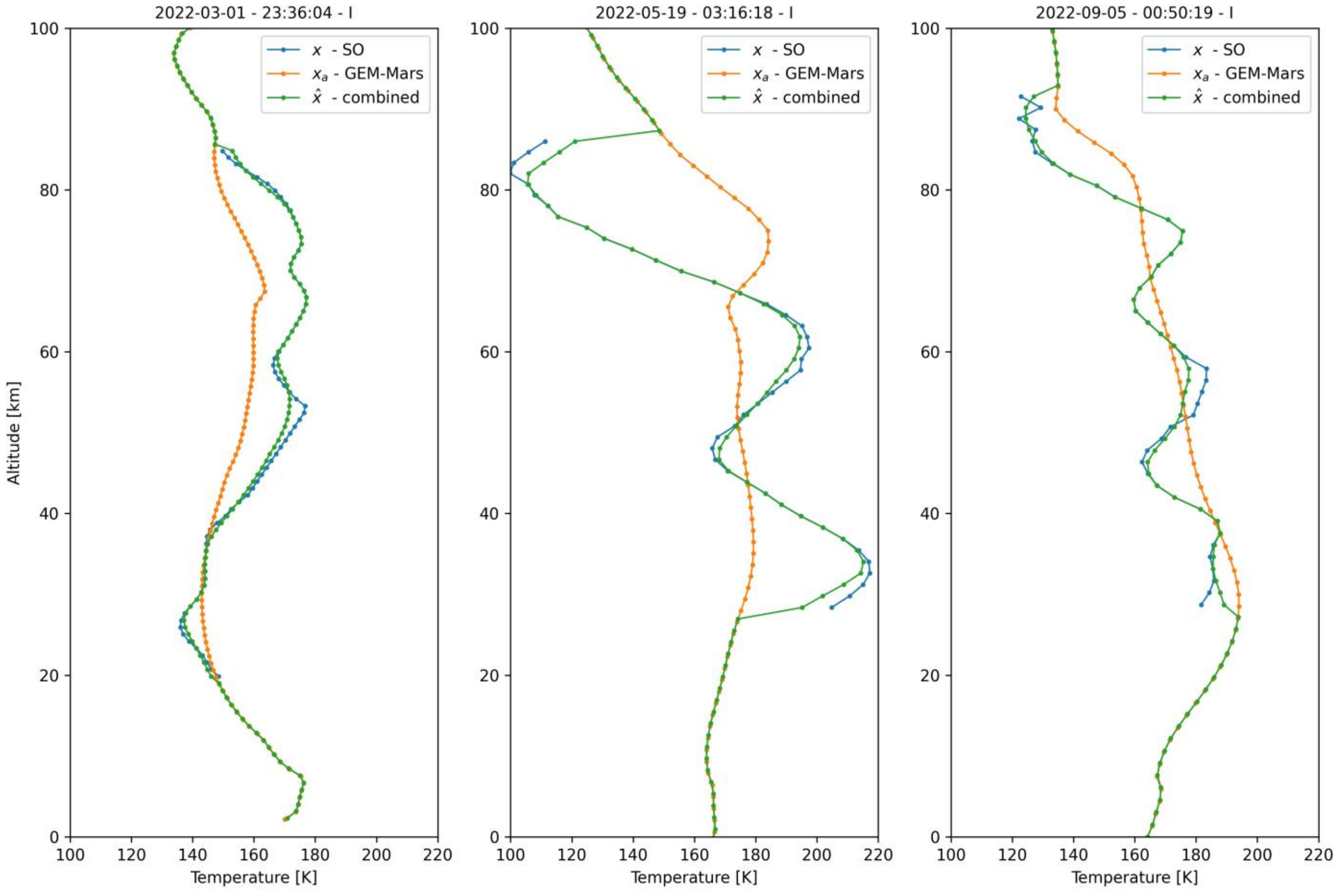
↔ : Linear part of the curve of growth

Combination of diffraction order 148 and 132

Convolution with triangular functions at bounds of profiles:

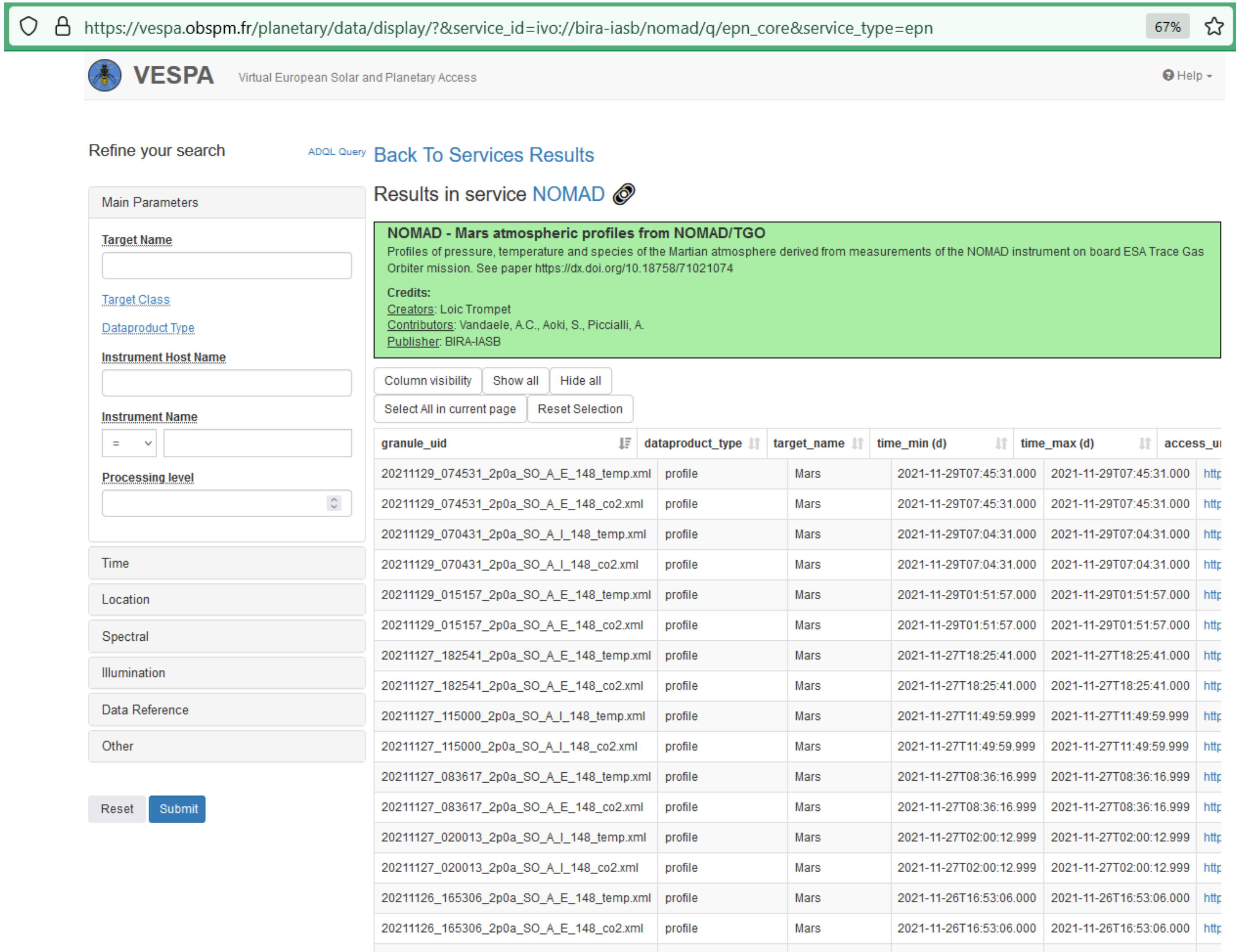
$$A_{ij} = \begin{cases} 0_{ij} & \text{if } z_i > z_{top} \text{ or } z_i < z_{bot} \\ \delta_{ij} & \text{if } z_{bot} + h < z_i < z_{top} - h \\ max\left(0, \frac{1}{a_i}\left(1 - \left|\frac{z_j - z_i}{a_i}\right|\right)\right) & \text{if } z_{bot} < z_i < z_{bot} + h \\ max\left(0, \frac{1}{b_i}\left(1 - \left|\frac{z_j - z_i}{b_i}\right|\right)\right) & \text{if } z_{top} - h < z_i < z_{top} \end{cases}$$

Spectra for 148 and 132 are automatically retrieved the same day than when we receive them.



Available data

- repository.aeronomie.be
- vespa.obspm.fr
  - H_2O: Aoki et al. 2022
  - O_3: Piccialli et al. 2023
  - CO_2 + T (148): Trompet et al. 2023 a,b
  - CO (soon): Yoshida et al., in rev.
  - Aerosols (soon): Flimon et al., in prep.
  - …
- loic.trompet@aeronomie.be



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20211129_074531_2p0a_SO_A_E_148_co2.xml	profile	Mars	2021-11-29T07:45:31.000	2021-11-29T07:45:31.000	http
20211129_070431_2p0a_SO_A_I_148_temp.xml	profile	Mars	2021-11-29T07:04:31.000	2021-11-29T07:04:31.000	http
20211129_070431_2p0a_SO_A_I_148_co2.xml	profile	Mars	2021-11-29T07:04:31.000	2021-11-29T07:04:31.000	http
20211129_015157_2p0a_SO_A_E_148_temp.xml	profile	Mars	2021-11-29T01:51:57.000	2021-11-29T01:51:57.000	http
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20211127_182541_2p0a_SO_A_E_148_temp.xml	profile	Mars	2021-11-27T18:25:41.000	2021-11-27T18:25:41.000	http
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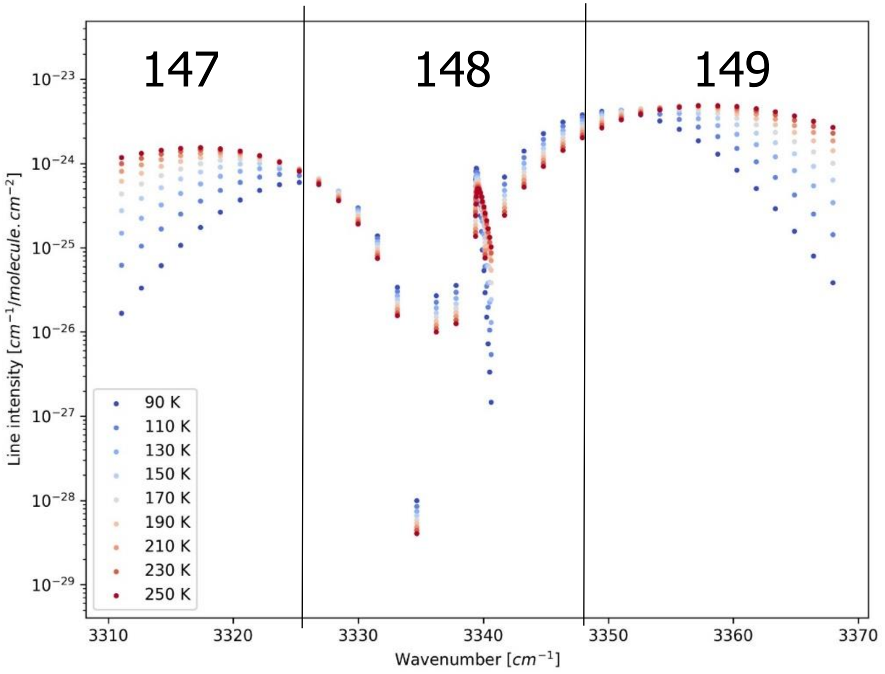
20211126_165306_2p0a_SO_A_E_148_co2.xml	profile	Mars	2021-11-26T16:53:06.000	2021-11-26T16:53:06.000	http

2.2 Comparison of two ways to retrieve the temperature

2.2 Comparison of retrieved temperature

- Implementation and tests on fit of temperature into ASIMUT by **Bastien Vispoel (UNamur)** in the framework of the ROADMAP project
- Now comparisons with temperature profiles retrieved from CO_2 fitted alone and temperature derived with the hydrostatic equilibrium equation
- Fit each spectrum individually



Tests for orders 148, 149, 132:

MY 36 L_S: 290°-300°

Only bin 2

No regularization

36 occ. order 148

10 occ. order 149

32 occ. order 132

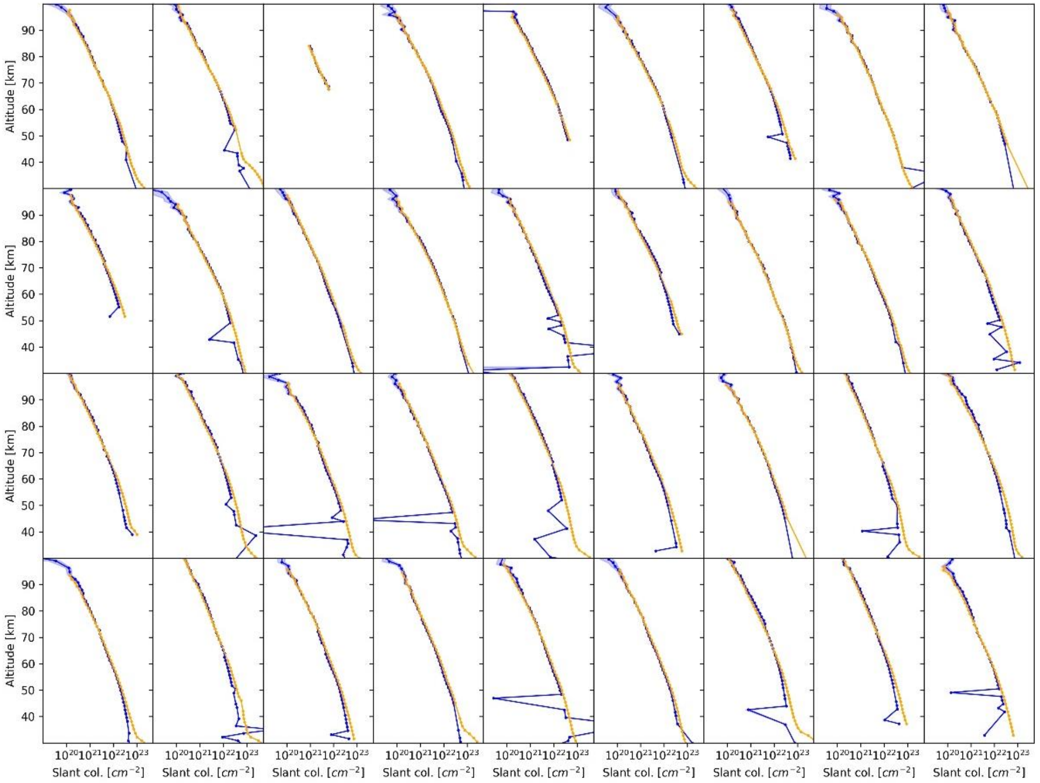
Fit c_{CO2} and T (and c_{H2O} below 60 km)

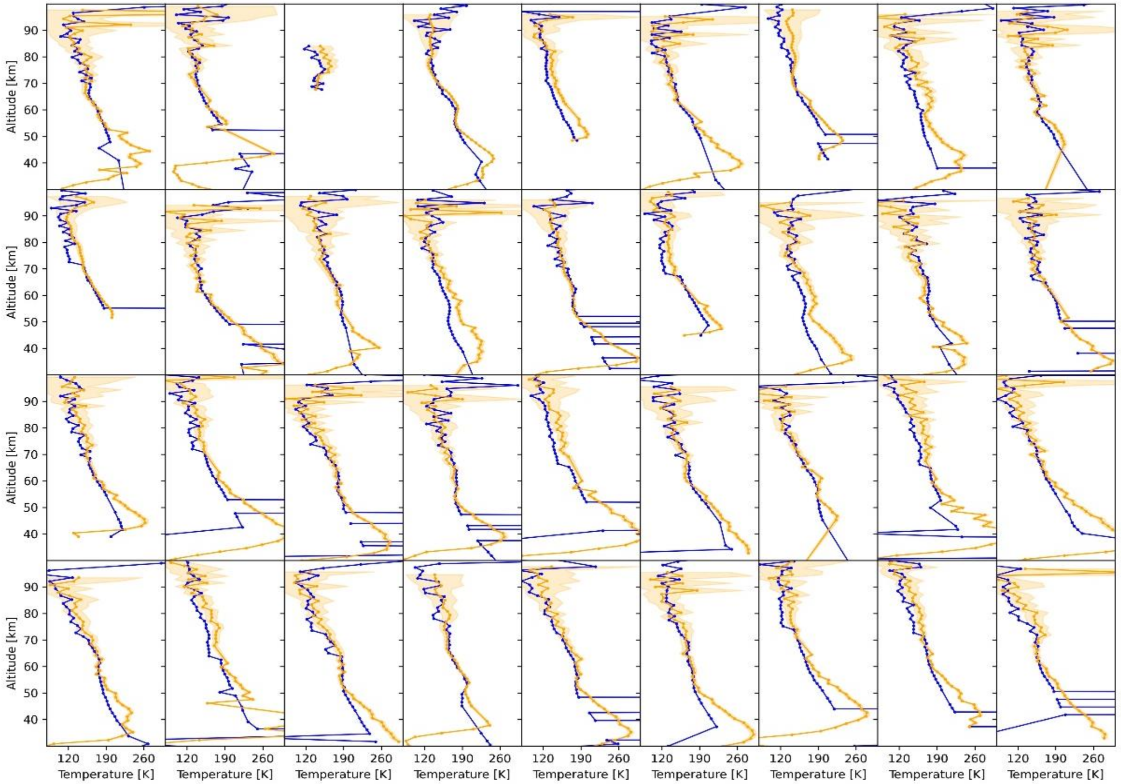
2.2 Comparison for diffraction order 148

36 profiles

Fit c and T

Fit c (T from hydro. eq.)





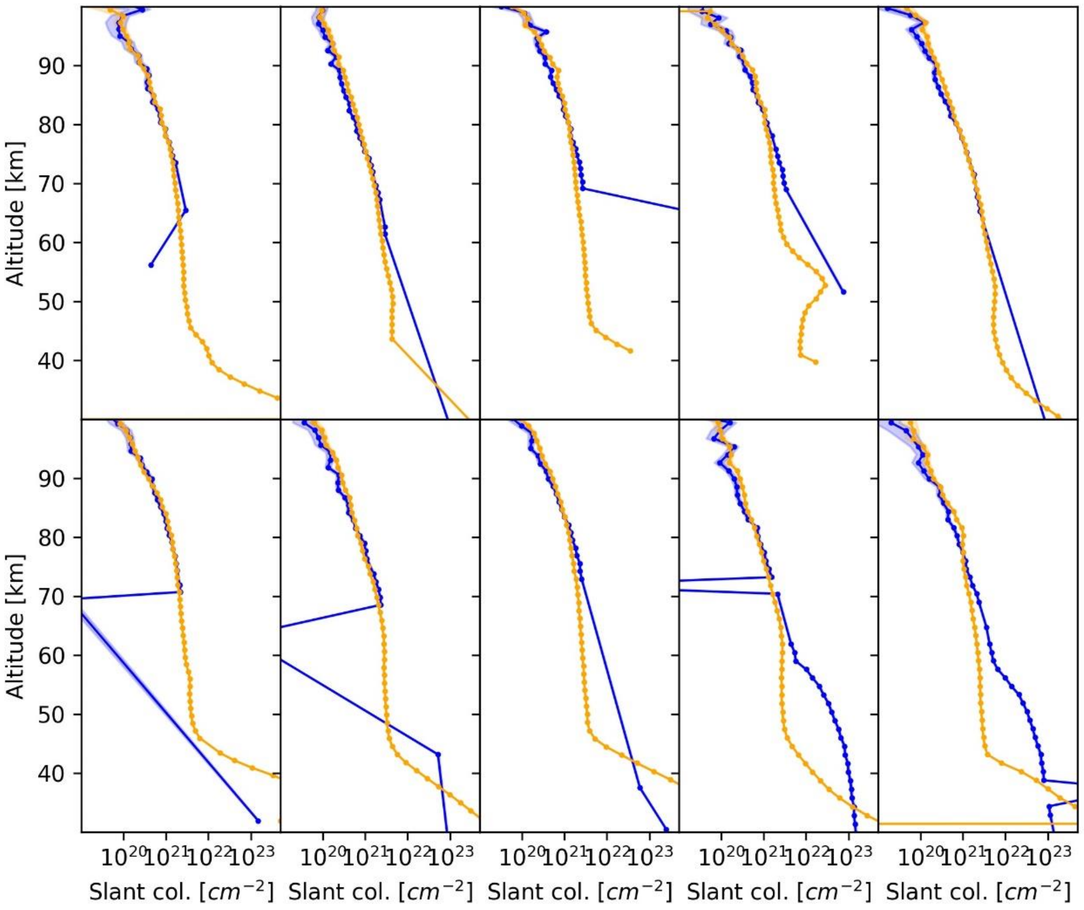
Reminder: saturation at ~50 km

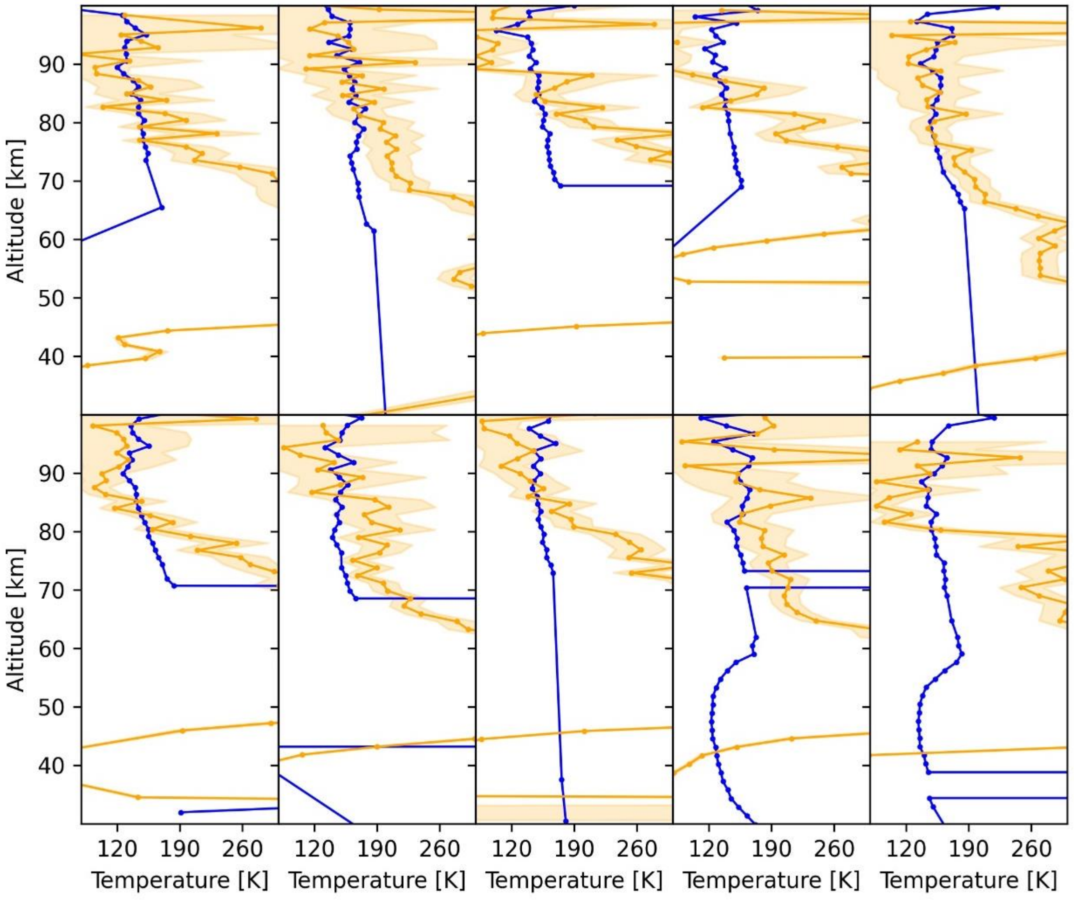
2.2 Comparison for diffraction order 149

10 profiles

Fit c and T

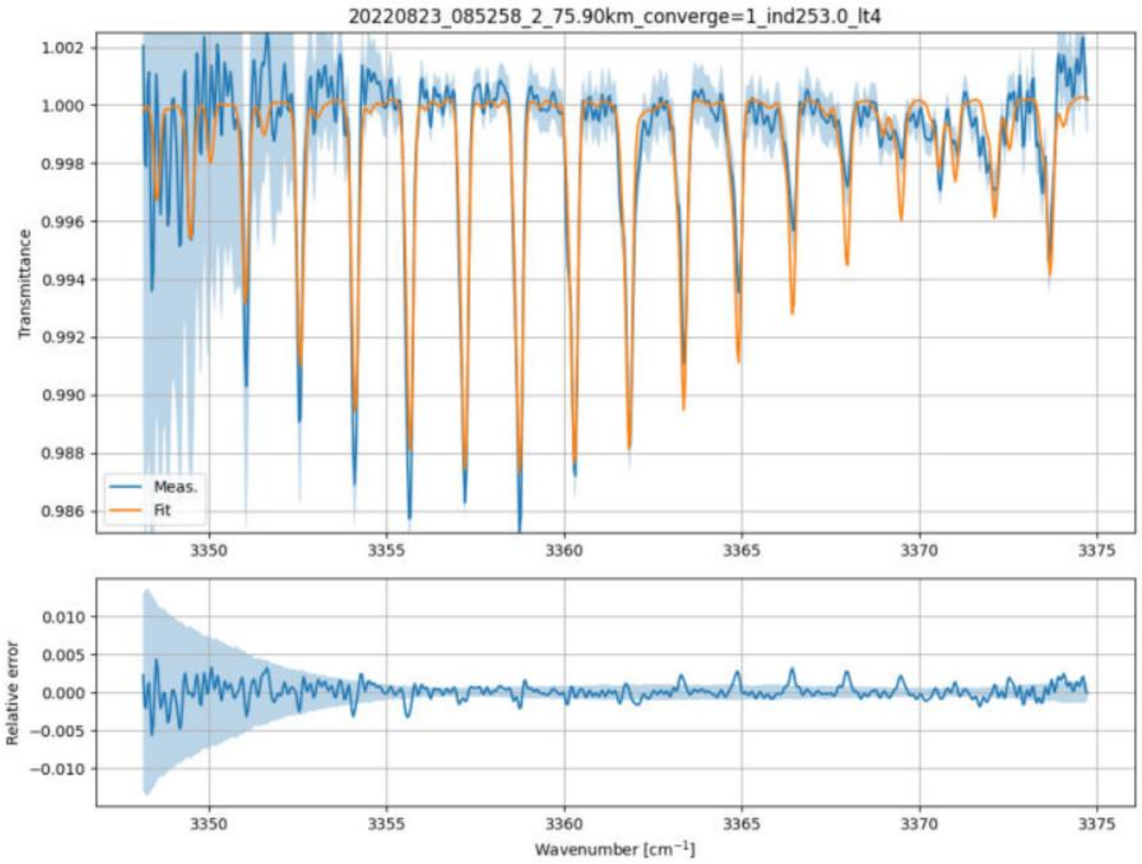
Fit c and T from hydro. eq.



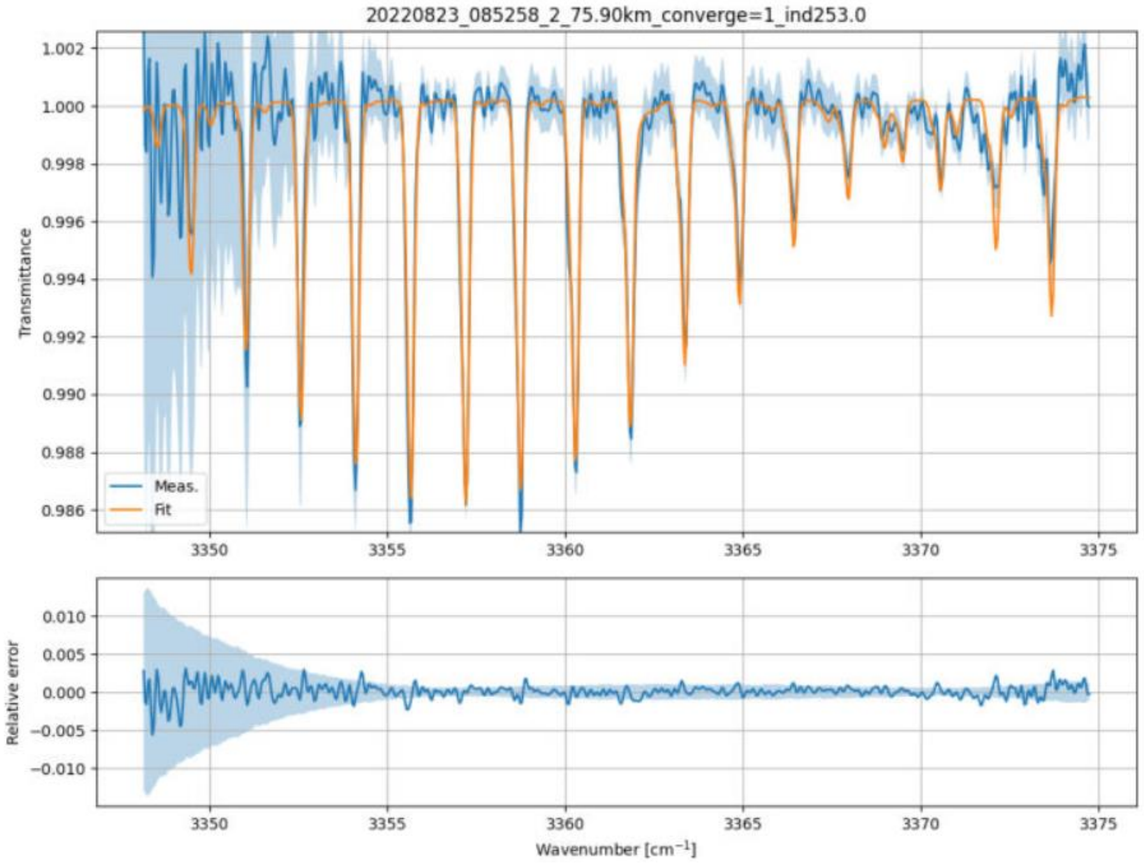


2.2 Comparison of fitted spectra - 149

Fit only c

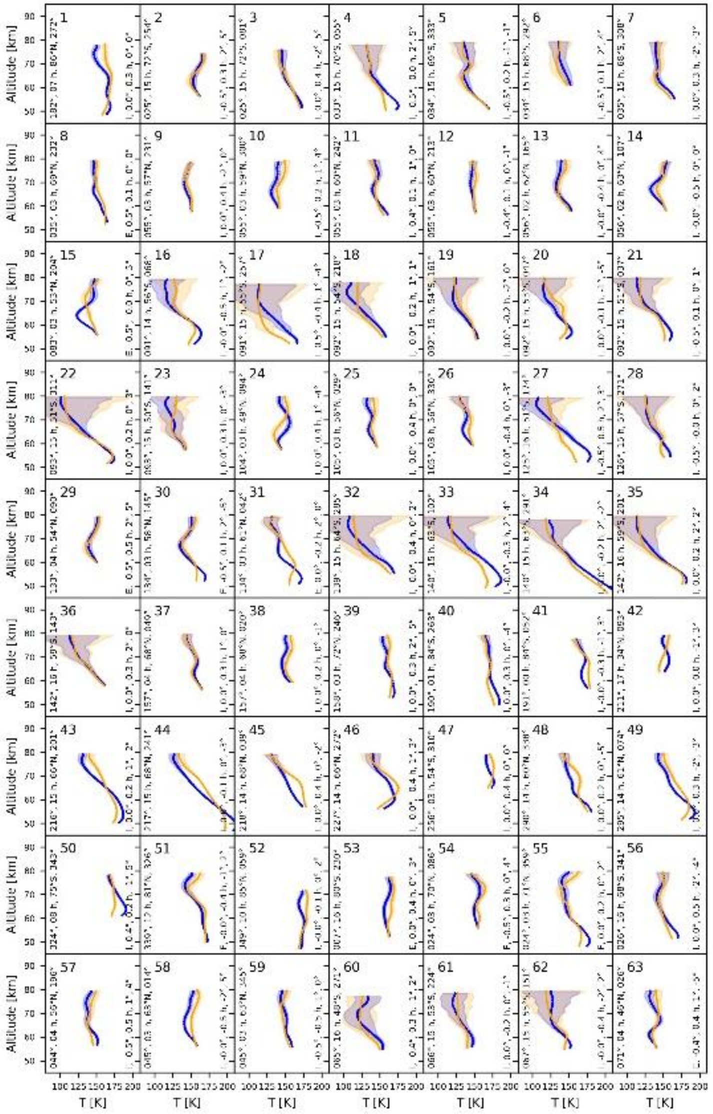


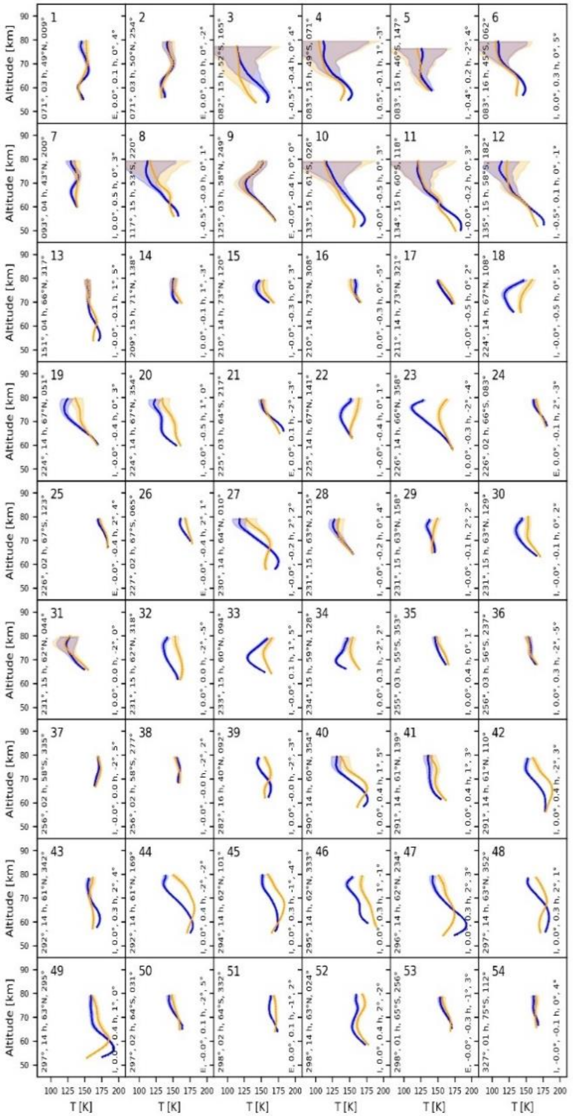
Fit c and T



3. How does it compares to other datasets ?

3. Comparison to MCS/MRO – order 148





SO
MCS

50-100 km altitude

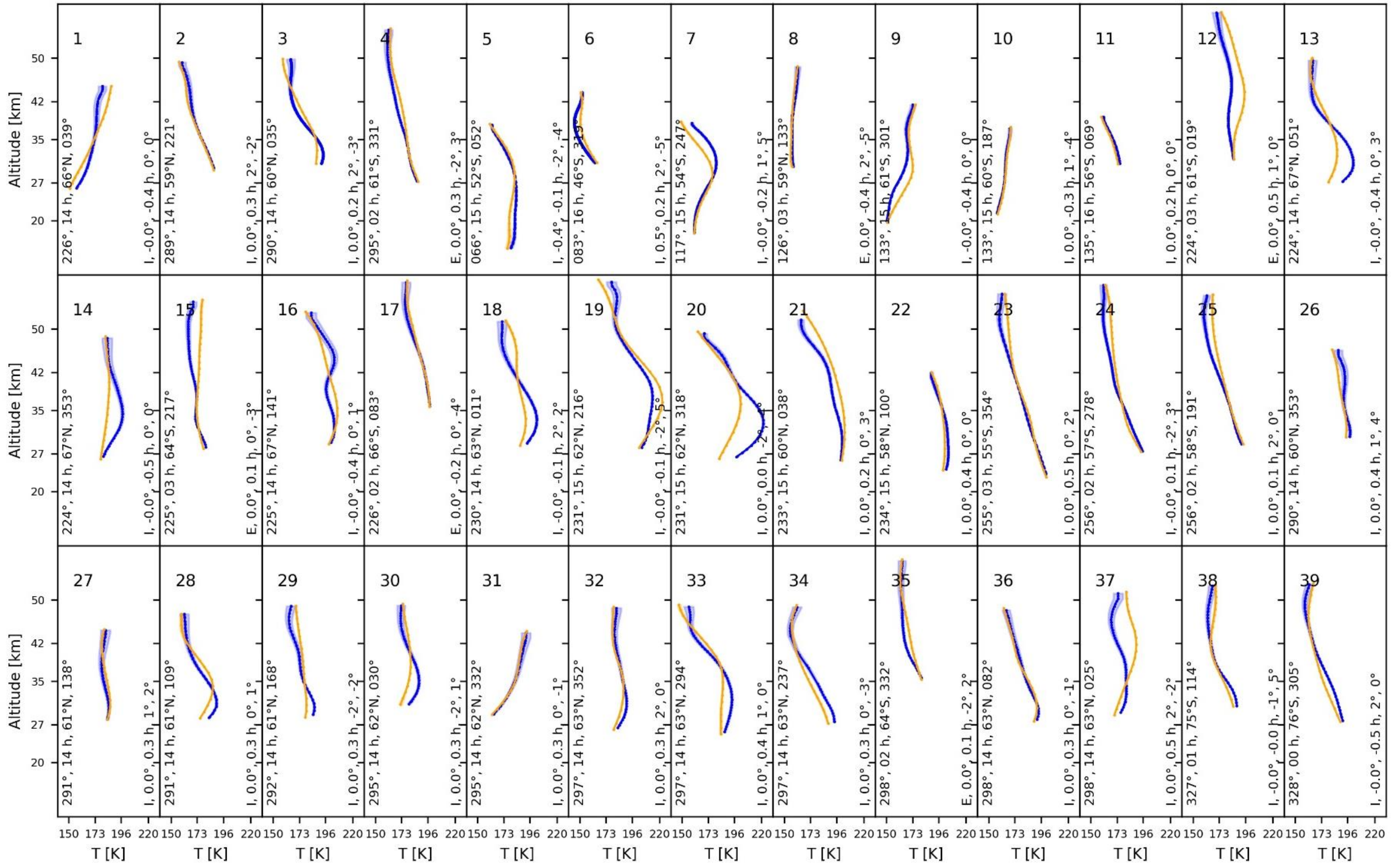
Co-location criteria: L_S 0.5°, LST 0.5 h, Lat. 3°, Lon. 6°

SO profiles are smoothed to 5 km vertical resolution

117 profiles (up to 10/2022)

Average difference: 0.1 K
Average absolute difference: 8.5 K

3. Comparison to MCS/MRO – order 132



SO
MCS

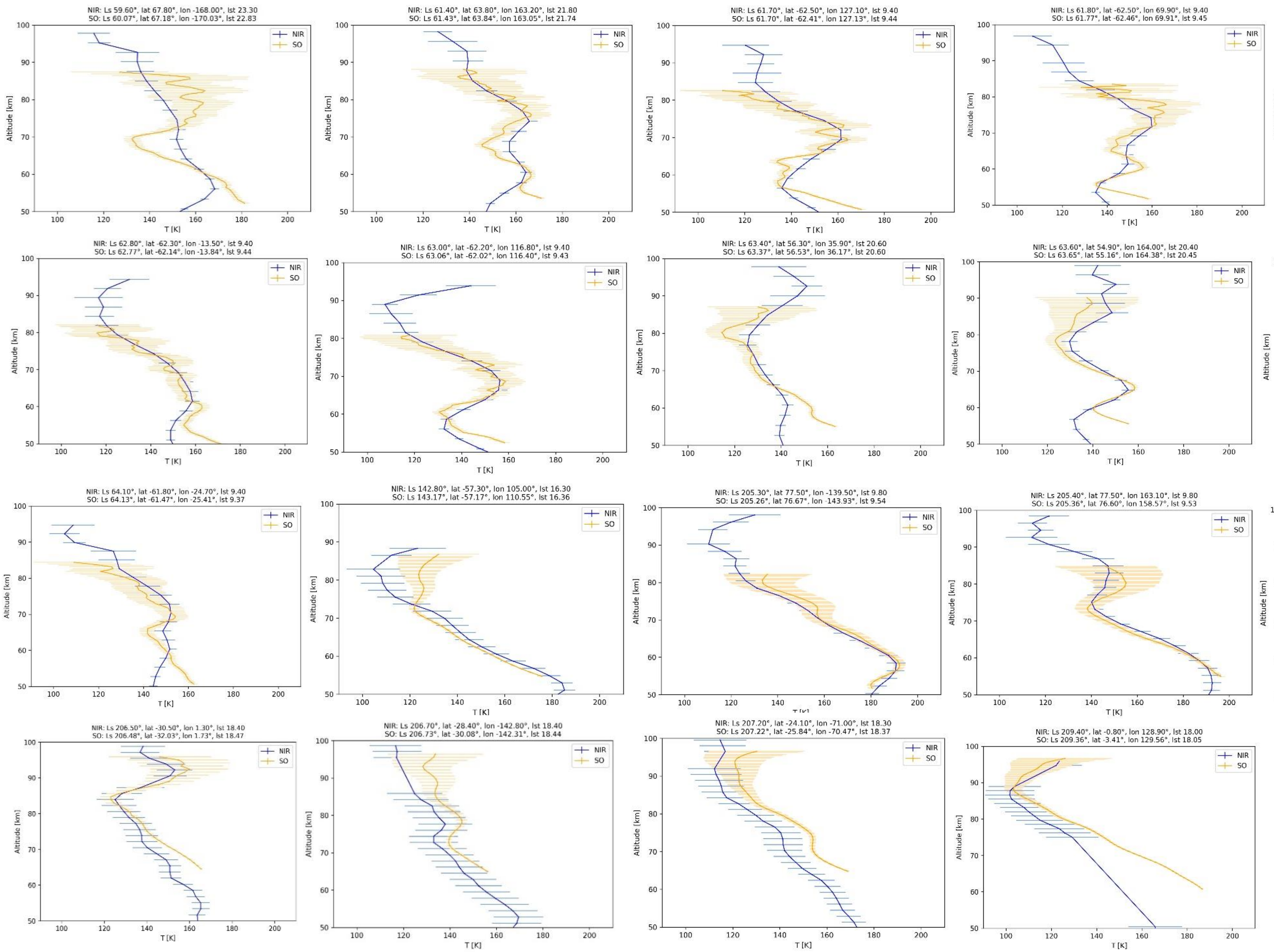
10-60 km altitude

39 profiles (up to 10/2022)

Average difference MCS-SO: -0.5 K
Average absolute difference: 4.4 K

3. Comparison with ACS-NIR/TGO (Fedorova et al., 2022)

NIR SO



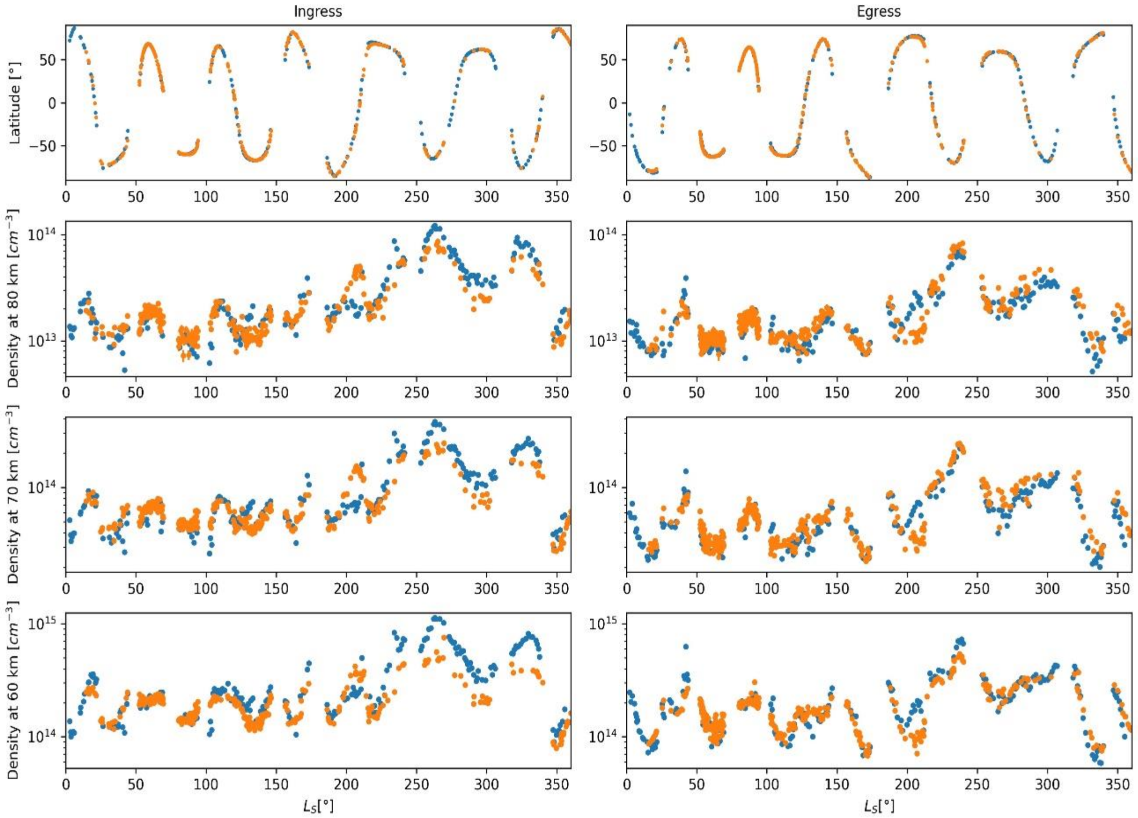
In MY 35, up to L_S 210°: 64 profiles
Simultaneous measurements
Average difference NIR-SO: -4.7 K
Average absolute difference: 6.7 K
(132: 9 profiles)

3. Comparison with ACS-MIR/TGO (Alday et al. 2021)

Not simultaneous measurements, difficult to quantify …

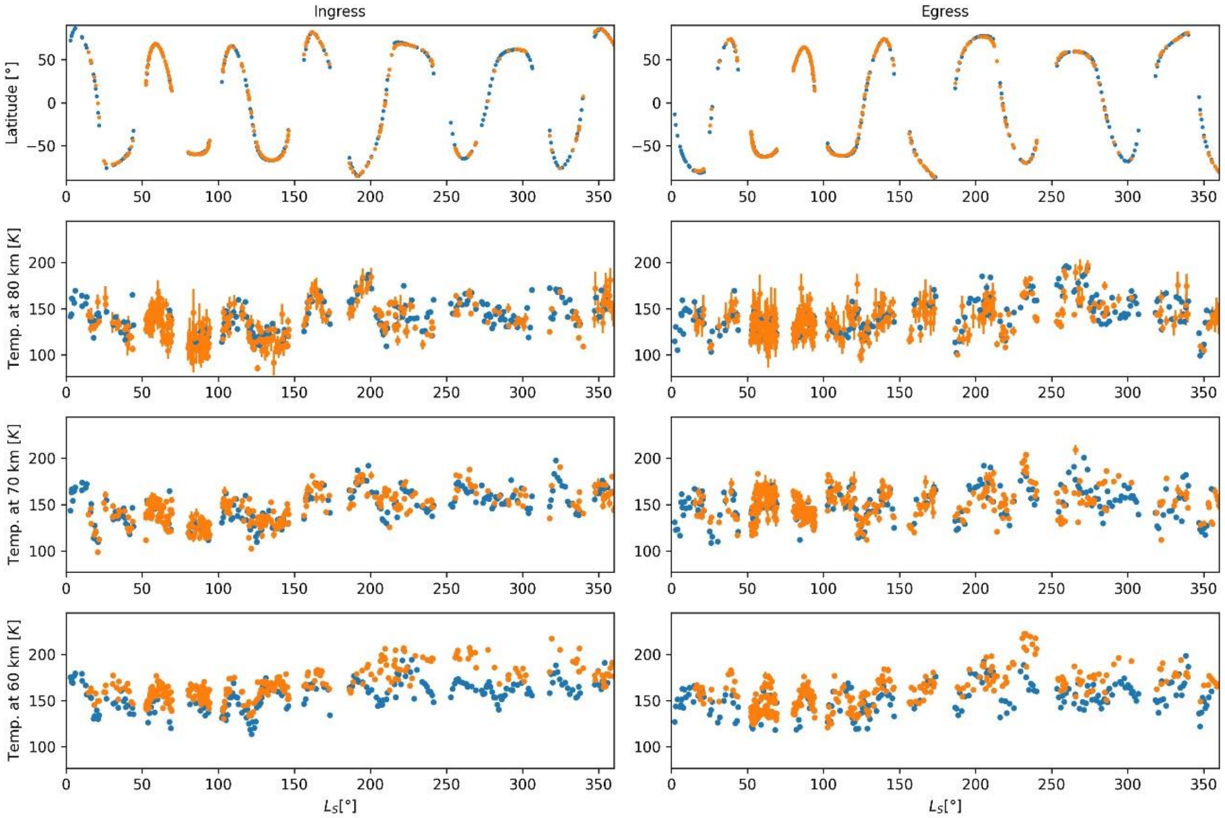
MIR
SO

CO_2



80 km
70 km
60 km

Temperature

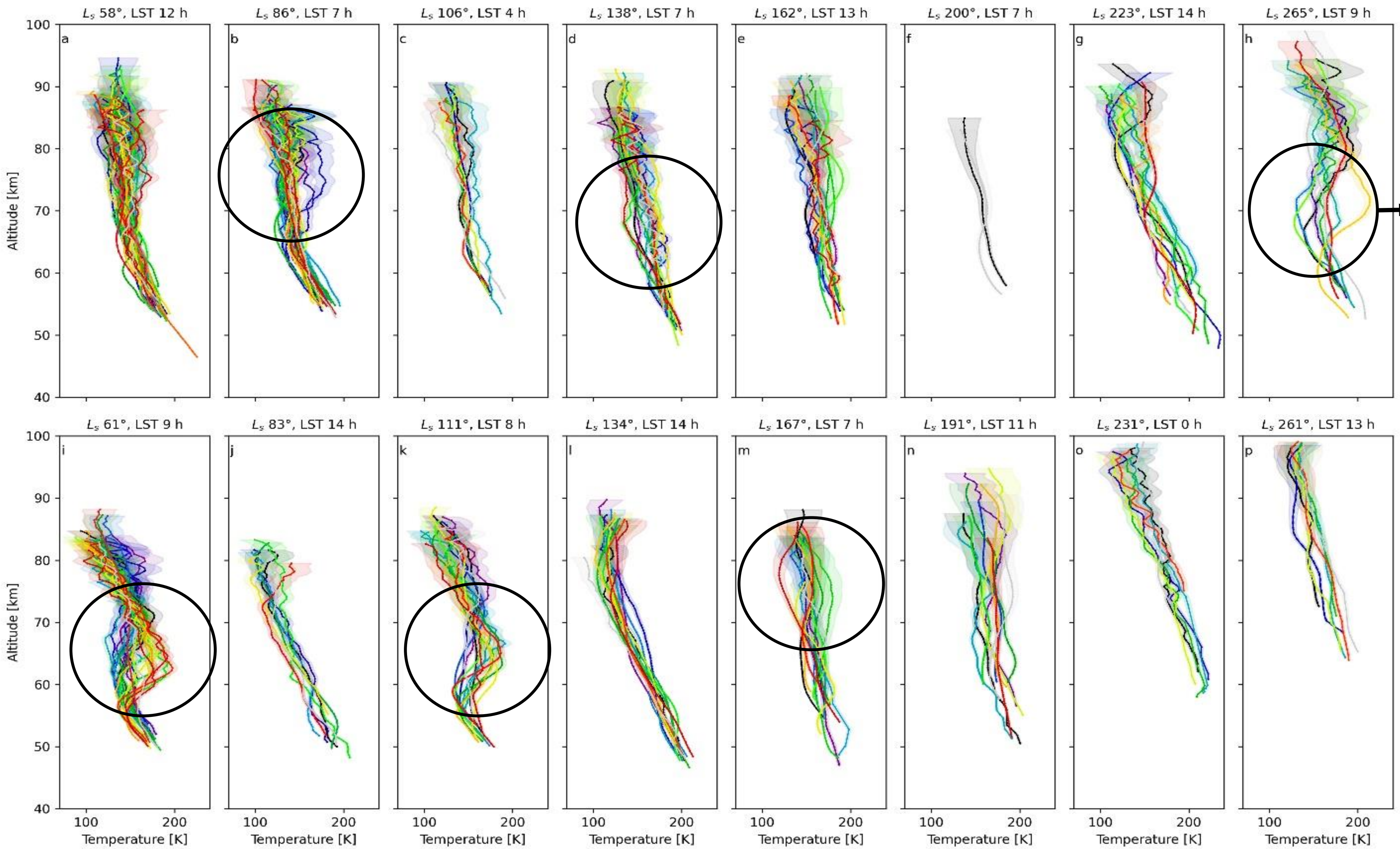


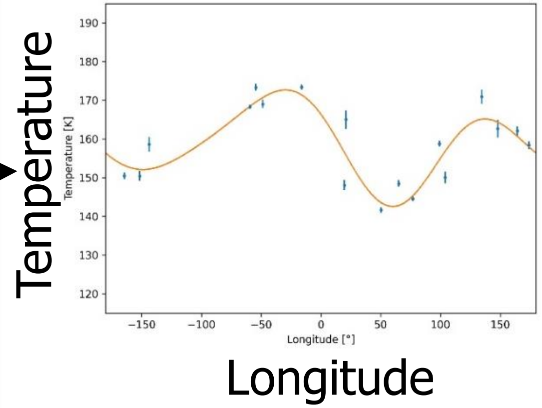
But we could check for co-located measurements …

4. A (very) few selected results

4. Longitudinal variations in MY 35

Bins of ± 15° L_S, 10° lat, 1 h LST.



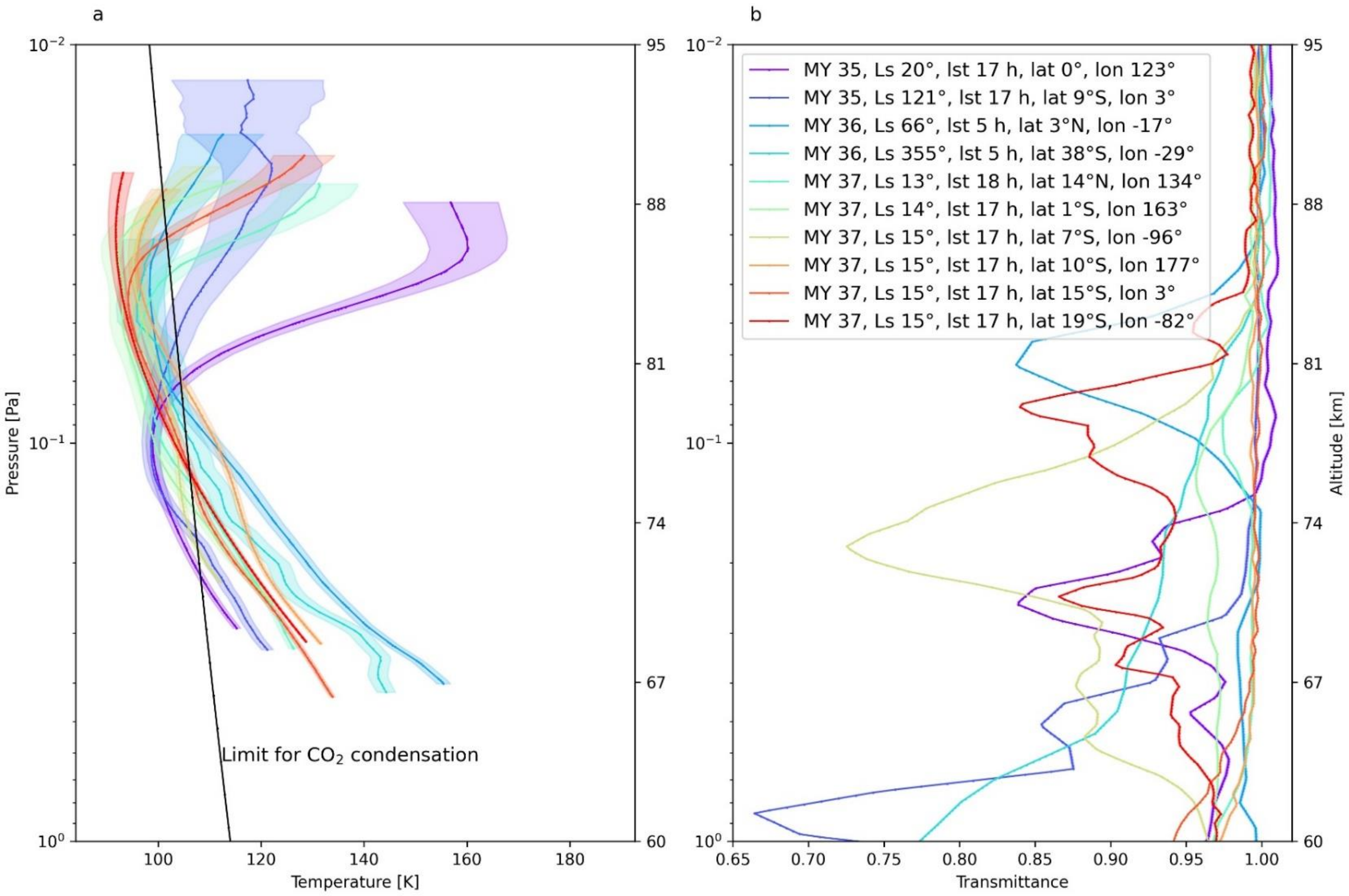


Longitudinal variations around alt 70 km and LST 7 h - 9 h

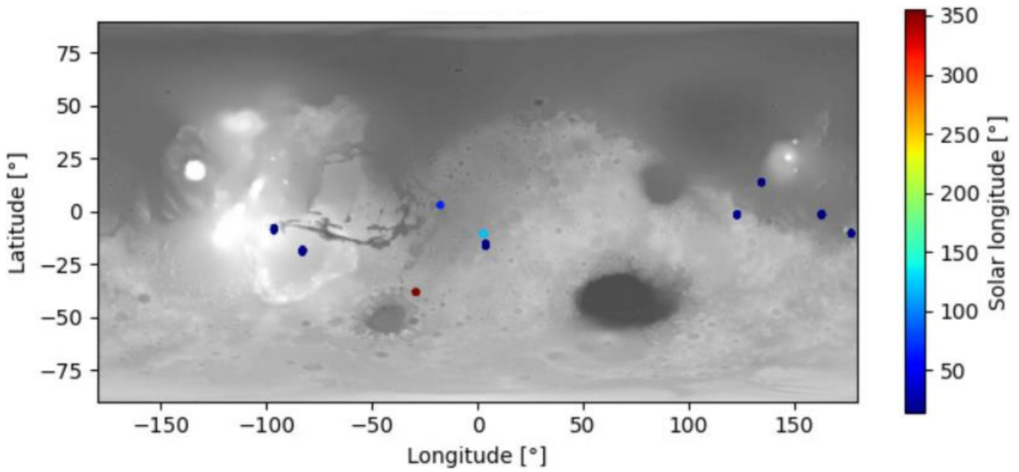
WN-1 (10%) + WN-3 (5%)

Trompet el al. a, b (2023)

4. Mesospheric CO_2 ice clouds



- Appears mainly at beginning (and the very end) of MY
- At low latitudes
- Longitudes 150°W to 10°E are well known
- Around 150°E as in Aoki et al. (2018) with PFS/MEx
- Liuzzi et al., (2021) with NOMAD-SO



5. (Coarse) Summary on temperature retrievals from NOMAD-SO

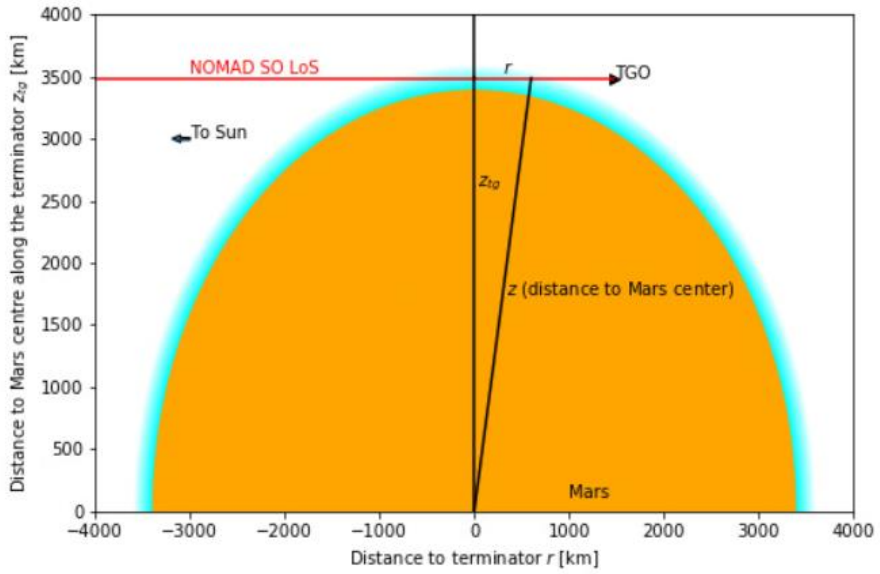
- Automatically retrieved the same day than when we receive the measurements
- Temperature is an important parameter for retrievals of minor species, especially for isotopic ratio
- There are two main retrieval schemes to retrieve temperature
  - Compare well
  - Fit of temperature is required for diffraction order 149 but not for 148 and 132
- Comparisons to other datasets show great similarities
  - With some differences that can be explained with differences in time and location or vertical resolution
- Temperature at terminator shows many variabilities
  - Many related to thermal tides, gravity waves, ...
  - Thermal tides are prominent in the morning terminator
  - Indicator of possible presence of CO_2 ice clouds
- Next
  - Comparison to aerosols
  - Continue tests with fit temperature: global fit, more diffraction orders, uncertainties, ...
  - Continue comparisons to other datasets
  - Continue analysis of thermal tides and gravity waves

Additional slides

The problem to solve: Abel transform

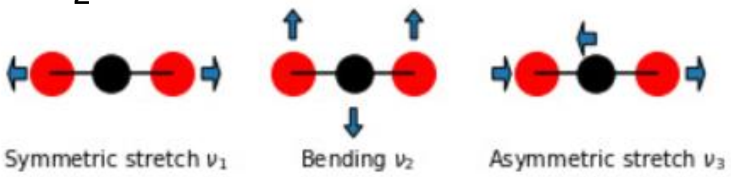
Beer-Lambert law

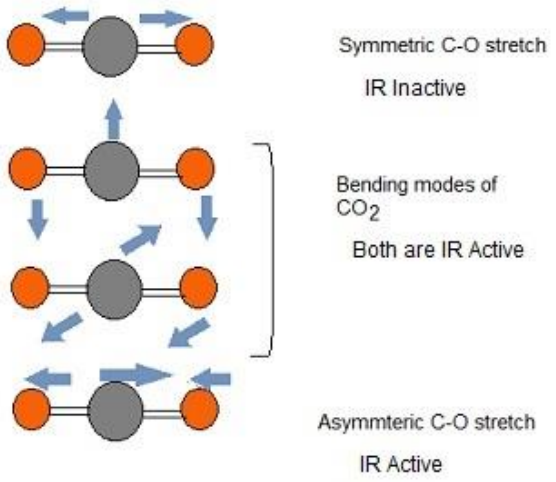
$$T(\nu, z_{tg}) = \frac{I(\nu, z_{tg})}{I_0(\nu)} = e^{-\tau(\nu, z_{tg})}$$

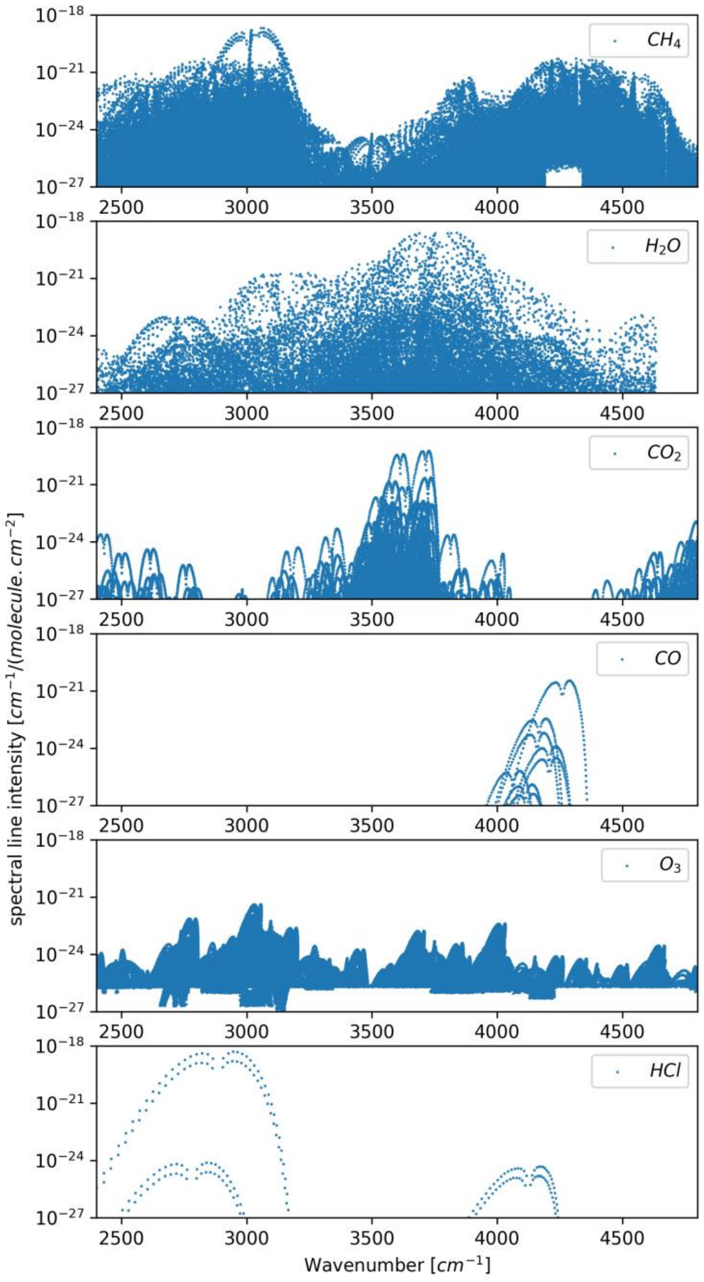


IR spectroscopy

For CO_2 :





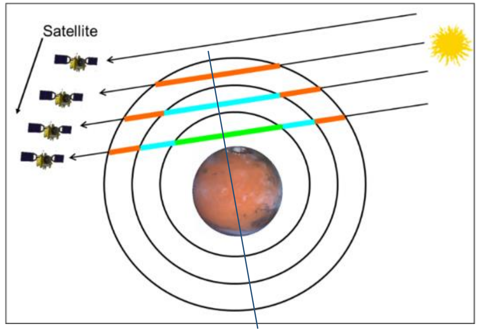


Transmittance calibration

For spectrum i at pixel j

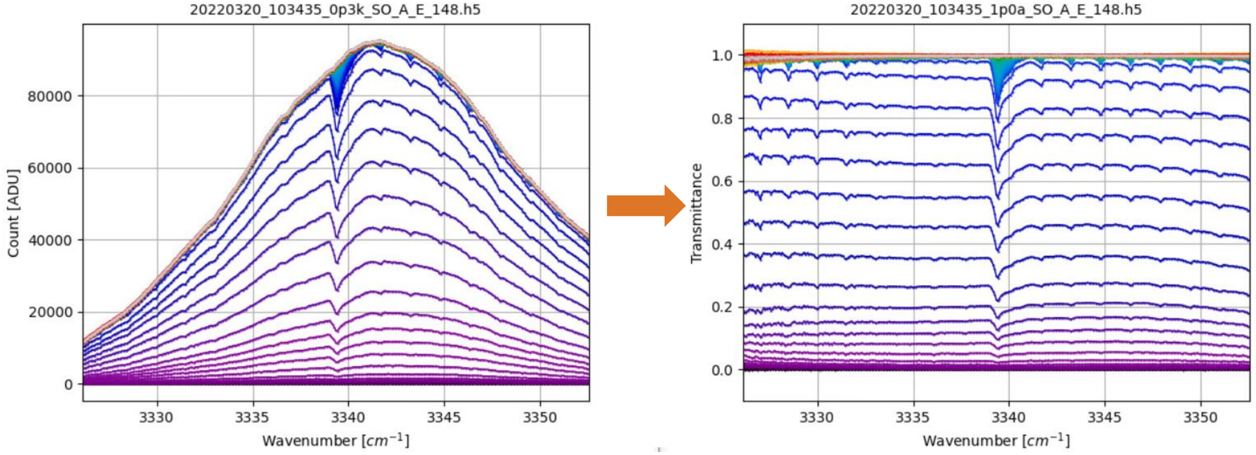
$$T_{ij} = \frac{A_{ij}}{S_{ij}}$$

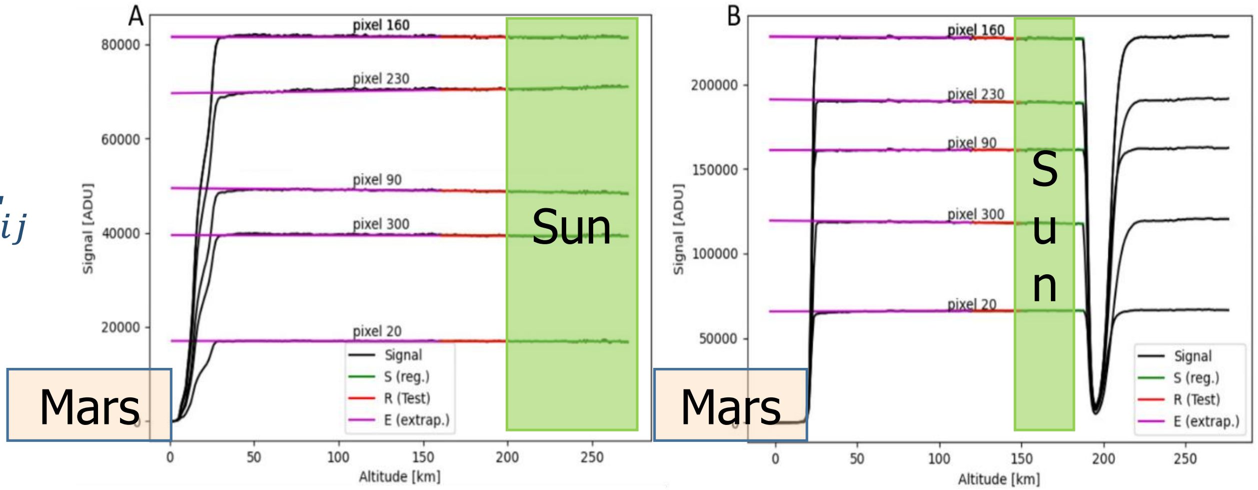
Solar occultation



Terminator

Diffraction order 148

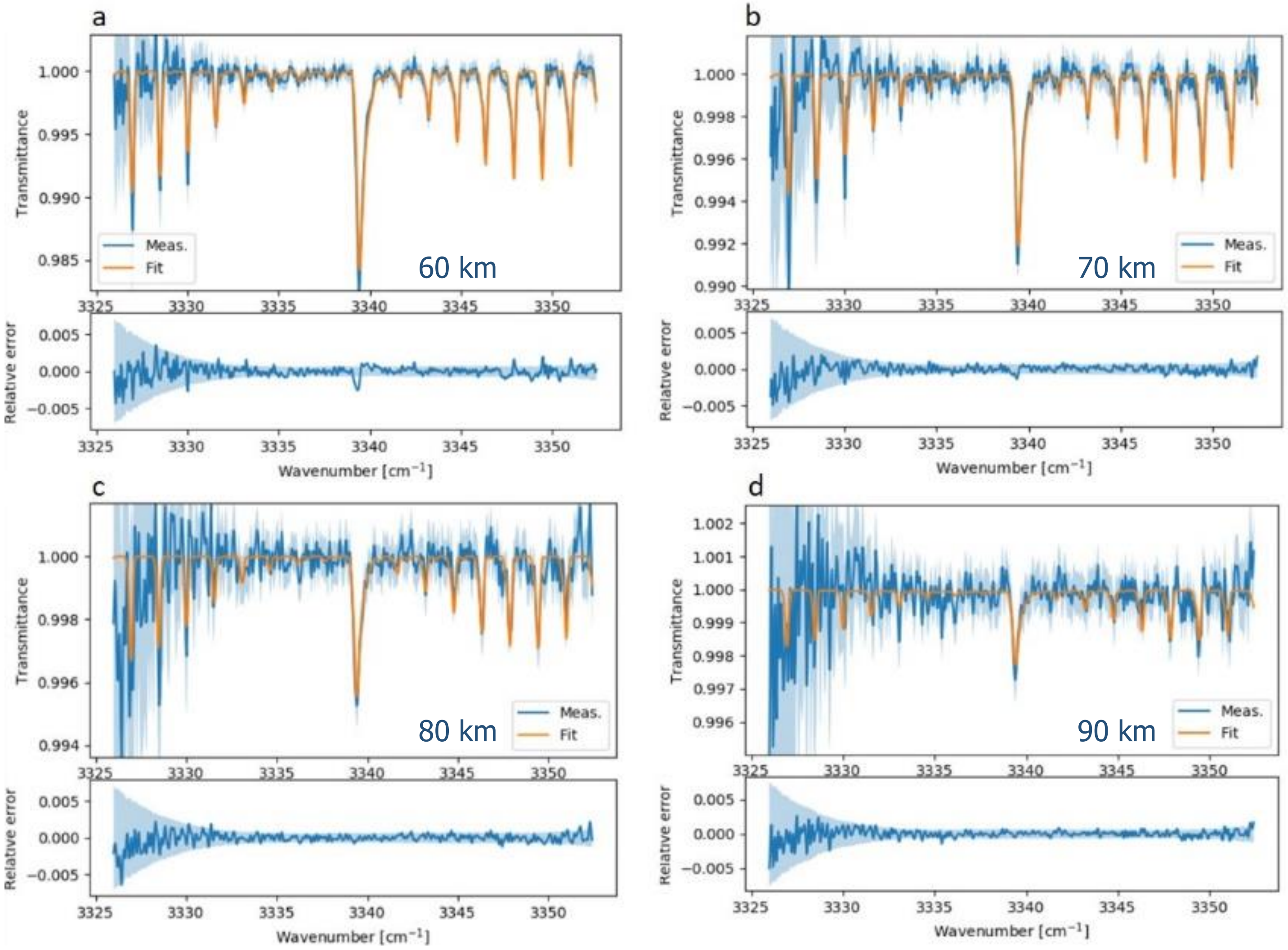




Criterion :

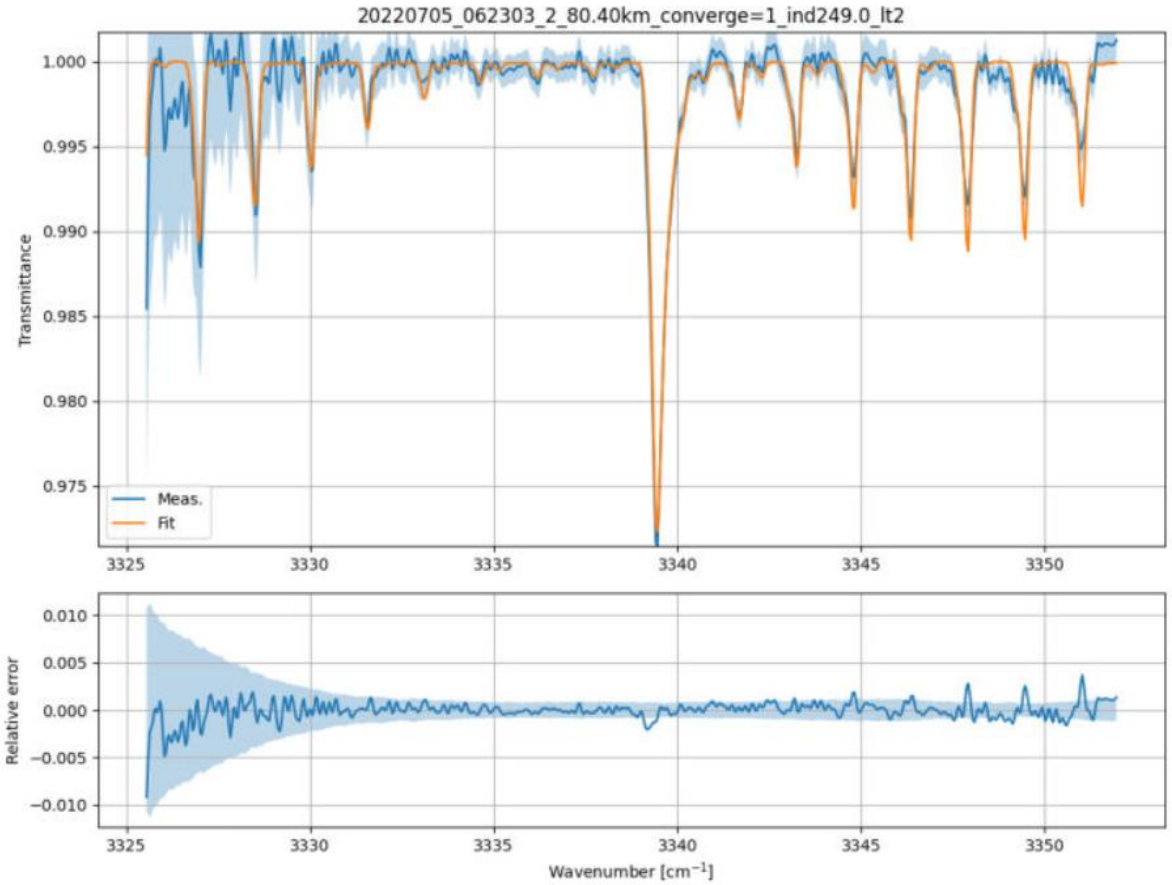
$$|1 - T_{ij}| < 2\, dT_{ij}$$

Examples of fit

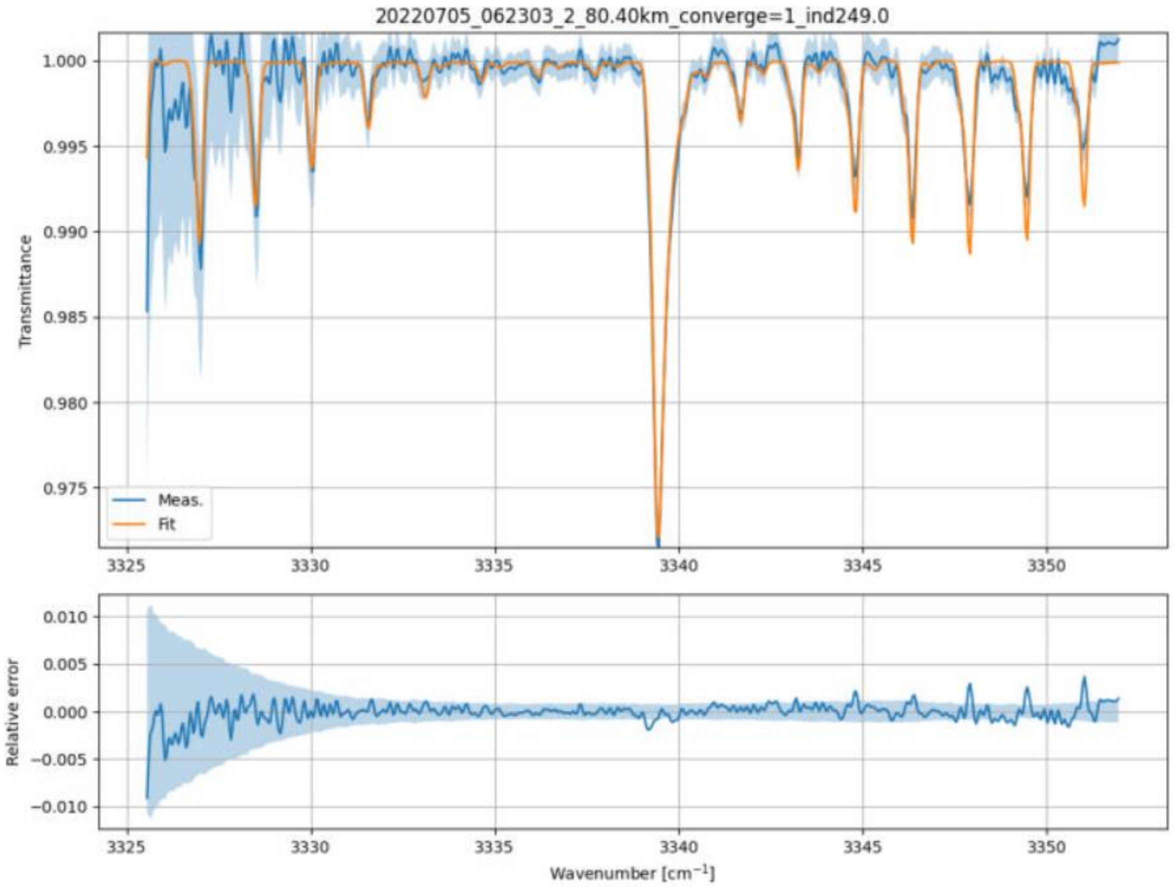


Comparison of fitted spectra - 148

Fit c

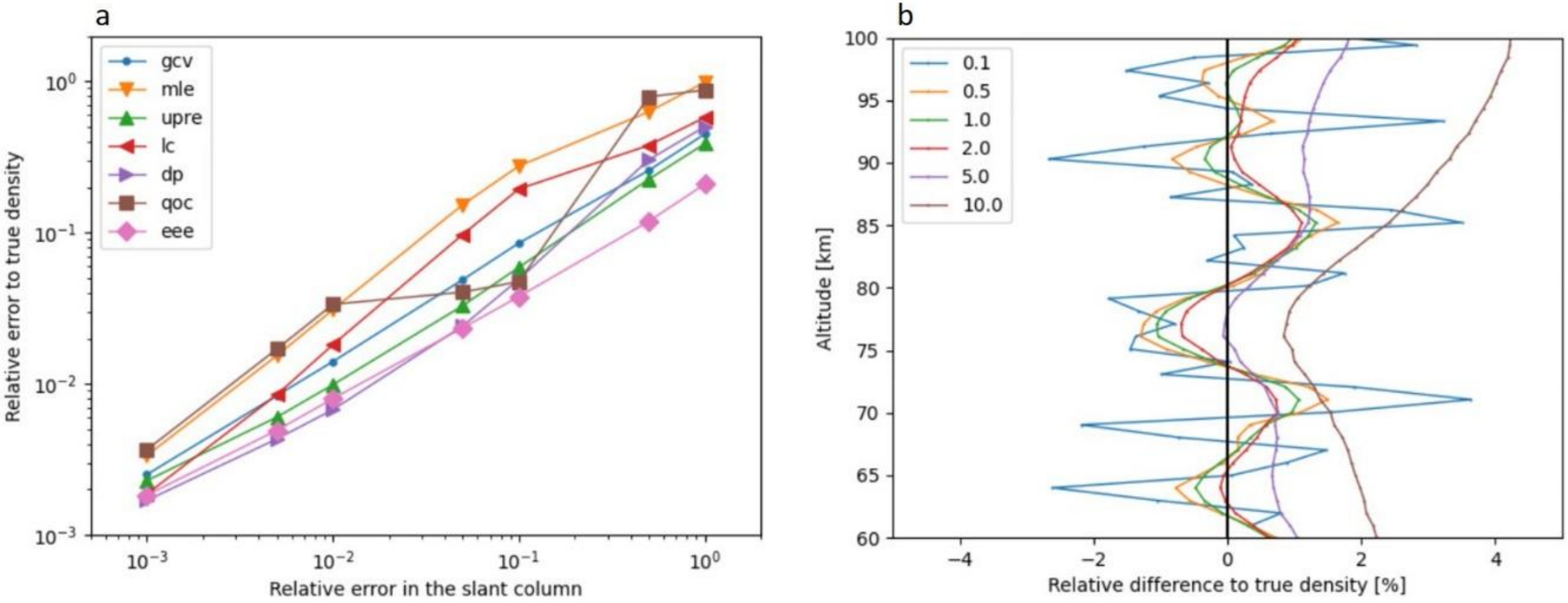


Fit c and T



Step 2: Regularization

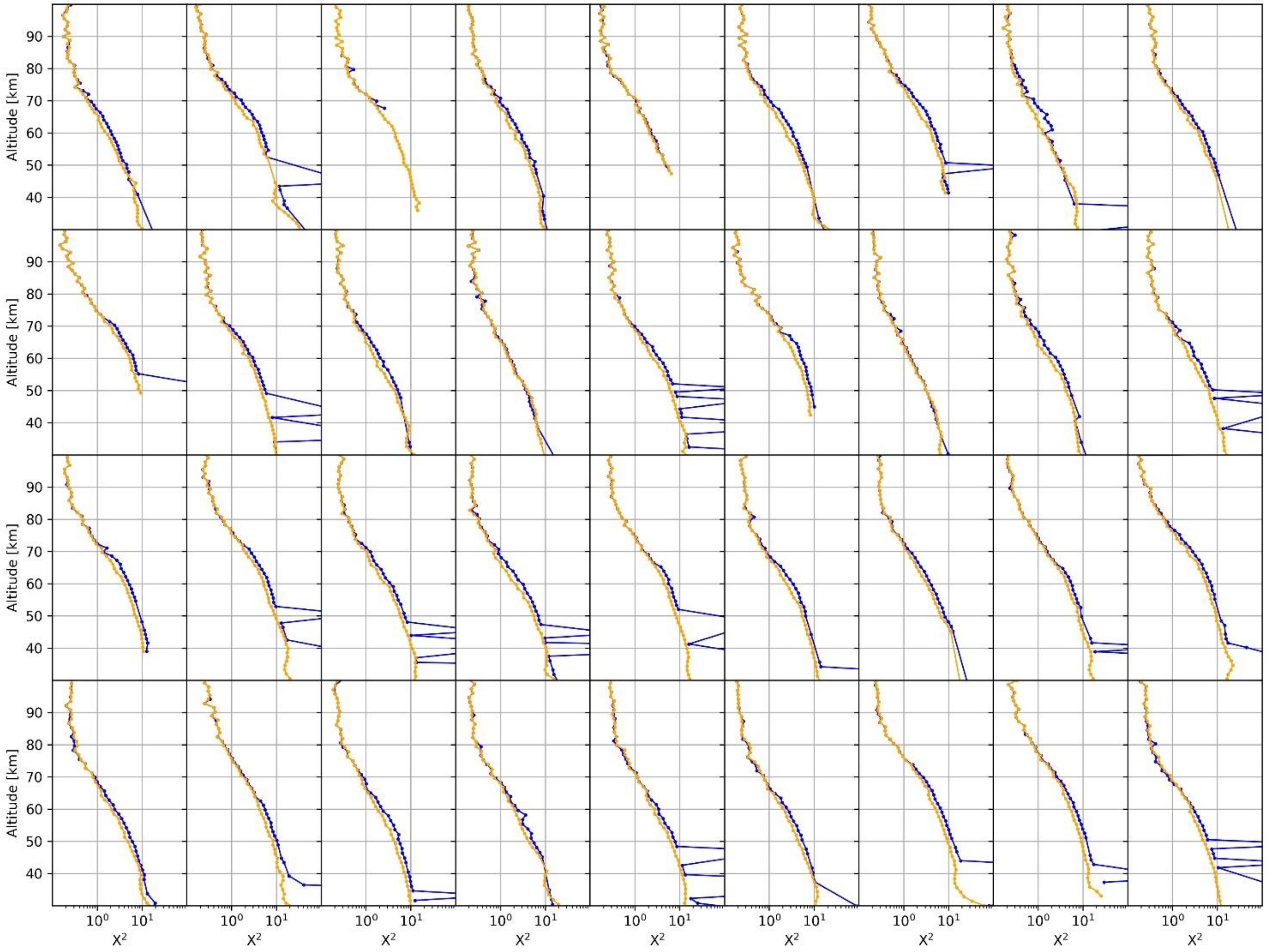
Different methods to find the best regularization parameter



3.1 Comparison of reduced X² - 148

X^2 must be as close as possible to 1
$X^2 < 1$: noise is overestimated
$X^2 > 1$: model must be improved

Fit c and T
Fit c

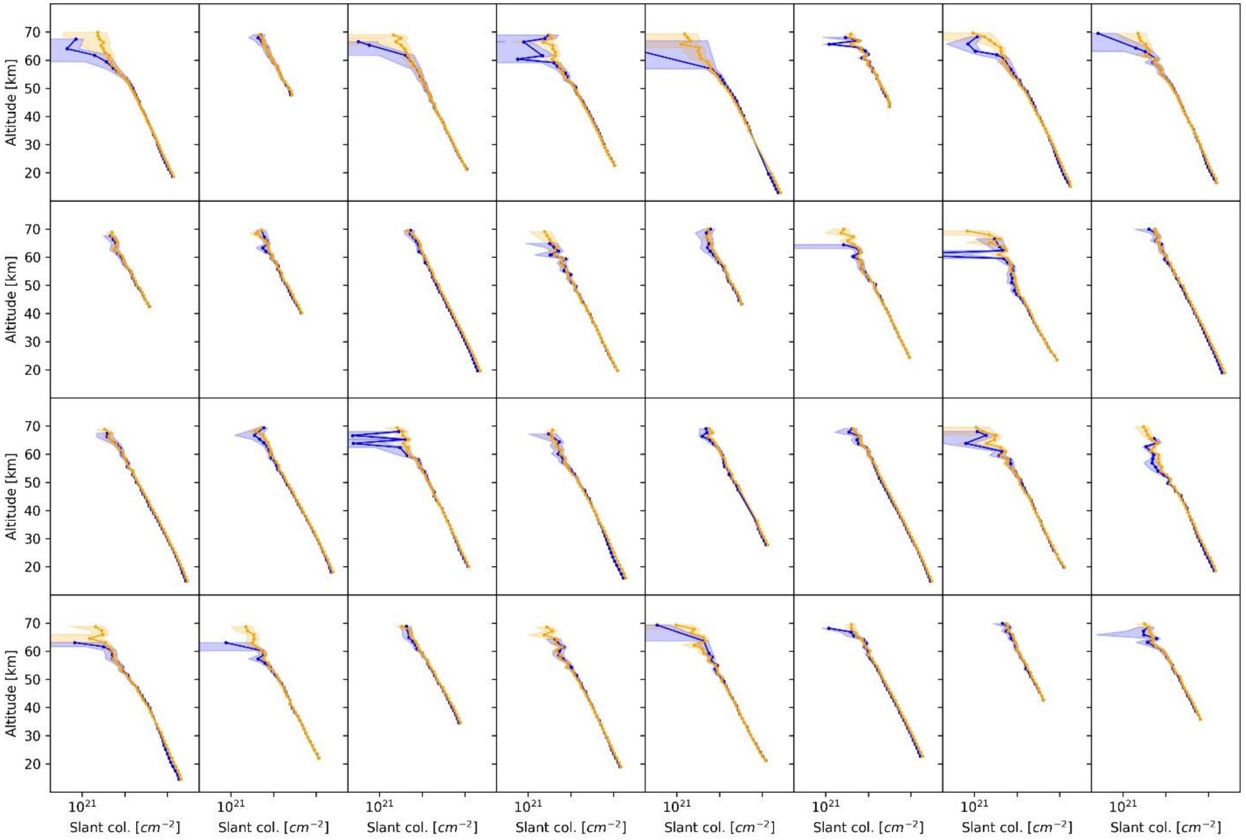


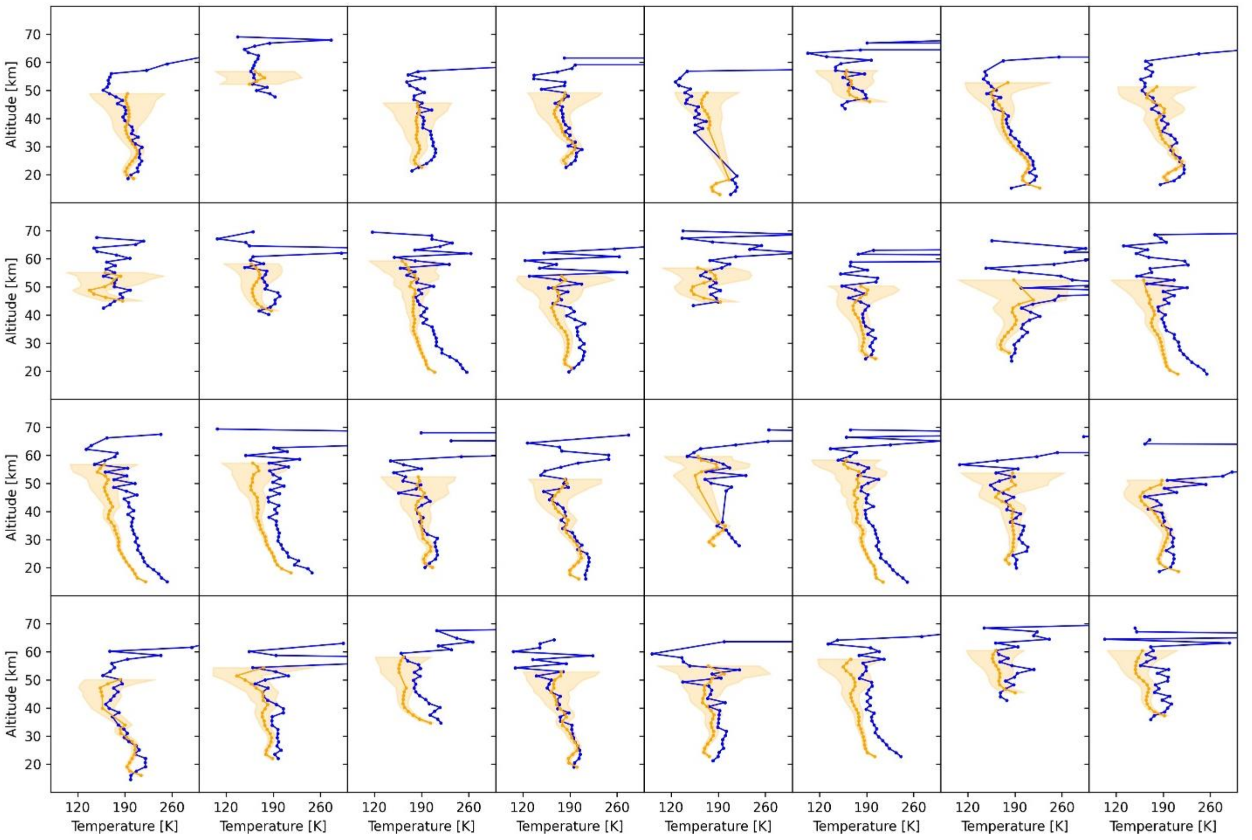
3.1 Comparison for diffraction order 132

32 profiles

Fit c and T

Fit c and T from hydro. eq.

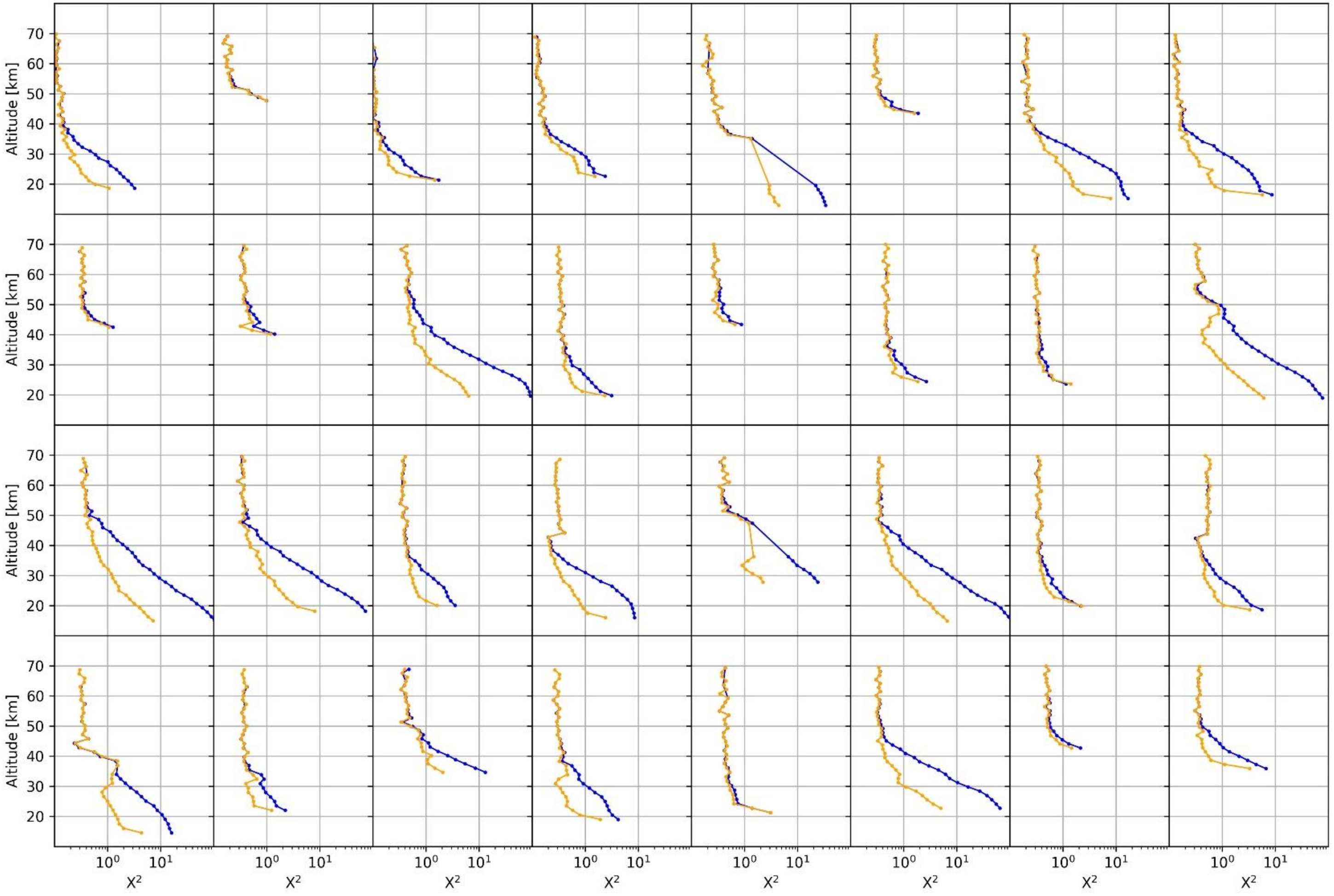




3.1 Comparison of reduced X^2 - 132

Fit c and T
Fit c

X^2 must be as close as possible to 1
$X^2 < 1$: noise overestimated
$X^2 > 1$: model must be improved



3.1 Summary on comparisons T_{HE} and T_{Fit}

- No constrain on T_{Fit} required during the spectral inversion
- Need to double check the computed uncertainties
- Order 148 compares well
- T_{HE} worse than T_{Fit} for order 149
- T_{HE} better than T_{Fit} for orders 148 and 132
- But still the fit of order 148 is better than 149
- Time of computation: only c: < 1 min/spectrum, c and T: < 2 min/spectrum
- Next:
  - Include fit of the temperature for P and R branches (149, 165)

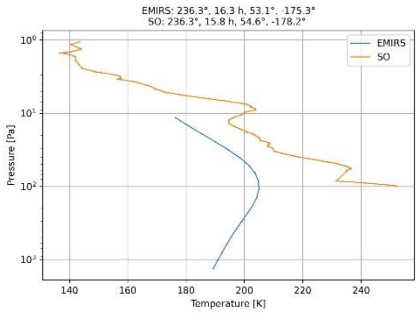
3.2 Comparisons

Contemporary datasets for comparisons of temperature

Reference (latest paper explaining ret.)	Instrument	Data available online	Rad. trans. code	Regularization method	A priori	Ret. method	Altitude range [km]	Resolution [km]
Pätzold+2016	RS/MEx	NO		None	None	Hydro. eq.	0-60	< 1 km
Kleinbhöl+2009	MCS/MRO	YES		OEM		Radiance	0-80	5
Smith+2022	EMIRS/EMM	YES		Conrath (2000)	Mars PCM	Radiance	0-40	10 – 15
Guerlet+2023	TIRVIM/ACS/TGO	YES		Conrath (2000)	Mars PCM	Radiance	0-50	10 – 15
Stone+2018	NGIMS/MAVEN	YES	/	/	/	Hydro. eq.	120-220	1
Gupta+2022	IUVS/MAVEN	YES		Tikhonov	None	Hydro. eq.	80-160	5
Thiemann+2018	EUVM/MAVEN	YES			None	Hydro. eq.	120-200	
Belyaev+2022	MIR/ACS/TGO	YES		LM+OEM+Tikhonov	Mars PCM	Intensity	0-190	1 – 3
Alday+2023	MIR/ACS/TGO	YES	NEMESIS	OEM	Mars PCM	Intensity	0-130 (190)	1 – 3
Fedorova+2022	NIR/ACS/TGO	YES		LM+Tikhonov	Mars PCM	Hydro. eq.	0-120	2.5 – 3
López-Valverde+2022	SO/NOMAD/TGO	YES	KOPRA	OEM+Tikhonov	Mars PCM	Intensity +Hydro. Eq.	0-100 (190)	
Trompet+2023	SO/NOMAD/TGO	YES	ASIMUT	Tikhonov	None	Hydro. eq.	(0) 60-100 (190)	1.6 – 3

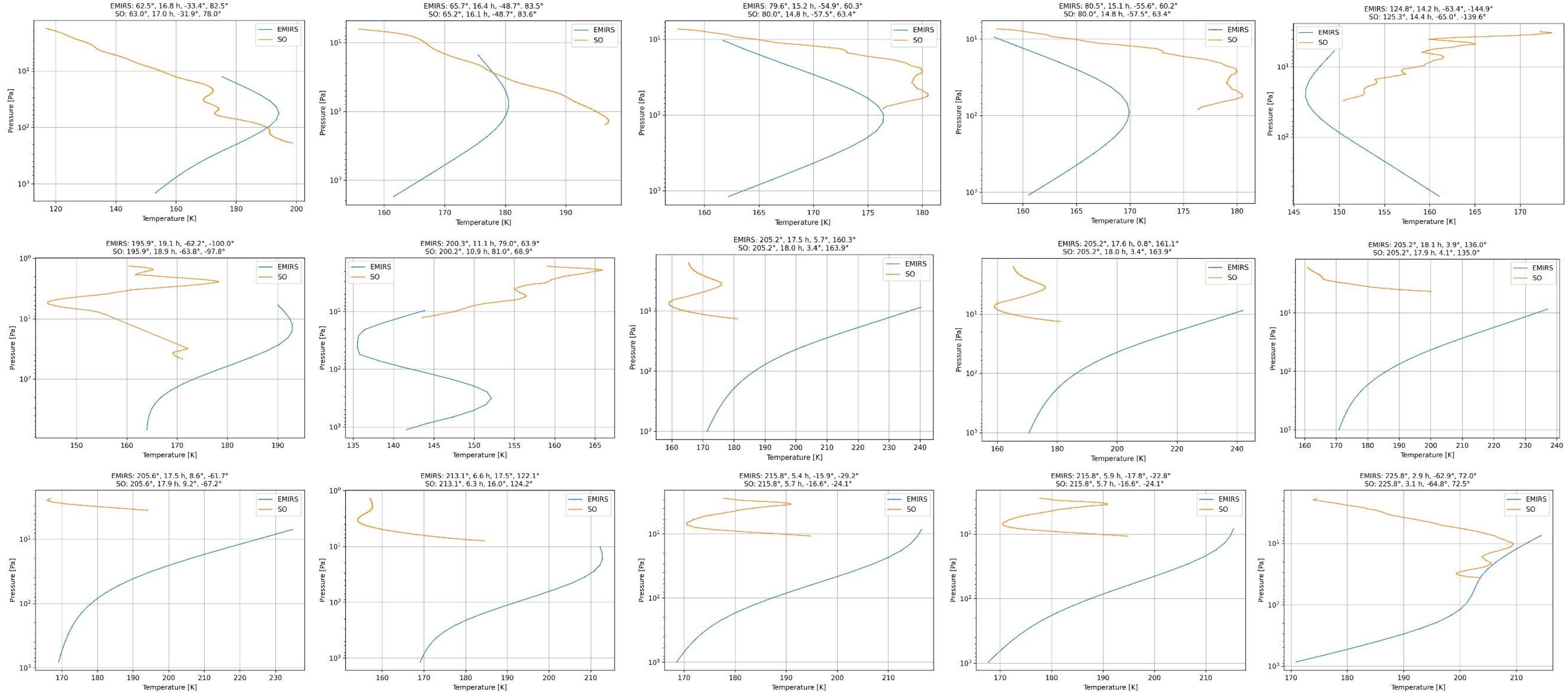
3.2 Comparison to EMIRS/EMM

Smith et al. 2022



16 profiles

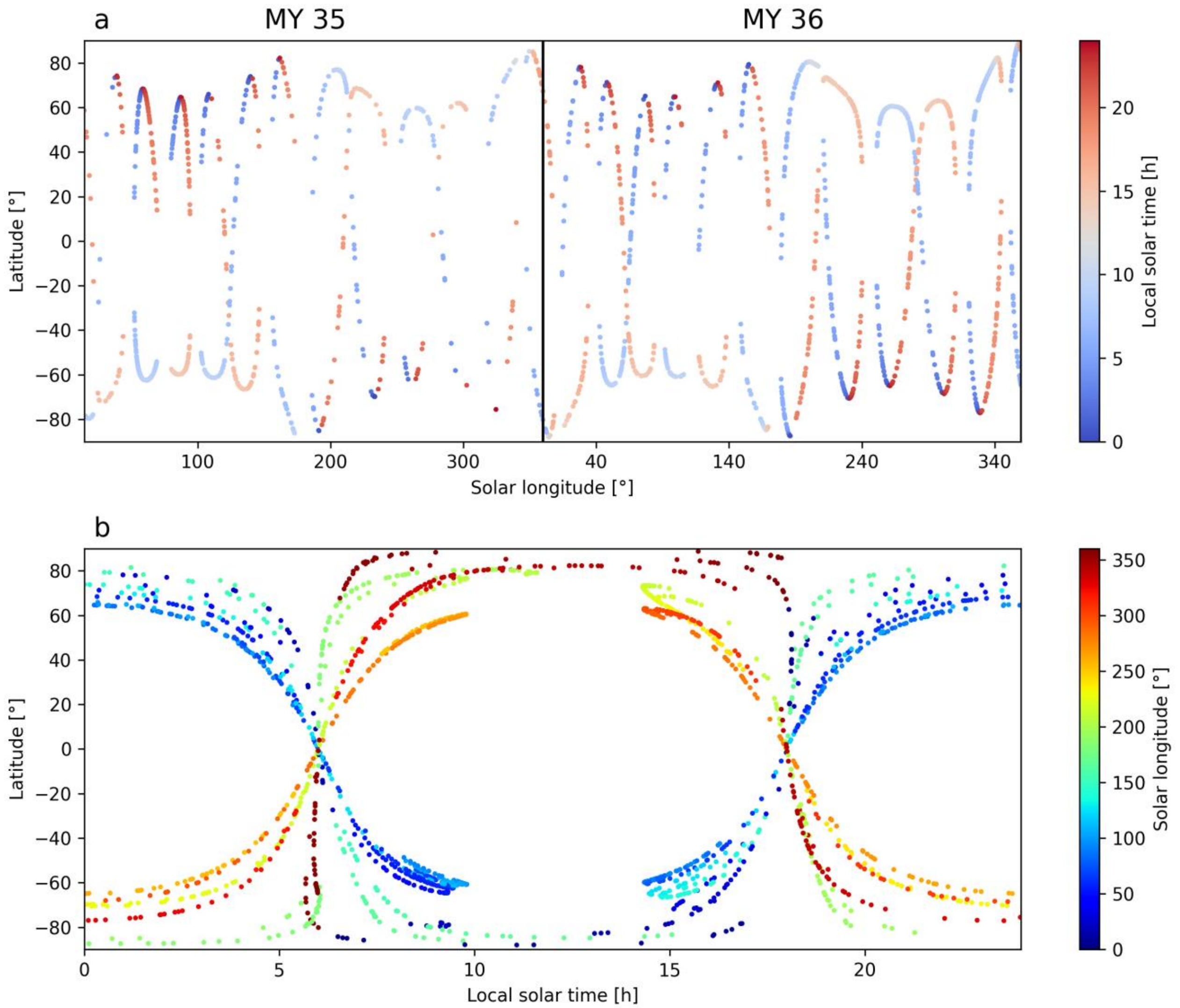
Differences in altitudes and vertical resolution



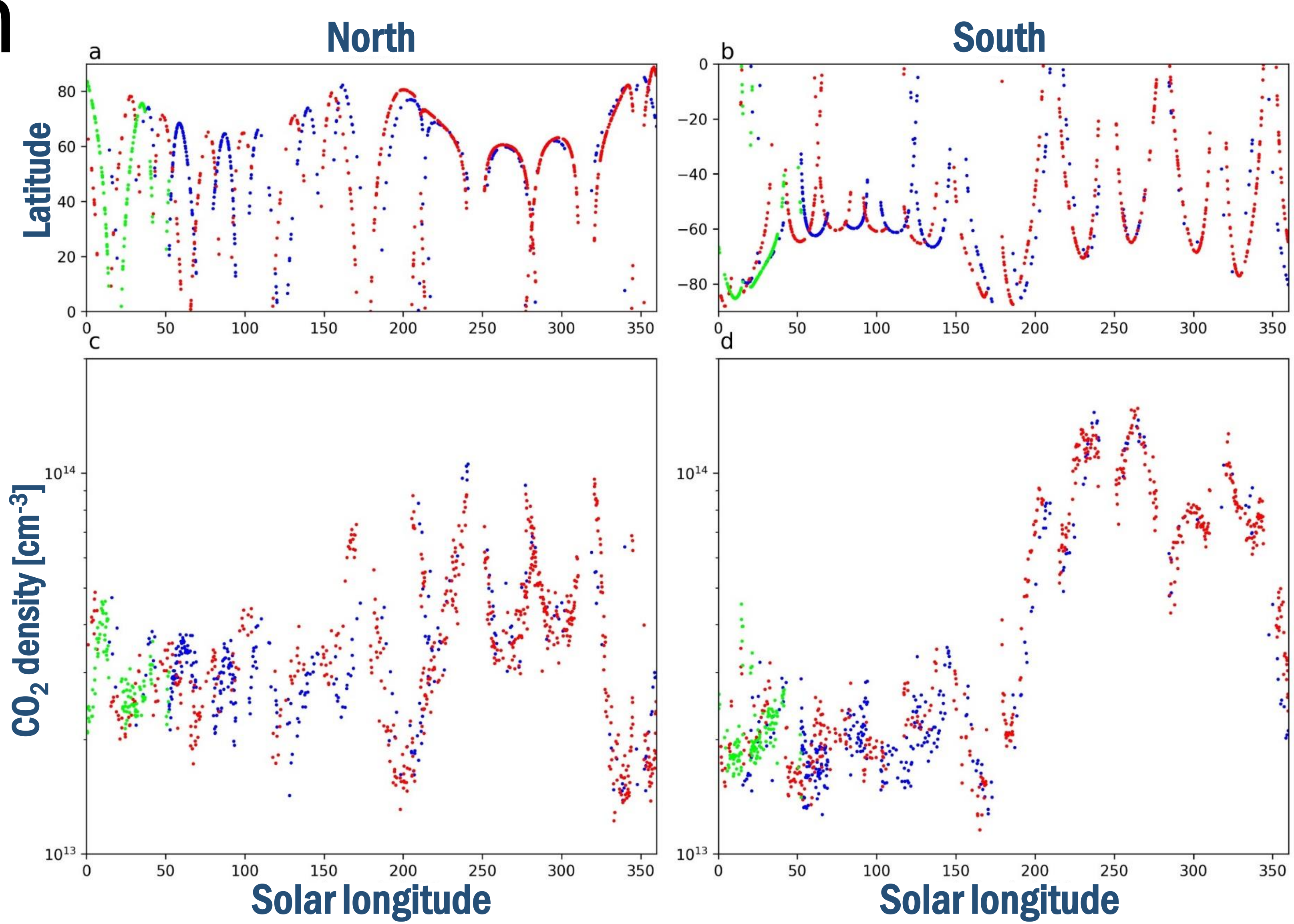
3. Summary on comparisons with other datasets

Other instrument X	NOMAD-SO order	# co-located profiles	average diff. X - SO [K]	absolute diff. [K]
MCS	148	117	0.1	8.5
MCS	132	39	-0.5	4.4
NIR	148	64	-4.7	6.7
NIR	132	9	-5.7	7.3
TIRVIM	132	0	No comparison possible	
EMIRS	132	16	Comparison difficult	

Coverage


a
MY 35
MY 36
Latitude [°]
Solar longitude [°]
Local solar time [h]
b
Latitude [°]
Local solar time [h]
Solar longitude [°]

Seasonal variation of CO_2 density @ 75 km

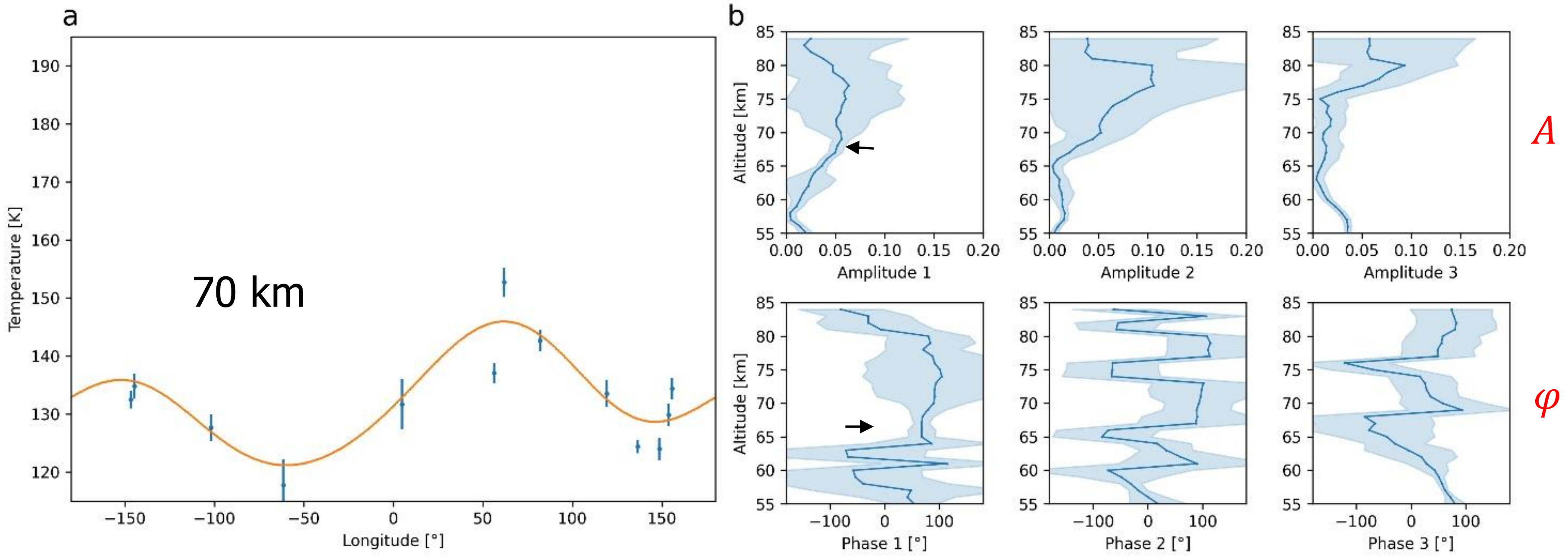


Mars year (MY) 1 started on 11/04/1955

1 MY ~ 687 days

4. Fit longitudinal components

Fit: $\sum_k A \cos(k * lon - \varphi)$



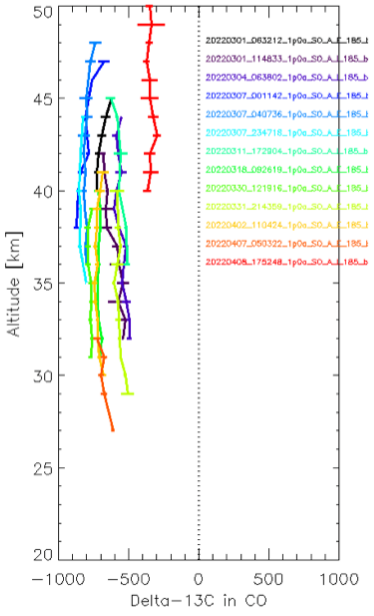
MY 35 L_s 126°-146°,
Lat 70°S-64°S,
LST 14.5 h - 16 h

~ 68 km: k=1 (5%)

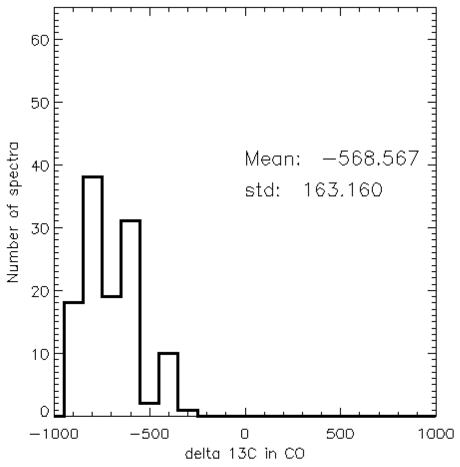
4.2 Sensitivity of CO retrievals to temperature

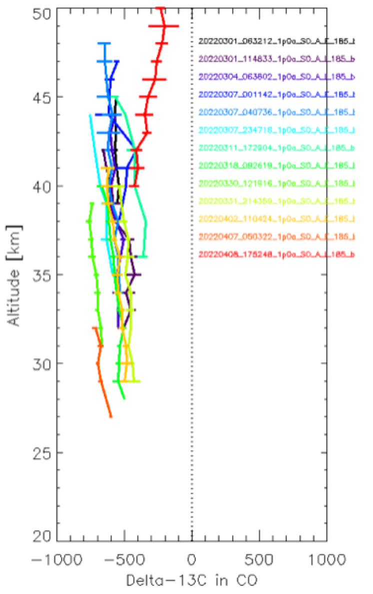
S. Aoki et al. (2023)

- CO isotopic ratio ($^{13}C/^{12}C$) has been selected for this subject as it is a key diagnostic for atmospheric evolution and the origin of organics on Mars.
- We found that weak ^{12}CO lines (whose intensities are comparable to ^{13}CO lines) are quite sensitive for the temperature.
- Comparison between retrievals with temperatures by a General circulation model and retrieved from simultaneously retrieved CO_2.
- The retrieved atmospheric temperature improves the quality of the retrievals of the isotopic ratio.



with GCM T





with retrieved T