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MIPAS database: Validation of HNO$_3$ line parameters using MIPAS satellite measurements

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Abstract

Using new and accurate experimental results concerning the spectroscopic properties of the HNO_3 molecule as well as improved theoretical methods it has been possible to generate an improved set of line parameters for this molecule in the spectral range covered by the MIPAS (**M**ichelson **I**nterferometer for **P**assive **A**tmospheric **S**ounding) experiment. These line parameters, which have been validated using broadband atmospheric spectra recorded by MIPAS, have been included in the last version of the MIPAS spectroscopic database to be used for future processing of the MIPAS spectra.

1 Introduction

The goal of this study which concerns the line positions, the line intensities and the broadening coefficients of the HNO_3 molecule, is to provide the best and the most consistent possible set of line parameters for the nitric acid molecule in the spectral range covered by the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) (Endemann, 1999). In a previous effort which has led to the MIPAS_PF3.1 version of the database (Flaud et al., 2003a) the spectral parameters of the hot band $v_5+v_9-v_9$ were improved using both laboratory spectra and atmospheric spectra recorded by the Atmospheric Trace Molecule Spectroscopy experiment (Flaud et al., 2003b). Also to account for new results concerning the intensities in the $11.2\,\mu$m region (Toth et al., 2003) the line intensities of the v_5, $2v_9$, v_3 and v_4 bands were multiplied by the factor 0.879 (Flaud et al., 2003a). Since that time new results (Chackerian et al., 2003) have been obtained and a careful survey of the literature together with new calculations have shown that new improvements can be made concerning the nitric acid line parameters. Also using broad-band emission spectra of the atmosphere recorded by MIPAS it has been possible to validate the consistency of the HNO_3 line parameters in the various spectral ranges covered by the MIPAS experiment. In order to facilitate reading the manuscript we give in Table 1 the usual spectroscopic notation together with the nota-

tion used in the MIPAS database as well as in the HITRAN database, up to the 2000 release (Rothman et al., 2003), and the band centers of the cold bands and of some hot bands or combination bands which will be included in the new version PF3.2 of the MIPAS database.

2   Line positions

The line positions have been improved in two spectral regions:

- around 11.2 μm for the ν_5 and the $2\nu_9$ cold bands for which a new extended study has been performed allowing to improve noticeably the P- and R- branch modeling for the high values of the rotational quantum numbers (Perrin et al., 2004);

- around 8.3 μm for the $\nu_8+\nu_9$ and $\nu_6+\nu_7$ bands for which it appears that the HI-TRAN database is not using the best Hamiltonian constants and energy levels available in the literature (Perrin et al., 1999).

In the 11.2 μm region a new analysis was performed by mixing the existing microwave data and a re-analysis of a series of infrared spectra recorded with different HNO_3 amounts and at various temperatures. Then, using an Hamiltonian model and an intensity model taking fully into account the various vibro-rotational resonances as well as the torsional effects and the axis switching effect, a new line list of positions and intensities (as far as the absolute intensities are concerned see next section) has been generated allowing one to better model the HNO_3 spectrum (Perrin et al., 2004). In particular, as it can be seen in Figs. 1 and 2 of Perrin et al. (2004) the new line parameters lead to a significant improvement in the wings of the 11 μm window from which one should now be able to retrieve more accurately the CFC-11 (CCl_3F) and CFC-12 (CCl_2F_2) atmospheric species at ~850 and ~920 cm^{-1}, respectively.

In the 8.3 μm spectral region the line positions and the line intensities included in HI-TRAN come from a private communication (Goldman, A.: $\nu_8+\nu_9$ band, 1990; originally

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generated by Maki, A. G., based on Maki, A., 1989) and only the strongest band absorbing in this region, the $\nu_8+\nu_9$, was accounted for, whereas this band is in interaction with another combination band $\nu_6+\nu_7$. This interaction was treated properly by Perrin et al. (1999) who has provided more precise and meaningful Hamiltonian constants.

5 Using these constants allows one to generate a better set of energy levels and hence of line positions.

3 Line intensities

The determination of accurate line intensities for nitric acid is an overarching problem and is still controversial since several previous and ongoing efforts in various labora-

10 tories give results which do not agree. The first studies concerned measurements of the integrated band intensities (see Appendix A for the relationship between the integrated band intensity and the cold band intensity) at 11 μm using low resolution spectra (Goldman et al., 1971; Giver et al., 1984; Massie et al., 1985; Hjorth et al., 1987). They led to integrated strengths at 300 K varying from 483 to 630 $\text{cm}^{-2}\,\text{atm}^{-1}$ (see Table 2).

15 The situation was not better for individual line intensity measurements since the results obtained using a diode laser technique (Brockman et al., 1978) are on the average 20% lower than those using Fourier transform spectra (Perrin et al., 1993). Also there exists a discrepancy between the low and high resolution measurements. For example the band strength derived at 11 μm from Perrin et al. (1993) is about 30% weaker than

20 the value measured by Giver et al. (1984). All these discrepancies show the difficulty of the problem. Finally it is worth stressing that the recommendation adopted for the preparation of the HITRAN2K database (Rothman et al., 2003) was to normalize the ν_5 and $2\nu_9$ linelist generated in Perrin et al. (1993) to the Giver 11 μm band intensity after a proper hot band correction[1].

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[1] As explained in Appendix A, the integrated band intensity S_{tot} can be related to the intensity of the cold band through the "approximate" relationship: $S_{tot}(T)=S_{cold\,band}(T){\ast}Z_{vib}(T)$. For HNO$_3$

Very recently two new studies were devoted to the measurement of HNO_3 line intensities at $11\,\mu$m:

– an extensive set of HNO_3 individual line intensities (733 and 402 for the ν_5 and $2\nu_9$ bands, respectively) were measured using Fourier transform spectra (Toth et al., 2003). The goal was once again to measure accurate absolute line intensities in the $11\,\mu$m region while adopting special experimental precautions to minimize and/or estimate correctly the HNO_3 decomposition. This new list of line intensities is rather complete providing one with a much more extended set of measured intensities and a larger range of rotational quantum numbers than previously (Perrin et al., 1993). On the average these new line intensities are weaker than those in the HITRAN2K linelist: $INT_{HIT2K}/INT_{NEW}\sim1.13\pm0.06$. We used this set of data to normalize the HNO_3 intensities at $11\,\mu$m for MIPAS_PF3.1. However it should be noted that the HNO_3 linelist used for MIPAS_PF3.1 was the linelist generated by Perrin et al. (1993) whereas in MIPAS_PF3.2 we used the improved linelist generated by Perrin et al. (2004).

– Fourier transform absorbances were measured at Pacific Northwest National Laboratory (Chackerian et al., 2003) for different samples of nitrogen-nitric acid mixtures at a spectral resolution of $0.112\,cm^{-1}$ and used to determine integrated cross sections in various spectral domains. For the $11\,\mu$m region, the integrated intensity is about 6% lower than the value reported by Giver et al. (1984) and about 7% higher than the intensities derived from the measurements of Toth et al. (2003).

Now, given all these various results one has to decide which sets of experimental intensity data should be used in the MIPAS database. Such a problem is not easy. If one performs the arithmetic mean of the experimental results quoted in Tables 2 and 3 one gets for the integrated total band intensity at $11.2\,\mu$m (these experimental

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we use $Z_{vib}(296)=1.29952$

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results are the more numerous) the following value: $2.31(23) \times 10^{-17}\,\text{cm}^{-1}$/(molecule cm^{-2}). This value, if it has a significant physical meaning, corresponds to the value measured by Toth et al. (2003). Also it is worth stressing that in the validation of the MIPAS nitric acid measurements using far infrared data from the IBEX (Infrared Balloon EXperiment) experiment it is shown that this value gives the best agreement between the two sets of atmospheric measurements (Mencaraglia et al.). As a consequence we retained the Toth et al. (2003) intensities at 11.2 μm.

For the other spectral domains, except the domain 1160–1240 cm^{-1}, there is a reasonable agreement between the Chackerian data and the Giver data; it is then suggested to use (since they are more accurate) the values measured by Chackerian et al. (2003) corrected taking into account the fact that at 11.2 μm the intensities of Toth et al. (2003) have been used.

We do not understand the origin of the rather strong discrepancy in the 1160–1240 cm^{-1} spectral domain. One argument could be that some impurity (such as N_2O_5) was existing in the Giver's sample leading to a measured integrated band intensity larger than it would be for a pure nitric acid sample. For this reason we suggest to use in this spectral domain the integrated band intensity value of Chackerian et al. (2003) corrected as explained above. Table 3 gives the band intensities derived from the line parameters included in MIPAS_PF3.1 (Flaud et al., 2003a) and MIPAS_PF3.2. Also it is worth noticing that the HNO_3 line intensities included in the last issue of HITRAN have also been modified. We give then the band intensities of HITRAN2K (Rothman et al., 1998, 2003) as well of HITRAN04 (Rothman et al., 2005).

4 Broadening coefficients

4.1 Self-broadening coefficients

Although the HNO_3 self-broadening coefficients are rather large, their precise knowledge is not really important given the nitric acid atmospheric concentrations. It is

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suggested to use an average value of 0.807(70) cm^{-1}/atm at 296 K based on the 4 microwave measurements of Zu et al. (2002).

4.2 Air-broadening coefficients

The only existing line broadening calculation was performed some years ago (Tejwani and Yeung, 1978). Since this historical work, which was performed using the Anderson-Tsao-Curnutte theory, to our knowledge no other line broadening calculation has been performed. It is however interesting to notice that, even if the calculations cannot be considered as being accurate, they show a strong dependence of the broadening parameters with respect to the rotational quantum numbers.

As far as experiments are concerned there exist rather few broadening measurements for HNO$_3$ in the literature. The most accurate were performed in the microwave or submillimeter spectral regions since it is then possible to observe well isolated lines (Goyette et al., 1988, 1991, 1998; Zu et al., 2002; Perrin et al., 2005). Table 7 of Perrin et al. (2005) gives a list of air-broadening coefficients (these coefficients were either measured directly or derived from the N$_2$- and O$_2$-broadening coefficients through the classical relationship: $\gamma_{air}(T)=0.79\,\gamma_{N_2}(T)+0.21\,\gamma_{O_2}(T)$) for various pure rotational transitions in the microwave or millimeter region.

From Table 7 of Perrin et al. (2005), it is evident that there exists a rather clear rotational dependence of the broadening coefficients which need to be modeled. In the absence of accurate theoretical calculations it was decided (Perrin et al., 2005) to rely on an empirical model which reproduces as well as possible the observed line broadening parameters. It was then proposed to model the rotational dependence of γ_{air} as follows (see Perrin et al., 2005, for more details):

– For $J = (J' + J'')/2$ values $< J^{Max} = 34.5$

$$\gamma_{air}(J) = a_{air} + b_{air} \cdot J$$

with a_{air}=0.1280 cm^{-1}atm^{-1} and b_{air}=−0.0008635 cm^{-1}atm^{-1}

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– For J values $> J^{Max}$

$$\gamma_{air}(J) = \gamma_{air}(J^{Max}) = 0.982\ cm^{-1}/atm\ \text{(constant value)}$$

Figure 1 of Perrin et al. (2005) shows that the observed air-broadening coefficients are rather well modeled with the empirical formulae given above.

5 ## 4.3 Temperature dependence of the line widths

There exist even rather few measurements concerning the temperature dependence of the broadening coefficients (the only n-temperature dependence obtained is n_{N_2}=0.64 to 0.74 and n_{O_2}=0.67 to 0.84 for N_2 and O_2, respectively; Goyette et al., 1991, 1998). From these measurements no clear dependence with respect to the rotational quantum
10 numbers could be derived for the n_{air} coefficient (Perrin et al., 2005). An average value of 0.725(90) can be derived not far from the theoretical value of 0.75. For this reason we suggest to use this last value for the MIPAS_PF3.2 database.

5 Validation of the new database

The new HNO$_3$ line parameters were validated by comparing MIPAS observed limb-
15 emission radiances with radiances simulated using alternatively the new (PF3.2) and the old (PF3.1) line parameters. The MIPAS observed radiances considered in this validation work were selected among the observations acquired during the "well-characterized" ENVISAT orbits 2081 and 2082 (from 24 July 2002), with nominal tangent altitudes of 12 and 24 km. Since our forward model is not able to simulate the effect
20 produced by clouds located within the instrument field-of-view, the observed spectra were preliminarily filtered to exclude the measurements affected by clouds (Remedios et al., 2003). This filtering led to the selection of 55 spectra with nominal tangent altitude of 12 km and 55 spectra with nominal tangent altitude of 24 km. For each of the selected spectra the corresponding simulation was calculated using a modified version

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of the forward model implemented in the Geofit code (Carlotti et al., 2001). Beyond the capabilities of the Geofit forward model, the used model (Ridolfi, M.: Accurate broad-band forward model for MIPAS, private communication, 2004) includes some additional functionalities, namely:

5   – modeling of heavy species with tabulated cross-sections,

     – modeling of line-mixing, pressure-shift and self-broadening,

     – modeling of gaseous continua of H$_2$O, O$_2$ and N$_2$,

     – capability of handling spectral intervals as broad as the full bands measured by MIPAS.

10 In the forward model calculations the atmospheric composition and the observation geometry were assumed as follows:

     – Line-of-sight pointing angles, pressure, temperature, and Volume Mixing Ratio (VMR) of H$_2$O, O$_3$, HNO$_3$, CH$_4$, N$_2$O and NO$_2$ had the values retrieved by the MIPAS off-line processor (Ridolfi et al., 2000).

15   – The VMRs of other chemical species were set equal to their climatological value specific for the month of July and the latitude band to which the observations refer.

The differences between observations and the corresponding simulations (residuals) relating to the same nominal tangent altitude were averaged in order to reduce the disturbance of the measurement noise. The averaged residuals were then character-
20 ized in terms of both their average value and root mean square (RMS) calculated in pre-defined spectral intervals.

Table 4 presents the results of the analysis of the average residuals for the two considered altitudes: 12 and 24 km. First, it is easy to recognize that for the two selected spectral intervals in MIPAS bands A and B, the new database provides results better
25 than the old database in terms of both average value and RMS of the residuals. This

is confirmed by the plots presented in Figs. 1 and 2 from which one can see that the residuals are smaller when using the new HNO_3 line parameters. To go one step further we have tried to see if using the MIPAS spectra it could be possible to improve the consistency of the HNO_3 intensities in the different spectral ranges. For that we have assumed that the line intensities in band A were correct and we have multiplied the HNO_3 intensities in bands B and C by factors ranging from 0.96 to 1.04. In both bands the average differences are decreasing when multiplying the HNO_3 intensities by factors of the order 1.02 or 1.04. On the other hand the corresponding RMS are either stable (12 km) or increasing (24 km). In fact we think that, since the average differences include contributions from other atmospheric species which are not perfectly modeled, the decrease of the average differences when changing the HNO_3 intensities is due to the fact that the increased HNO_3 contributions compensate some deficiencies in the modeling of the other species. As a consequence it is not possible, with the present MIPAS spectra, to improve the consistency of the HNO_3 line parameters in the various spectral intervals covered by MIPAS. However one can say that the HNO_3 line intensities are consistent to within 4–5%. Table 5 gives detailed information on the new HNO_3 line parameters included in the last version of the MIPAS database (MIPAS_PF3.2).

6   Conclusion and update of the MIPAS database

Using the most recent and precise experimental results concerning HNO_3 spectroscopic parameters as well as improved theoretical method it has been possible to generate an improved set of line parameters for this molecule in the spectral range covered by the MIPAS experiment. These line parameters which have been validated using broadband atmospheric spectra recorded by MIPAS have been included in the last version of the MIPAS database MIPAS_PF3.2 and will be provided to the HITRAN database.

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Appendix A

The line intensity (in $cm^{-1}/(molecule\ cm^{-2})$) for a given vibration- rotation transition is given by the following expression:

$$k = (8\pi^3 v/3hc4\pi\varepsilon_0)\exp(-E_L/kT)[1 - \exp(-hcv/kT)]1/Z(T)| < \Psi''|\mu|\Psi' > |^2 \qquad (A1)$$

where $< \Psi''|\mu|\Psi' >$ is the matrix element of the transition dipole moment operator corresponding to the band, $Z(T)$ is the rotation-vibration partition function calculated at the temperature T. E_U and E_L are the upper and lower energy levels of the transition and v is the line position.

If the assumption that rotation and vibration can be separated is valid it is possible to sum all the rotational transitions belonging to a single band to get the vibrational band intensity given by:

$$S_{vib} = (8\pi^3 v_v/3hc4\pi\varepsilon_0)\exp(-E_L^v/kT)[1 - \exp(-hcv_v/kT)]1/Z_{vib}(T)| < \Psi_v''|\mu|\Psi_v' > |^2$$

$$(A2)$$

where v_v is the band center, $Z_{vib}(T)$ is the vibrational partition function and $|<\Psi_v''|\mu|\Psi_v'>|^2$ is the vibrational transition moment squared. For a given vibrational mode one has:

$$Z_{vib}(T) = \Pi[1/(1 - \exp(-E_v/kT))]$$

In the harmonic approximation $|<\Psi_v''|\mu|\Psi_v'>|^2$ is equal to $(v_i+1)\ (\partial\mu/\partial q_i)^2$ where $\partial\mu/\partial q_i$ is the change in dipole moment with respect to the normal coordinate q_i. Also in the harmonic approximation $E^v=v_i\omega_i$ and $v_v=v_0$ the band center of the cold band.

Accordingly, the intensity of a given band can be written as:

$$S_{v\leftarrow v+1} = (8\pi^3 v_0/3hc4\pi\varepsilon_0)\exp(-v\omega/kT)[1 - \exp(-\omega/kT)](v + 1)/Z_{vib}(T)(\partial\mu/\partial q_i)^2$$

$$(A3)$$

or

$$S_{v \leftarrow v+1} = (8\pi^3 v_0 / 3hc4\pi\varepsilon_0)[\exp(-v\varpi/kT) - \exp(-(v+1)\varpi/kT)](v+1)/Z_{\text{vib}}(T)(\partial\mu/\partial q_i)^2$$
(A4)

The integrated band intensity $S_{\text{tot}} = \sum S_{v \leftarrow v+1}$ is then given by:

$$S_{\text{tot}} = (8\pi^3 v_0 / 3hc4\pi\varepsilon_0)(\partial\mu/\partial q_i)^2 1/Z_{\text{vib}}(T) \sum [\exp(-v\varpi/kT) = (8\pi^3 v_0 / 3hc4\pi\varepsilon_0)(\partial\mu/\partial q_i)^2$$
(A5)

On the other hand the intensity of the cold band $S_{\text{cold band}}$ is equal to:

$$S_{\text{cold band}} = (8\pi^3 v_v / 3hc4\pi\varepsilon_0)(\partial\mu/\partial q_i)^2 [1 - \exp(-\varpi/kT)]1/Z_{\text{vib}}(T)$$
(A6)

Combining Eq. (A5) and Eq. (A6) leads to:

$$S_{\text{tot}} = S_{\text{cold band}} \times Z_{\text{vib}}(T)/[1 - \exp(-E_U^{v=1}/kT)] \sim S_{\text{cold band}} \times Z_{\text{vib}}(T)$$
(A7)

As a consequence it is possible to use Eq. (A7) to link the intensity of the cold band with the integrated band intensity knowing the vibrational partition function (for HNO_3 $Z_{\text{vib}}(296)=1.29952$ according to the band centers given in Table 1).

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Table 1. Notations and band centers.

Spectroscopic notation	MIPAS_PF3/HITRAN2K notation	Band center (cm^{-1})
Pure rotation	14–14	0.0
ν_9	19–14	458.229
ν_7	31–14	580.304
ν_6	26–14	646.826
ν_8	32–14	763.154
$3\nu_9 - \nu_9$	23–19[a]	830.675
$\nu_5 + \nu_9 - \nu_9$	24–19	885.425
ν_5	18–14	879.108
$2\nu_9$	21–14	896.447
$\nu_8 + \nu_9$	33–14	1205.707
$\nu_6 + \nu_7$	25–14[b]	1222.679
ν_4	17–14	1303.518
ν_3	27–14	1325.735
ν_2	16–14	1709.568
ν_1	15–14	3550.0

[a] Not included in HITRAN2K
[b] Not included in HITRAN2K and MIPAS_PF3.1 but included in MIPAS_PF3.2

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Table 2. Comparison of measured HNO$_3$ integrated band intensities in the 11.2 μm spectral region.

References	Integrated band intensity	
	cm^{-2} atm^{-1}	cm^{-1}/(molecule cm^{-2})
Goldman et al. (1971)	585	2.48(37)$\times 10^{-17}$
Giver et al. (1984)	637	2.57(13)$\times 10^{-17}$
Massie et al. (1978)	483	1.95(30)$\times 10^{-17}$
Hjorth et al. (1987)	541	2.18(33)$\times 10^{-17}$

The band intensities are given in the two most commonly used units.

Table 3. HNO_3 integrated band intensities.

Range (cm^{-1})	Assignment[a]	Integrated band intensity (cm^{-1}/(molecule cm^{-2}))					
		Chackerian et al. (2003)	Giver et al. (1984)	HITRAN 2K	MIPAS PF3.1	HITRAN 04	MIPAS PF3.2
820–950	18–14, 21–14, 23–19, 24–19	$2.424(65) \times 10^{-17}$	2.57(13)	2.564	2.266	2.267	2.308
1160–1240	33–14, 25–14	$1.263(81) \times 10^{-18}$	1.64(15)	1.592	1.587	1.589	1.235
1240–1400	17–14, 27–14	$5.09(18) \times 10^{-17}$	5.15(26)	4.780	4.201	5.095	4.960
1480–1570	$\nu_5 + \nu_6$, $2\nu_8$	$9.01(81) \times 10^{-19}$			0.	0.	0.
1640–1770	16–14	$5.71(19) \times 10^{-17}$	5.70(37)	5.693	5.693	5.693	5.693
2460–2710	$\nu_2 + \nu_5$, $2\nu_3$, $2\nu_4$	$1.42(20) \times 10^{-18}$		0.	0.	0.	0.

[a] The assignments are given in HITRAN2K notation when the bands are included in the existing databases, in spectroscopic notation otherwise.

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Table 4. Results of the comparison of MIPAS observed and simulated spectra for tangent heights of 12 and 24 km.

MIPAS database version	Scaling factor	MIPAS band	Spectral interval (cm^{-1})	Tangent Height: 12 km		Tangent Height: 24 km	
				Average difference[a] (r.u.)	RMS (r.u.)	Average difference (r.u.)	RMS (r.u.)
3.1	**1.0**	**A**	**840–930**	**209.00**	**54.40**	**20.76**	**22.52**
3.2	**1.0**	**A**	**840–930**	**203.06**	**51.02**	**17.85**	**20.04**
3.2	0.96	B	1270–1360	21.14	18.36	7.09	14.83
3.2	0.98	B	1270–1360	21.14	18.36	7.09	14.83
3.1	**1.0**	**B**	**1270–1360**	**24.53**	**20.62**	**11.72**	**15.09**
3.2	**1.0**	**B**	**1270–1360**	**20.08**	**17.81**	**5.6**	**15.08**
3.2	1.02	B	1270–1360	19.56	17.57	4.86	15.27
3.2	1.04	B	1270–1360	19.04	17.35	4.13	15.49
3.2	0.96	C	1670–1740	5.85	4.86	2.32	3.66
3.2	0.98	C	1670–1740	5.85	4.86	2.32	3.66
3.1	**1.0**	**C**	**1670–1740**	**5.71**	**4.83**	**2.09**	**3.66**
3.2	**1.0**	**C**	**1670–1740**	**5.61**	**4.82**	**2.01**	**3.66**
3.2	1.02	C	1670–1740	5.50	4.81	1.86	3.67
3.2	1.04	C	1670–1740	5.38	4.79	1.71	3.69

[a] r.u.: Radiance Units, nW/(cm^2 sr cm^{-1}).

Table 5. HNO$_3$ line parameters in MIPAS_PF3.2.

BAND[a]	XMIN[b]	XMAX[b]	SMIN[c]	SMAX[c]	STOT[d]	NB[e]
31 14	600.0003	613.6181	0.2425D-22	0.1652D-21	0.6853D-19	1200
26 14	615.0260	677.9806	0.2830D-22	0.8540D-21	0.1262D-17	8379
32 14	722.5331	809.9647	0.1211D-22	0.1090D-20	0.1242D-17	7101
23 19	769.6870	884.4384	0.3838D-24	0.6717D-21	0.5290D-18	17720
18 14	806.2073	963.9949	0.9830D-24	0.6600D-20	0.1027D-16	57108
21 14	806.7087	963.4347	0.9830D-24	0.3880D-20	0.7503D-17	55310
24 19	832.1165	942.9013	0.9870D-24	0.7000D-21	0.1067D-17	14521
27 14	1098.3760	1387.8490	0.1037D-22	0.3133D-19	0.2537D-16	21308
33 14	1133.5516	1258.8061	0.3706D-24	0.4448D-21	0.9284D-18	40119
25 14	1147.5084	1250.1141	0.3713D-24	0.3535D-22	0.1570D-20	559
17 14	1229.8670	1387.5610	0.1037D-22	0.1867D-19	0.1277D-16	19584
16 14	1650.0136	1769.9822	0.2119D-23	0.2119D-19	0.4381D-16	32340

[a]: Band notation in the HITRAN2K format (see Table 1)
[b]: Lower and higher line position for the band
[c]: Lower and higher line intensity for the band
[d]: Total band intensity
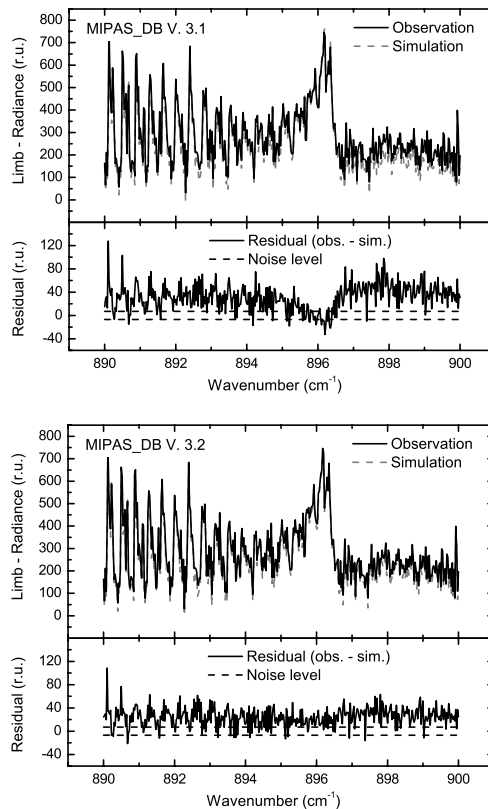[e]: Number of transitions for the band

Fig. 1. Comparison of observed and simulated MIPAS spectra in band A for an altitude of 24 km. The lower part of each panel gives the difference between the average of 55 spectra at 24 km tangent height acquired during orbits 2081 and 2082 (black) and the average of the corresponding broadband simulations (dash) with the old (upper panel) and the new (lower panel) HNO$_3$ spectroscopic line data. The MIPAS specified measurement noise level for the average in this spectral interval is about 7 nW/(cm^2 sr cm^{-1}).

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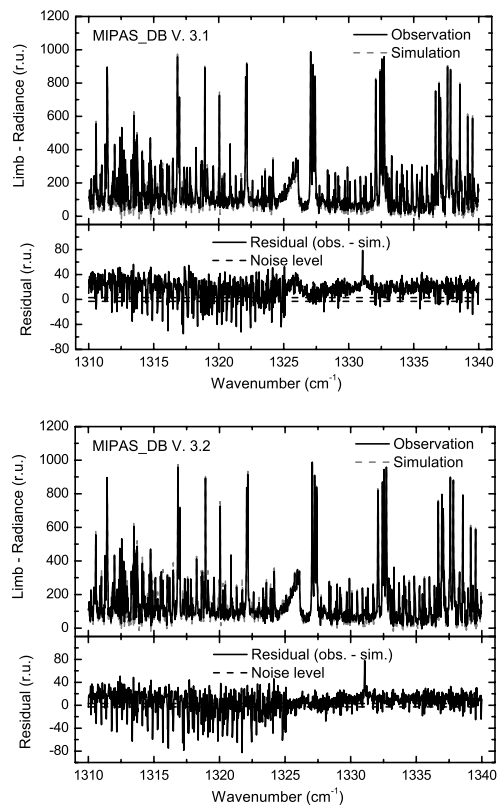
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Fig. 2. Comparison of observed and simulated MIPAS spectra in band B for an altitude of 24 km. The format is the same as in Fig. 1. The MIPAS specified measurement noise level for the average in this spectral interval is about 3 nW/(cm^2 sr cm^{-1}).

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