

A Spectroscopic Database for MIPAS

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ABSTRACT

The analysis and interpretation of atmospheric limb spectra such as those recorded by MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) require good knowledge of the molecular parameters of the atmospheric species. This is why a spectroscopic database dedicated to the MIPAS experiment has been generated. The new spectroscopic parameters were first validated through a comparison between atmospheric simulations and ATMOS (Atmospheric Trace Molecule Spectroscopy) measurements. Then, whenever possible, a further validation using MIPAS measurements has been made. The spectroscopic parameters which are reviewed in this paper are those of the main target species: water vapour (H₂O), carbon dioxide (CO₂), ozone (O₃), methane (CH₄), nitrogen dioxide (NO₂) and nitric acid (HNO₃).

INTRODUCTION

Since the quality of line-by-line radiative transfer calculations depends on the availability of comprehensive and accurate molecular spectral line data compilations, various atmospheric databases, which result mainly from experimental and theoretical laboratory studies, were generated. They are periodically up-dated and, among them, there are currently three widely used spectroscopic databases:

- HITRAN (High-resolution TRANsmission) molecular absorption database [1];
- GEISA (Gestion et Etude des Informations Spectroscopiques Atmospheriques) database [2];
- JPL (Jet Propulsion Laboratory) catalogue and atlas of microwave and submillimeter transmission [3].

Since we are dealing with infrared measurements, the HITRAN96 database, which was the last version of HITRAN well documented, was adopted as a starting point to generate a database dedicated to the MIPAS experiment.

The 1996 HITRAN edition contains line parameters for 37 molecules, each of which is assigned an identification number (the numbering of the species is simply by chronological entry into HITRAN database). The parameters include molecule and isotope code number, positions in cm⁻¹, line intensities in cm⁻¹/(molecule·cm⁻²) at 296K, the weighted transition moment squared in Debye², air-broadening and self-broadening coefficients in cm⁻¹/atm at 296K, lower state energies in cm⁻¹, the temperature-dependence exponent of the air-broadening coefficients *n*, the air-broadened pressure shifts in cm⁻¹/atm at 296K, the upper and lower vibrational state index codes, the upper and lower rotational quantum numbers and the accuracy and the reference code numbers.

Also when line parameters are difficult to obtain (heavy molecules such as chlorofluorocarbons, N₂O₅, ClONO₂, ...), absorption cross-section data are given as an alternative.

TOWARDS A MIPAS DATABASE

In this paper the molecules for which the spectroscopic database is reviewed are the main target species that are retrieved from MIPAS measurements. This section describes then in a synthetic manner the recommendations and the modifications made to HITRAN96 in order to generate a dedicated MIPAS database (a detailed description can be found in [4]). Also some information is given about the validation of the data using ATMOS or MIPAS atmospheric spectra. Finally it is worth noting that changes not described here were also performed for non target species such as HOCL, COF₂ (see ref. [4] for details).

Water vapour (H₂O)

In our study, four sets of spectral parameters were taken into account for the H₂O molecule:

- the HITRAN 96 parameters denoted in the following as HIT96,
- the HITRAN 2K parameters denoted in the following as HIT2K,
- the updated parameters that can be found on the HITRAN website and which are denoted in the following as HIT01,

- the parameters derived for the main isotope from recent calculations using new experimental data [5] and a new theoretical model [6-8] and denoted in the following as CAL02.

As far as the less abundant water vapor isotopic species are concerned it was shown [4] that the HIT01 file is the most complete and accurate.

As far as the main isotopic species is concerned it was first shown [4] that the HIT01 file was more precise than HIT96. Then simulations of ATMOS spectra at 23km were performed using HIT01 and CAL02 and Table 1 presents a statistical analysis of the residuals obtained using these two sets of data. The statistics was made for 3 cm⁻¹ wide intervals covering the spectral MIPAS bands, excluding those regions in which the observed ATMOS spectra were opaque. For each spectral band three columns are given. The first column shows the spectral intervals of the band in which the statistics was performed, the second column shows the RMS of residuals using the two different sets of data, and the third column shows the number of intervals where the new data (in this case CAL02 data) give better results, compared with the total number of intervals.

Table 1
Comparison of simulated and observed ATMOS spectra using
CAL02 and HIT01 data for the H₂¹⁶O molecule at 23 km

Band	Spectral domain (cm ⁻¹)	RMS · 10 ⁻² CAL02/HIT01	Number of intervals where CAL02 give better results
A	745-970	2.3581/2.4941	45 of 75
AB	1041-1170	1.9230/1.9229	16 of 38
B	1215-1500	2.2379/2.2357	29 of 91
C	1573-1750	2.6402/2.6583	32 of 59
D	1820-2240	1.8160/1.8444	85 of 160
Total	-	2.1275/2.1644	207 of 423

Except the results in band AB and B in which the overall RMS of the residuals are comparable, considering the total effect it is possible to conclude that there is some indication that the CAL02 data set is likely to give better results than HIT01.

As a conclusion the H₂O line parameters included in the MIPAS database are: (i) the line parameters of HIT01 for all isotopic variants of H₂O except H₂¹⁶O, (ii) the line parameters of CAL02 for H₂¹⁶O and (iii) the line parameters of HIT01 for the band HIT6-3 of the main isotope.

Carbon dioxide (CO₂)

The last version of the HITRAN database (HITRAN2K) includes for carbon dioxide the same spectral parameters than HITRAN96 [1]. These data were mainly derived using the DND (Direct Numerical Diagonalization) method [9]. However recently an analogous method based on global fits of observed frequencies and line intensities using the effective operator approach [10-17] was developed and used to generate new line parameters for the four most abundant isotopic species of carbon dioxide, namely ¹²C¹⁶O₂, ¹³C¹⁶O₂, ¹⁶O¹²C¹⁸O and ¹⁶O¹²C¹⁷O (Carbon Dioxide Spectroscopic Databank (CDS)).

To check the quality of the new CO₂ spectral parameters the same strategy as for H₂O was applied. More precisely first the CDS data and the HITRAN96 data were compared and then both sets of data were used to simulate the ATMOS spectra.

The comparison of the two databases [4] showed that the CDS database is more extensive and includes bands which are not included in HITRAN. However it is to be noted that generally the new bands are rather weak.

The comparisons with the ATMOS spectra were performed for three tangent altitudes, namely 15, 27 and 43 km to estimate the effects in the change of the weak, medium and strong lines. The comparisons were done using on the one hand the HITRAN database and on the other hand the CDS database complemented by the HITRAN line parameters for the isotopomers of CO₂ not accounted for in CDS. As in the case of the analysis of the water vapor, the statistics was made for 3 cm⁻¹ wide intervals and for each spectral band three columns are given. From this comparison [4] it appears that, even if the percentage of intervals in which the new data are better is not decisive, the overall RMS in all bands together is better with the new data (CDS) than with the HITRAN data. Also a more detailed analysis [4] showed that it is difficult to discriminate between the two sets of data except for band D for which the new set gives significantly better agreement.

The new data were also validated using MIPAS data. More precisely p, T retrievals were performed using orbit 2081 and the results are presented in Table 2. In this table four columns are given: the first column shows the altitude for which pressure and temperature were retrieved, the

second column shows the number of scans along the orbit for which the chi-squared values have been averaged, the third and fourth columns show the average chi-squared values derived from retrievals using on the one hand the previous spectroscopic data (HITRAN2K) and on the other hand the new data (CDS). The last row of [Table 2](#) shows the total chi-squared values averaged over all altitudes using the two different databases. It is clear that at all altitudes (except 24 km) the CDS data give better results.

Table 2
Average chi-squared values as a function of altitude obtained when retrieving p, T profiles, using the HITRAN2K and the CDS database (Orbit 2081 of MIPAS)

ALT (km)	No scans	HITRAN2K	CDS
68	50	2.47	2.47
60	50	2.46	2.45
52	51	3.93	3.91
47	45	3.15	3.07
42	51	6.33	6.27
39	51	12.26	12.11
36	51	9.75	9.64
33	51	12.27	12.25
30	51	10.84	10.82
27	51	8.73	8.71
24	51	14.78	14.85
21	49	1.81	1.79
18	49	2.82	2.81
15	49	4.64	4.51
12	49	4.28	4.12
Total		6.05	6.01

Established that the CDS database is consistent from a spectroscopic point of view since it results from global fits, that the comparison with the ATMOS spectra shows either analogous simulations or better ones (in band D) and that better results are obtained with MIPAS spectra, it is possible to conclude that CDS set gives better results than HITRAN. As a conclusion the CO₂ line parameters included in the new version of the MIPAS database are (i) the line parameters of CDS for the four most abundant isotopic variants of CO₂ (¹²C¹⁶O₂, ¹³C¹⁶O₂, ¹⁶O¹²C¹⁸O and ¹⁶O¹²C¹⁷O) and (ii) the line parameters of HITRAN for the other isotopic variants of CO₂.

Ozone (O₃)

The ozone molecule ¹⁶O₃ was recently the subject of extensive laboratory studies in the 10 μm region in order to improve line positions and intensities. This spectral region is extensively used for atmospheric retrievals by several instruments and in particular by MIPAS. A comparison between four sets of experimental data obtained by four different groups [18-21] was performed and the following conclusions were reached: (i) the four sets are highly consistent on a relative basis (agreement better than 2%) and (ii) the absolute intensities of three sets [19-21] are consistent within a dispersion of ~0.8% (1σ standard deviation of ~1.7%), whereas the intensities of the fourth set [18] are ~4% higher.

Considering these results [22], a new line list was generated for the two bands absorbing at 10 μm, namely ν₁ (HIT4-1) and ν₃ (HIT5-1). The relative intensity between HITRAN96 and the new calculations is on average 1.044(35) for ν₁ (HIT4-1) band and 1.035(14) for ν₃ (HIT5-1) band. Further tests were performed using ATMOS measurements. As for the water vapour and carbon dioxide cases, the ATMOS broadband spectra corresponding to MIPAS bands have been divided into 3 cm⁻¹ spectral intervals covering the overall spectral range. The comparison between ATMOS measurements and the atmospheric simulations was performed in each spectral interval for both the HITRAN96 parameters and the new line list parameters. The statistical comparisons at two different tangent altitudes, at about 34 km and 26 km, shows that for more than 90% of the intervals the new line list gives better results [22]. This indication denotes that, on a relative basis, the new line list parameters allow to perform better atmospheric simulations than HITRAN96.

As a consequence of these tests, it was decided to include the new data of the cold bands ν₁ (HIT4-1), ν₃ (HIT5-1) and ν₂ (HIT2-1) in the MIPAS database, complemented by the intensities of all

the other bands in HITRAN96 (hot bands, isotopic species) divided by 1.04 to account the change in the absolute intensities of the cold bands [4].

The last versions of the HITRAN database do not include any spectral parameters for the ozone isotopic species in the 4.8 μm . There are 3 interacting bands, namely $\nu_1 + \nu_3$, $2\nu_1$ and $2\nu_3$, absorbing around 4.8 μm . Recently these bands were studied at high resolution for the $^{16}\text{O}^{18}\text{O}^{16}\text{O}$ and $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ species [23] and the $^{16}\text{O}^{17}\text{O}^{16}\text{O}$ and $^{16}\text{O}^{16}\text{O}^{17}\text{O}$ species [24]. The spectroscopic analyses were performed taking into account the vibro-rotational resonances affecting the energy levels and the line intensities. However, the main problem is that only the $\nu_1 + \nu_3$ bands were observed (they are strong bands) whereas the two other bands were not. As a consequence, the line positions and intensities for the weak $2\nu_1$ and $2\nu_3$ bands are not precise and these bands were not introduced in the MIPAS database. On the other hand it is worth stressing that, since the line intensity calculations for the $\nu_1 + \nu_3$ bands of $^{16}\text{O}^{18}\text{O}^{16}\text{O}$, $^{16}\text{O}^{16}\text{O}^{18}\text{O}$, $^{16}\text{O}^{17}\text{O}^{16}\text{O}$ and $^{16}\text{O}^{16}\text{O}^{17}\text{O}$ were performed using the transition moments of the main isotopic species $^{16}\text{O}_3$, their absolute intensities cannot be assumed at this stage to be better known than 30-40% (conservative estimation). The corresponding line parameters have however been introduced in the MIPAS line list since the lines are observable in the atmospheric spectra.

Methane (CH_4)

The file 06.HIT01.par, which is not included in HITRAN2K, and which has been recently updated by L. Brown (JPL, USA) is a total replacement of the 1996 spectroscopic parameters for the three isotopic species of methane ($^{12}\text{CH}_4$, $^{13}\text{CH}_4$, CH_3D). In this new file the most recent studies for all three isotopes have been merged and include line shape assessments.

Many lines weaker than $1 \times 10^{-24} \text{cm}^{-1}/(\text{mol} \cdot \text{cm}^{-2})$ were also included for the benefit of planetary and stellar applications. The main changes are in the region between 850 cm^{-1} and 4810 cm^{-1} .

Recently, the IMK group [25] reported that in the 1202 cm^{-1} spectral region the fit quality of ground based FTIR atmospheric spectra was decreased in terms of spectral residuals when using the updated spectral parameters. For some lines, there were problems with the new pressure shifts and to a lesser extent with the new pressure broadening coefficients. It turned out that some of the parameters were inadvertently changed and a new line list was provided [26].

These new spectroscopic parameters have been compared with the HITRAN96 parameters using ATMOS spectra, in the 1050-1899 cm^{-1} and 2149-2500 cm^{-1} spectral regions (divided in 3 cm^{-1} wide intervals). Table 3 shows the results of the statistical analysis performed through the comparison of ATMOS spectra at altitude of about 23 km, and confirms that the new data are more reliable.

Table 3
Comparisons of simulated and observed ATMOS spectra using HITRAN96
and the new methane data at 23.3 km

Band	Spectral domain (cm^{-1})	Number of intervals where the new data set gives better results
AB	1065 - 1170	34 of 35
B	1215 - 1278 & 1350 - 1500	45 of 71
C	1570 - 1690	27 of 36
D	2123 - 2258	30 of 46

Accordingly in the MIPAS database the HITRAN96 parameters of CH_4 have been replaced by the new spectroscopic parameters [26].

Nitrogen dioxide (NO_2)

The 6.2 μm region is widely used to retrieve atmospheric NO_2 profiles from balloon borne or satellite instruments since it corresponds by far to the strongest absorption of this molecule: ν_3 (HIT5-1) band. In the infrared the vibration-rotation lines of NO_2 appear as doublets, due to the spin-rotation interaction. This spin-rotation interaction can be treated either through a perturbation method or directly, the latter method giving much more accurate results.

In HITRAN96 only two bands appear in the 6.2 μm region: the fundamental ν_3 (HIT5-1) band [27] and the first hot band $\nu_2 + \nu_3 - \nu_2$ (HIT8-2) [28]. No other hot band is available and this prevents the possibility of dealing with possible Non-Local Thermodynamic Equilibrium (NLTE) phenomena. Based on recent spectroscopic studies, new spectral parameters were generated and included in the MIPAS database: the first hot band $\nu_2 + \nu_3 - \nu_2$ (HIT8-2) [29], the band $\nu_1 + \nu_3 - \nu_1$ (HIT13-4) [30], the

bands $2\nu_3 - \nu_3$ (HIT14-5) and $2\nu_2 + \nu_3 - 2\nu_2$ (HIT11-3) [31], the bands $3\nu_3 - 2\nu_3$ (HIT27-14) and $2\nu_2 + 2\nu_3 - (2\nu_2 + \nu_3)$ (HIT23-11) [32].

Recently a number of studies have dealt with the line widths of the NO_2 molecule. A careful comparison of the various studies [33- 38] was made [4] and we suggest, until new experimental or theoretical results are available, to use in the MIPAS database:

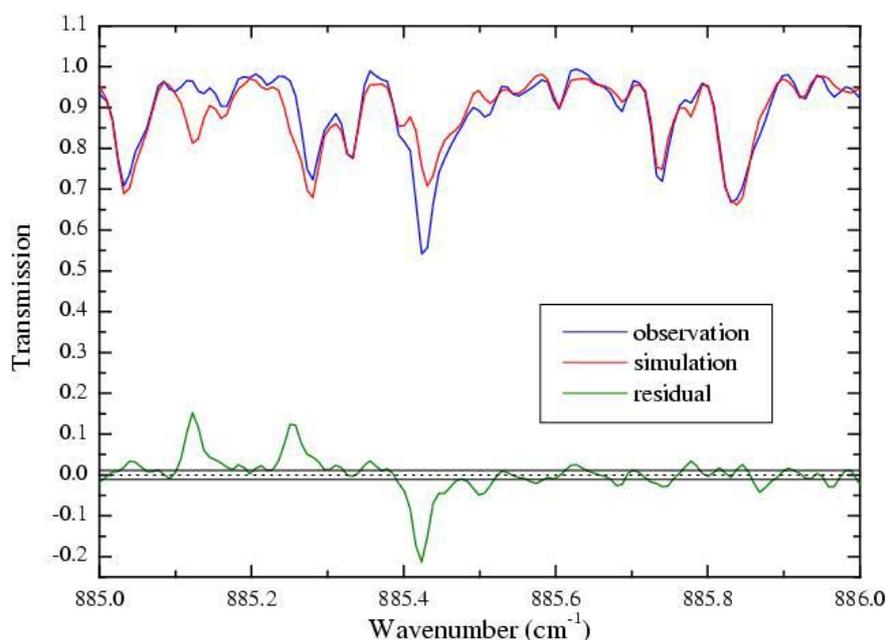
$$\gamma_{\text{air}}(296\text{K}) = 0.074/0.71 * \gamma_{\text{air}}(\text{HITRAN01}), n = 0.97$$

Also instead of no value, HITRAN01 gives a value of $0.095 \text{ cm}^{-1}/\text{atm}$ for the self-broadening coefficient. This value seems reasonable and we have introduced it in the MIPAS database.

Nitric Acid (HNO_3)

The $11 \mu\text{m}$ bands of nitric acid are widely used by infrared remote sensing techniques since they are centered in an atmospheric window and therefore present the advantage of being relatively free from interfering lines from other species. The $11 \mu\text{m}$ spectral region involves mainly two interacting cold bands ν_5 and $2\nu_9$ and two hot bands $\nu_5 + \nu_9 - \nu_9$ and $3\nu_9 - \nu_9$ located at 885.424 cm^{-1} and 830.6 cm^{-1} respectively.

A simulation of the ATMOS spectra using HITRAN96 demonstrated that in particular around 885 cm^{-1} the agreement with the observations was rather poor as indicated in [Fig.1](#).



[Figure 1](#)
Simulation of an ATMOS spectrum around 885.5 cm^{-1} using HITRAN96

A careful analysis showed that this was due to very poor spectral parameters for the hot band $\nu_5 + \nu_9 - \nu_9$ of HNO_3 (HIT24-19). A new version of the spectral parameters is available in HITRAN2K, but, even if the residuals are improved, the agreement proved to be far from satisfactory (line shift of the absorption peak and shape of the absorption peak not correct).

It was then decided to perform an improved theoretical modelling of the hot band [39] that led to an excellent agreement between the laboratory observations and calculations. This improvement on the HNO_3 (HIT24-19) band parameters was confirmed by the comparison between the ATMOS observations and the atmospheric simulations made with the new spectroscopic data, as illustrated in [Fig.2](#).

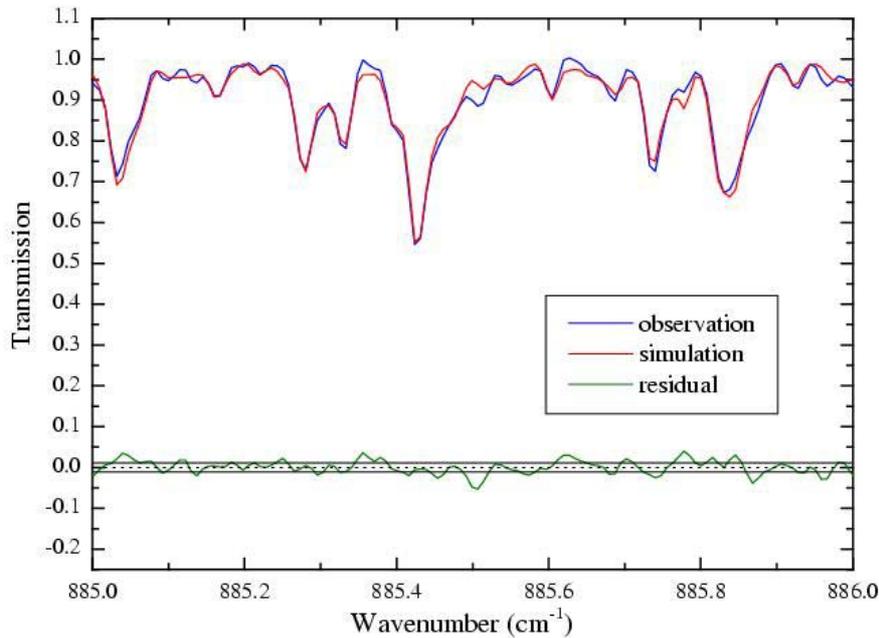


Figure 2
Simulation of an ATMOS spectrum around 885.5 cm^{-1} using
the new parameters for the hot band $\nu_5 + \nu_9 - \nu_9$

The improvement of the residual is evident when compared to the previous results shown in [Fig.1](#).

Accordingly the new spectroscopic parameters for the hot band $\nu_5 + \nu_9 - \nu_9$ of HNO_3 (HIT24-19) band were included in the MIPAS database. The $3\nu_9 - \nu_9$ band (HIT23-19) was also calculated and included in the MIPAS database.

However, recent simulations of the MIPAS spectra [4] using these new data showed that there was still an inconsistency between the spectral parameters of this hot band and those of the cold bands absorbing in the same spectral region, namely ν_5 (HIT18-14) and $2\nu_9$ (HIT21-14). A careful analysis, for different altitudes and sequences of the microwindow HNO30006 ($885.1 - 888.1 \text{ cm}^{-1}$), which contains this hot band, showed that either the hot band intensity is too weak by about 13% or that the cold band intensities (which are those of HITRAN2K) are too large by the same amount.

New measurements of HNO_3 line intensities were performed at JPL [40], providing a total band intensity of $560(5\%) \text{ cm}^2/\text{atm}$ for the two cold bands ν_5 and $2\nu_9$, value lower than the value of $637 \text{ cm}^2/\text{atm}$ used in the HITRAN database. Given the quality of the spectroscopic studies of the authors of the recent paper it has been decided to use this new value for the total band intensities of the cold bands at $11 \mu\text{m}$. Accordingly the individual line intensities of the bands ν_5 (HIT18-14), $2\nu_9$ (HIT21-14), ν_3 (HIT27-14) and ν_4 (HIT17-14) have been multiplied by the factor 0.879. The consistency of the cold bands and the hot band line parameters was checked using preliminary MIPAS data. [Fig.3](#) shows the percentage difference between retrievals obtained with the previous band intensities and the new values for the orbit 2081 of MIPAS. It is important to notice that this change in the line intensities leads to a more or less systematic increase of the HNO_3 abundances of about 13%.

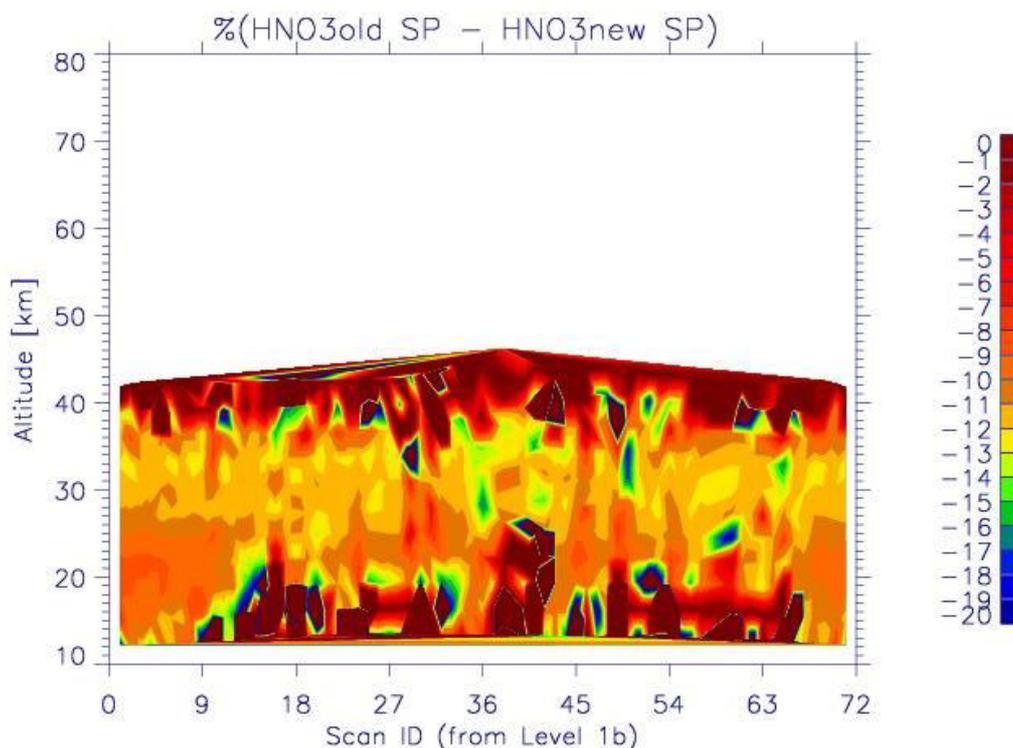


Figure 3
Percentage difference between retrievals from orbit 2081 of MIPAS using the old and the new intensities for the hot band $\nu_5 + \nu_9 - \nu_9$

CONCLUSION

This paper gives an overview of the MIPAS database as of January 2003 (version 3.0 of the spectroscopic database) noting that the MIPAS operational retrieval code [41] is presently using an intermediate version (2.0) that does not include some of the most recent updates. The efforts were mainly devoted to the improvement of the line parameters of the CO_2 molecule (pressure and temperature profiles) and of the target species (O_3 , H_2O , CH_4 , HNO_3 , NO_2). The paper discusses mainly the previously unpublished line parameters and how they were assessed. Finally, even if we are aware that no compilation is perfect, we hope that the new database represents an improvement for the analysis and retrieval of MIPAS spectra.

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