MIPAS database: New HNO_3 line parameters at 7.6 µm derived from laboratory intensity measurements and MIPAS satellite measurements

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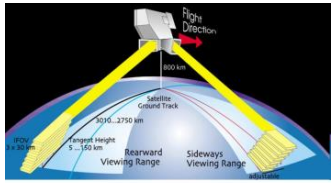
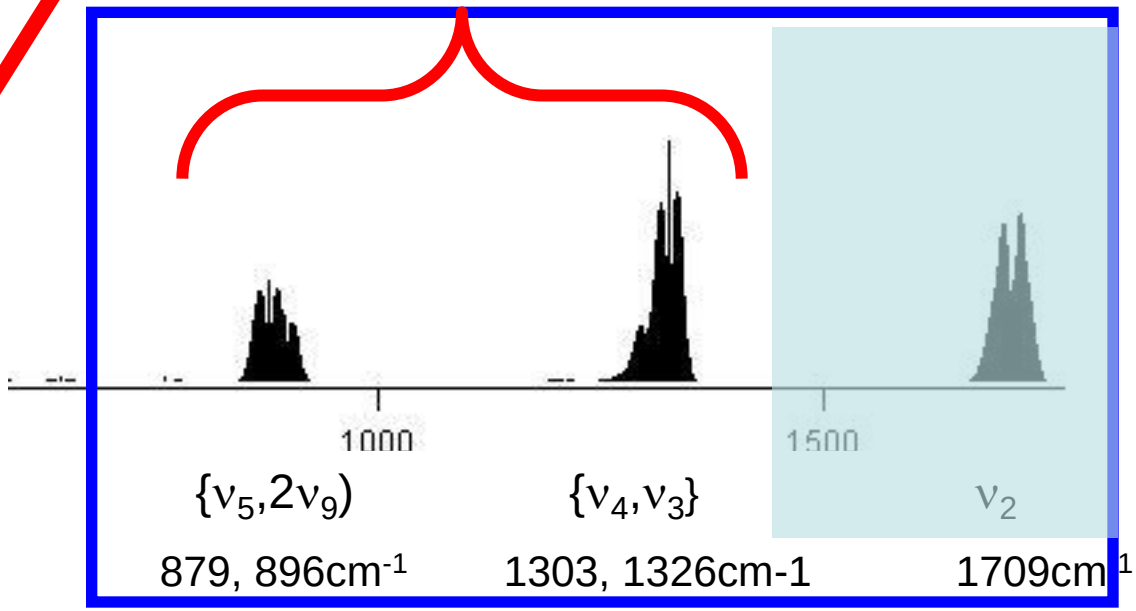
IASI on METOP



MIPAS on ENVISAT sattellite

Preparation of **IASI-New Generation** (2020)



11µm 7.6µm

Goal for **IASI -NG**: to enable simultaneous detection of HNO_3 both at 11 µm & 7.6 µm using MIPAS spectra

The source for the line positions & relative intensities parameters for HNO_3 @7.6 µm in the HITRAN-2012 database:

¤ Perrin, Lado-Bordowski and Valentin, « The ν3 and ν4 bands of HNO_3 ».Mol. Phys 67 p249 (**1989**)

¤ Perrin, et al. « Line intensities in the 11µm & 7.6 µm bands of HNO_3 » J. Mol; Spectrosc. 160, p524 (**1993**)

The « **bad quality** » of the HNO_3 parameters in HITRAN or GEISA at 6.3 µm … originates from « **our imperfect 1989-1993 linelist**»

A.Perrin: « New Analysis of the ν_3 and ν_4 bands of HNO_3 in the 7.6 µm region

J. Phys. Chem. A 2013, 117, 13236−13248

- FTS spectra recorded at high resolution in the 7.6 µm, 11 µm and 22 µm regions.
- New theoretical model => the ν_3 and ν_4 cold bands, and four dark bands (the $2\nu_6$, $3\nu_9$, $\nu_5+\nu_9$, $\nu_7+\nu_8$)
- First observation of the $\nu3+\nu9-\nu9$ hot band

A 2013 **preliminary** linelist for $H^{14}NO3$ (ν_3 and ν_4 cold bands, four dark bands ($2\nu_6$, $3\nu_9$, $\nu_5+\nu_9$, $\nu_7+\nu_8$) and the $\nu3+\nu9-\nu9$ hot band

Strategy:

¤ As a starting point, we use the 2013 preliminary list of line positions and **relative** line intensities at 7.6 µm

¤We kept the **11 µm** band line parameters as they are in GEISA or HITRAN

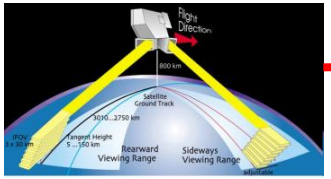
¤ We performed the intercalibration of the new 7.6 µm parameters (line positions and relative intensities) relatively to those at **11 µm**.

$Perrin: *J. Phys. Chem. A* 2013, 117, 13236−13248

Strategy for the 11µm and 7.6 µm regions (HNO_3)

We used and **combined** three sets of experimental data

- ¤ A list of laboratory experimental (individual) line intensities measured in the 7.6 µm region using FTS spectra recorded in 2004 at Giessen (a)
- ¤ The Pacific Northwest Laboratory (PNNL) cross sections (https://secure2.pnl.gov/nsd/nsd.nsf/Welcome) (b)
- ¤ MIPAS spectra (orbit 04712 from 24 january 2003)



Here we present the final 7.6 µm database « **MIPAS-2015** » which is a compromise resulting from these 3 studies)

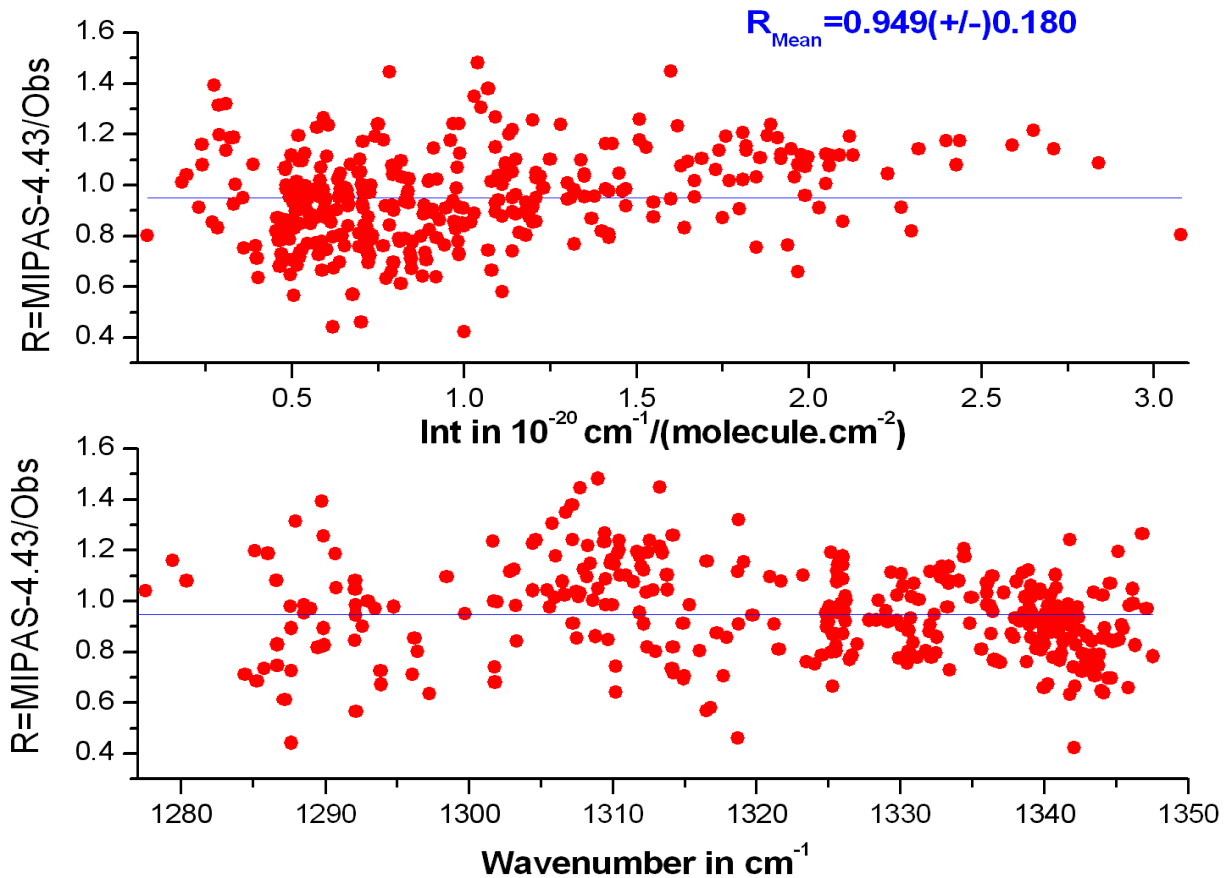
References :
(a) Perrin, Orphal, Flaud, Klee, Mellau, Mäder, Walbrodt & Winnewisser, J. Mol. Spect 228 (2004)
(b) Sharpe, Johnson, Sams, Chu, Rhoderick, & Johnson, Appl. Opt. 58 (2004) p1452.

(1)

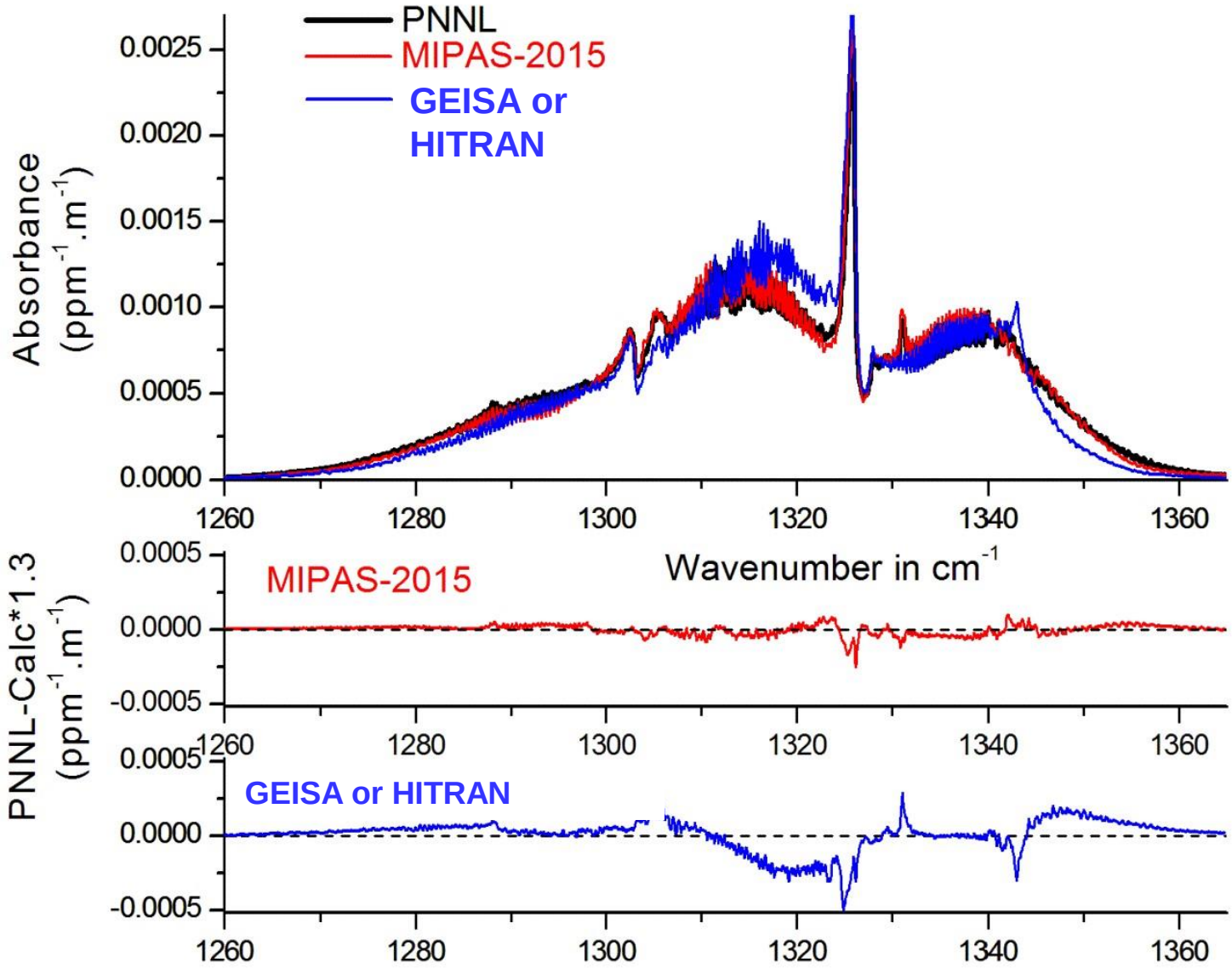
¤ A set of ~ 350 line intensities were measured for well isolated lines in the 7.6 µm region using the program "WSpectra" (ULB Belgium software)

(FTS spectra recorded in Giessen)

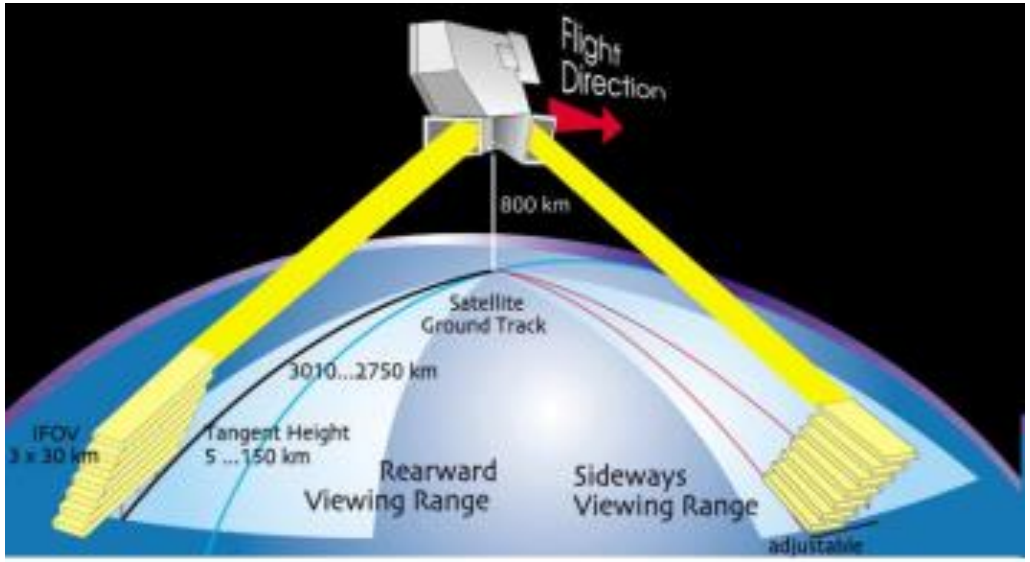
Ratio R=MIPAS-2015/ Measured line intensities



(2) The Pacific Northwest Laboratory cross sections (https://secure2.pnl.gov/nsd/nsd.nsf/Welcome)

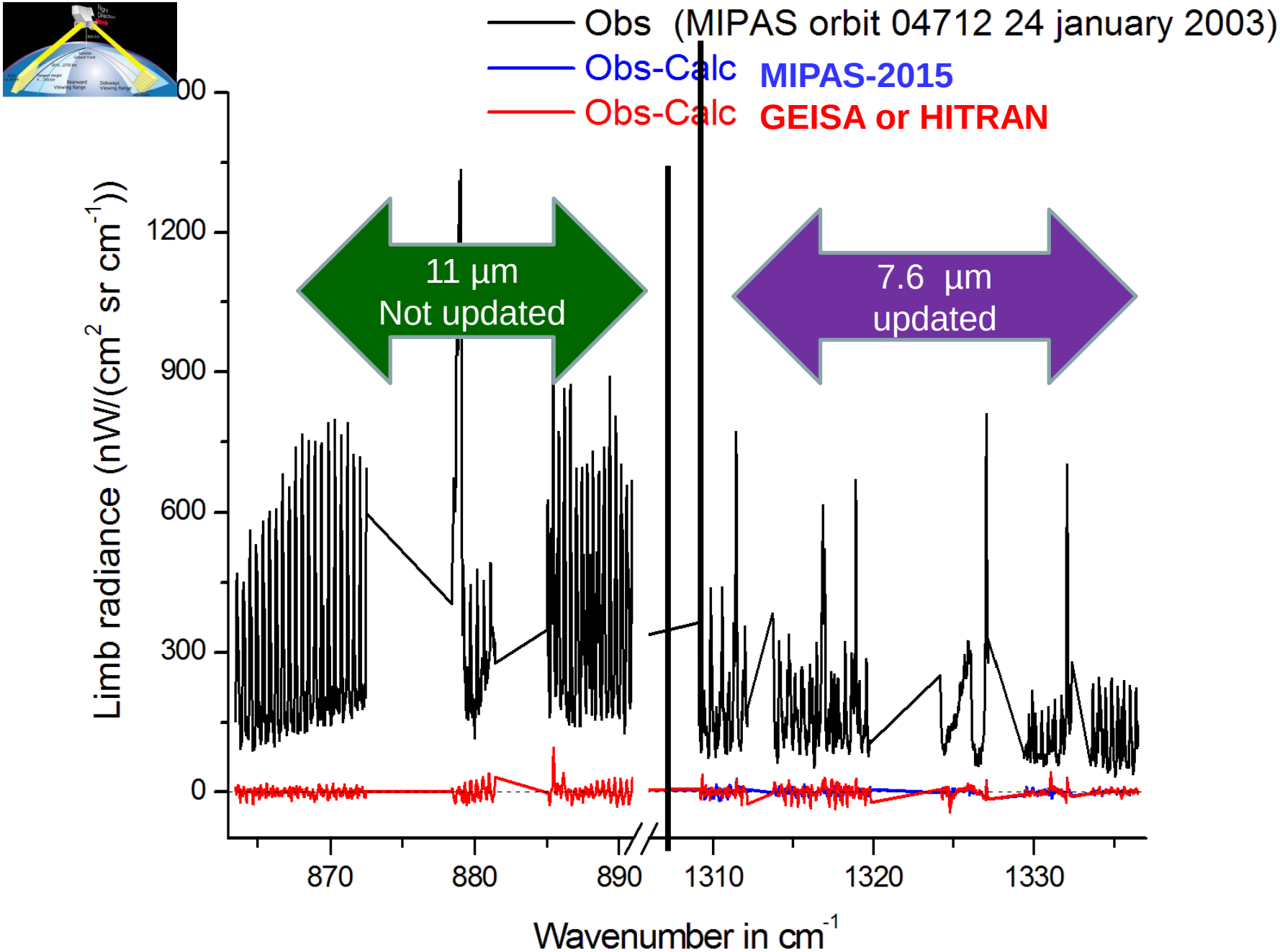


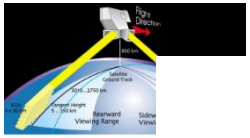
(3) Intercalibration of the 7.6 µm ⇔ 11 µm spectral region using MIPAS spectra

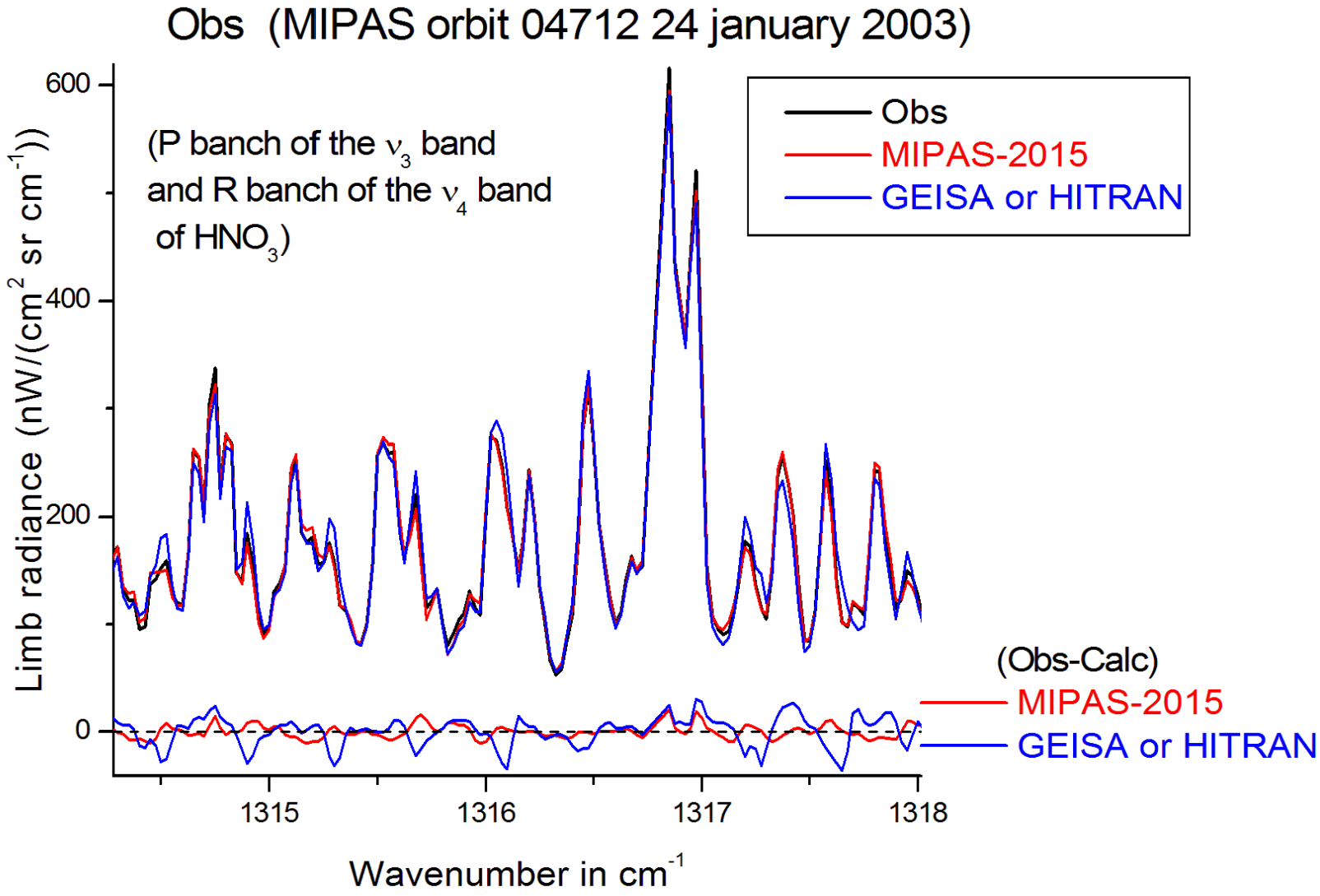


The **M**ichelson **I**nterferometer for **P**assive **A**tmospheric **S**ounding (MIPAS) was a FTS spectrometer for the detection of limb emission spectra in the middle and upper atmosphere. On **ENVISAT** (died in 2012)

A.Perrin IASI conference 2016


Obs (MIPAS orbit 04712 24 january 2003)
Obs-Calc MIPAS-2015
Obs-Calc GEISA or HITRAN
11 µm
Not updated
7.6 µm
updated
Limb radiance (nW/(cm^2 sr cm^{-1}))
1200
900
600
300
0
870
880
890
1310
1320
1330
Wavenumber in cm^{-1}





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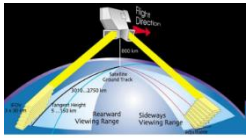
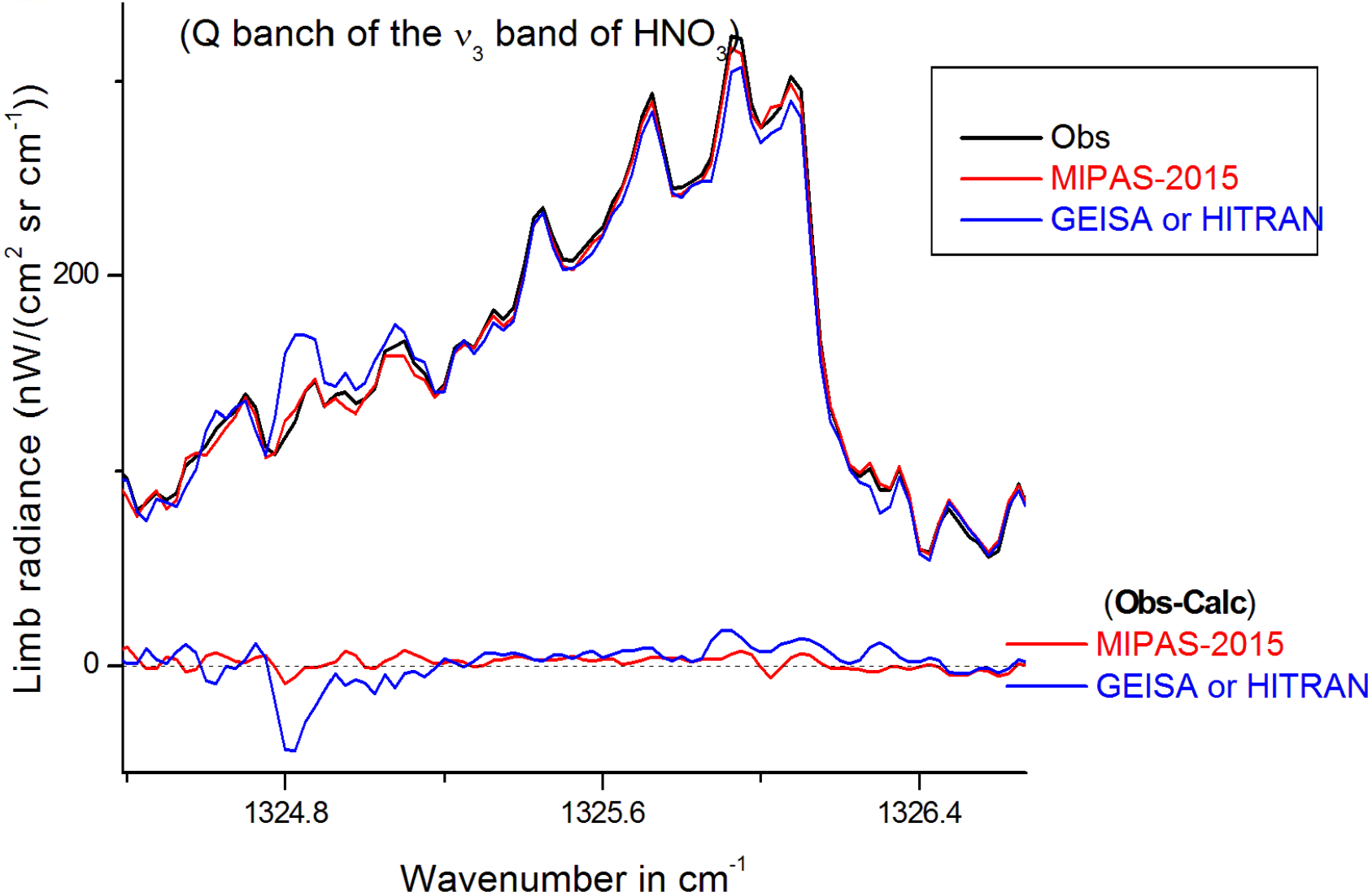
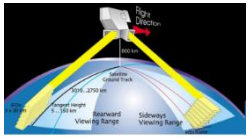
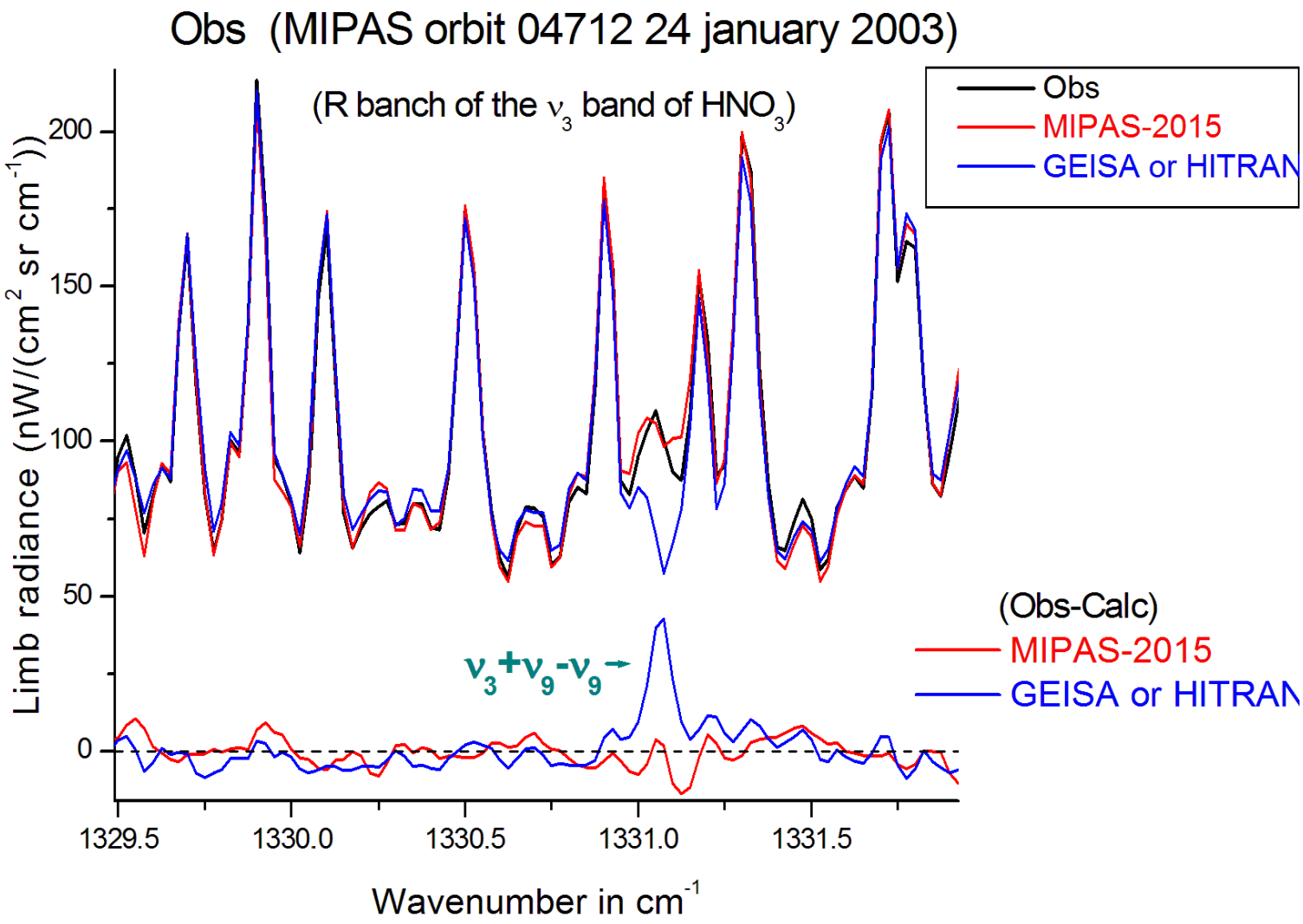


Obs (MIPAS orbit 04712 24 january 2003)







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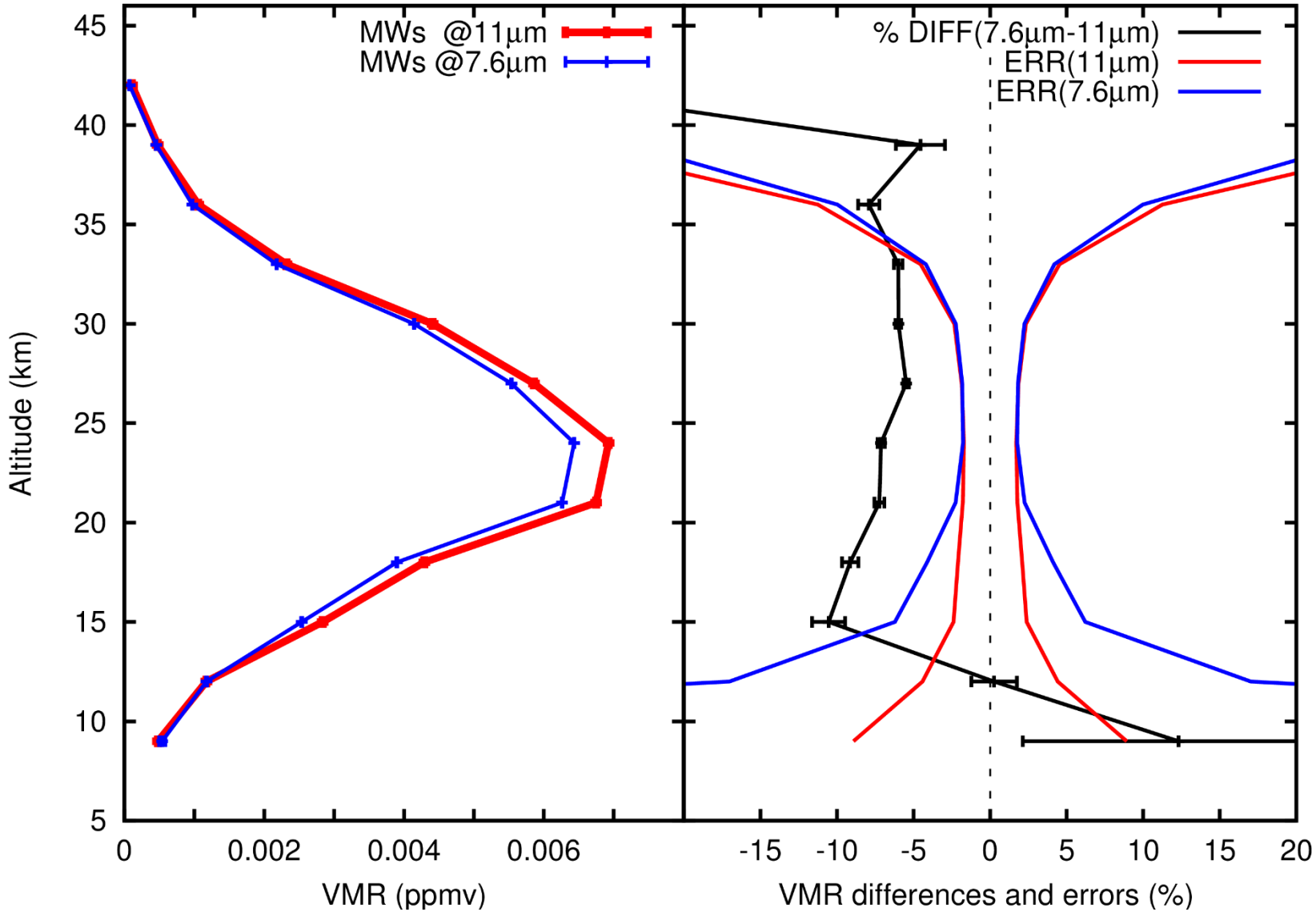
HNO_3 concentration profile (v.s. altitude) using the « old » database…



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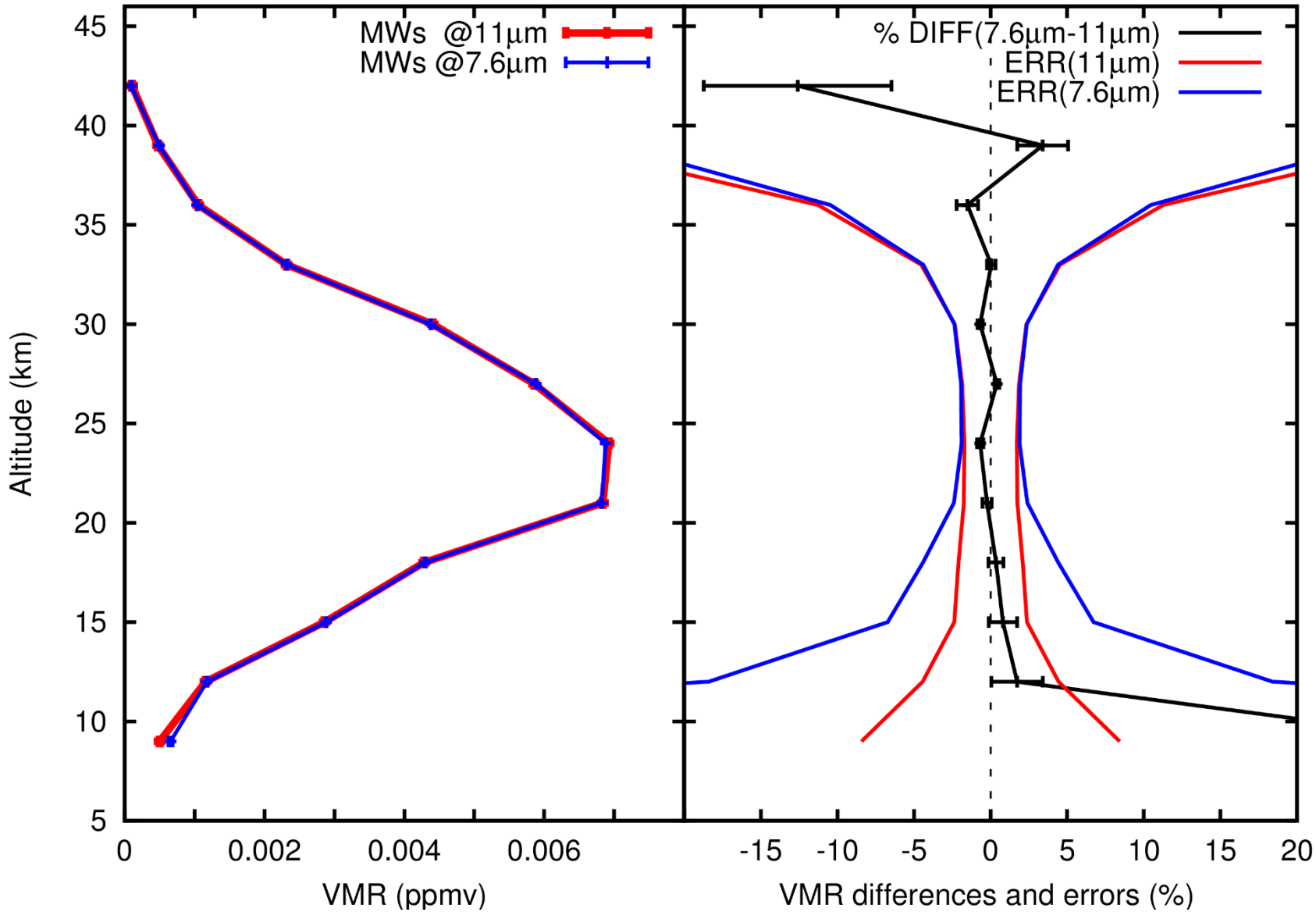
HNO_3 concentration profile (v.s. altitude) using the « new » database…



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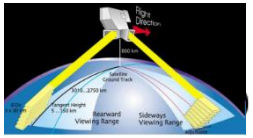
Conclusion

Improved line positions and intensities have been generated for the 7.6 µm spectral region of nitric acid. They were obtained relying on:

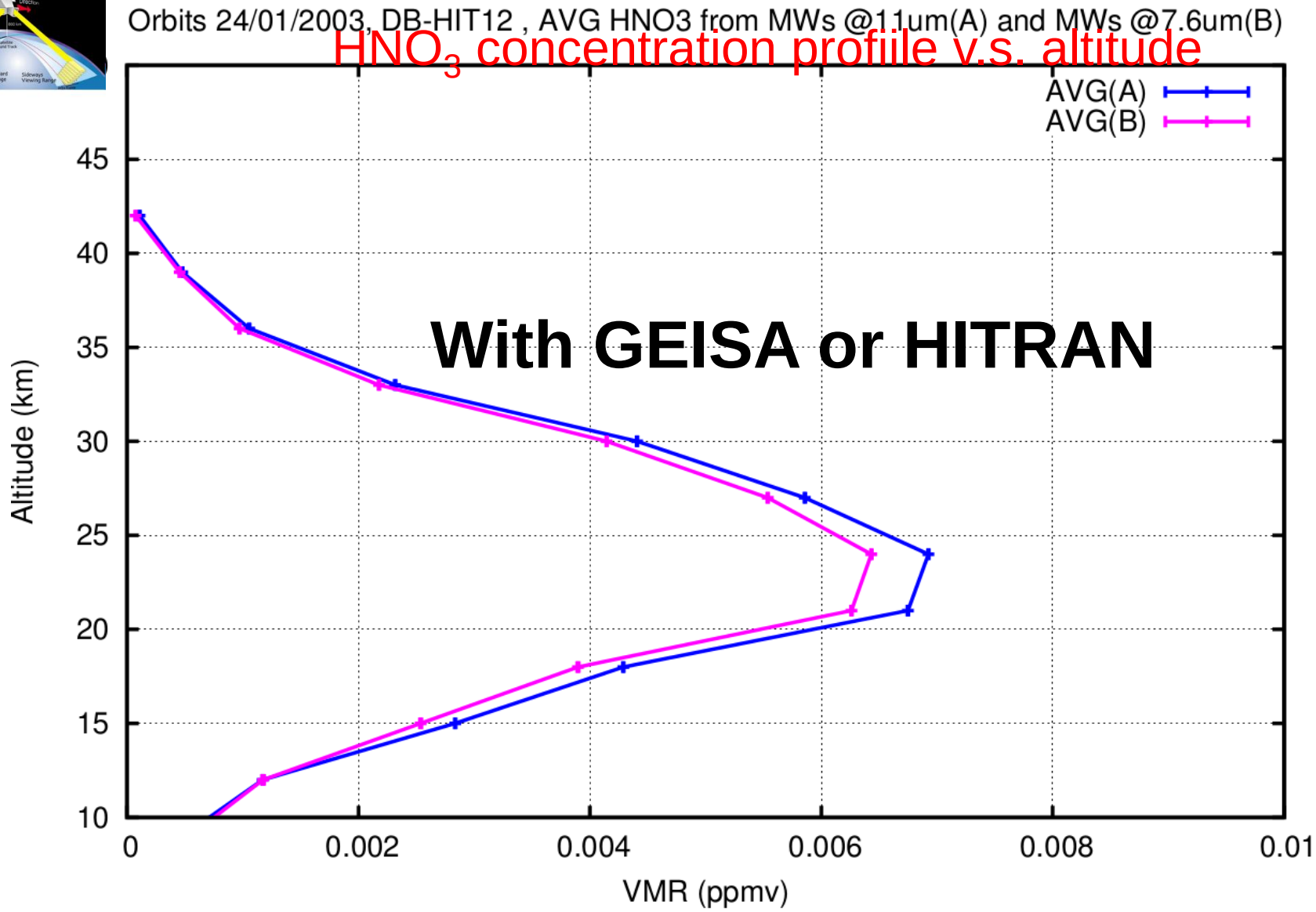
A recent reinvestigation of the nitric acid band system at 7.6 µm, followed by calibration of the intensities using:

- Line intensity measurements in laboratory conditions
- Validation using the PNNL cross sections
- Comparisons of HNO_3 concentration profiles retrieved from "Michelson Interferometer for Passive Atmospheric Sounding" (**MIPAS**) limb mission radiances in the 11 and 7.6 mm domains.

Financial support from CNES (Centre National de la Recherche Spatiale, France) is gratefully acknowledged
Part of this work was also performed within the **GDRI Hi*Res*MIR network**



HNO_3 concentration profiile v.s. altitude



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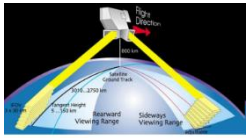

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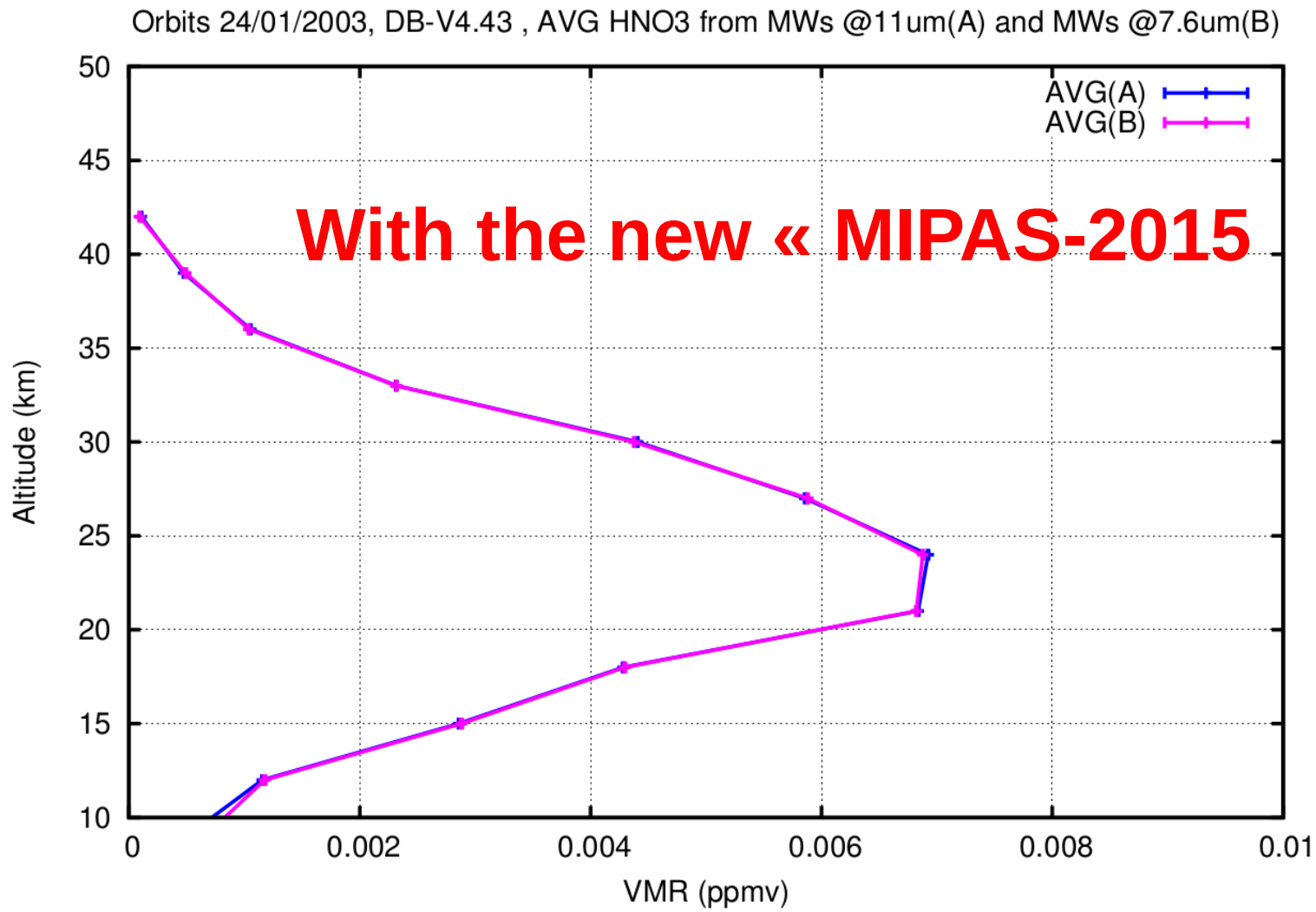

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Hamiltonian matrix

E_v= (cm^{-1})	1289.2	1293.2	**1303.1**	**1326.2**	1339.2	1342.9
sym:	A'	A"	A'	A'	A"	A"
	6^2	9^3	4^1	3^1	$5^1 9^1$	$7^1 8^1$
6^2	W		**Fermi+C**	**Fermi+C**		
9^3		W+Torsion	**B**	**B**	**strong Fermi**	
4^1	**Fermi+C**	**B**	**W**	**Anh**		
3^1	**Fermi+C**	**B**	**Anh**	**W**	**A+B**	**A+B**
$5^1 9^1$		**strong Fermi**	**A+B**	**A+B**	W	**A+B**
$7^1 8^1$			**A+B**	**A+B**		W