Technical Note on:

MIPAS_03: an update of the MIPAS.PF2 database

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1. Reference documents

[RD1]	TN-LPM-IROE-001, Issue 1a Title: “Spectroscopic Database Updates”

2. Introduction

A dedicated spectroscopic database for MIPAS experiment has been built starting from HITRAN96 with additional improvements obtained through new laboratory studies or new calculations. The first version of the MIPAS database which is called *hitran_mipas_pf2.0* includes updates for the HOCl, HNO_3, O_3, NO_2, CH_4 and H_2O molecules that have been validated performing comparisons between atmospheric simulated spectra and atmospheric ATMOS spectra [RD1].

This report describes the new version of the spectroscopic database called *hitran_mipas_pf3.0* (referred below as *MIPAS_03*) through the changes that have been done to hitran_mipas_pf2.0 in order to further improve the actual parameters for the MIPAS experiment using new laboratory spectroscopy or new calculations. Some updates have been validated against ATMOS observations, other using preliminary MIPAS measurements.

This report is written molecule by molecule because the recommendations and changes are different for each molecule. The molecules for which the spectroscopic database is reviewed are CO_2, HNO_3, CH_4, NO_2, O_3 and COF_2.

3. Updates of MIPAS database hitran_mipas_pf2.0

3.1. Carbon dioxide CO_2

The last version of the HITRAN database (HITRAN2K) includes for carbon dioxide the same spectral parameters as HITRAN96 [1]. These data were mainly derived using the DND (Direct Numerical Diagonalization) method [2]. However more recently an analogous method based on global fits of observed frequencies and line intensities using the effective operator approach [3-10] was developed and used to generate new line parameters for the four most abundant isotopic species of carbon dioxide, namely $^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{16}O^{12}C^{18}O$ and $^{16}O^{12}C^{17}O$. Thanks to the courtesy of J.-L. Teffo [11], this new line parameters were made available to us.

To check the quality of the new CO_2 spectral parameters the same strategy as for H_2O or CH_4 was applied [RD1]. More precisely we have first compared the new data with the HITRAN96 ones and then both sets of data were used to simulate the ATMOS spectra.

SUMMARY OF THE NEW CO_2 DATA AND COMPARISON WITH HITRAN

Table 1 in the annex gives a summary of all the bands included in the new Carbon Dioxide Spectroscopic Databank (CDSD) together with the same information for the HITRAN data. For each band it gives, for the spectral interval of interest for MIPAS (600-2500 cm^{-1}), the name of the band (in HITRAN notation), the minimum and maximum wavenumbers of the lines of the band, the minimum and maximum line intensities, the band intensity (sum of all the lines of the band appearing in the databases) and the number of lines of the band.

In CDSD both the numbers of bands and of lines are larger than in HITRAN showing that the former database is more extensive and includes bands, which are not included in HITRAN. However, it should be noticed that generally the new bands are rather weak. Table 2 in the annex summarizes the results of the comparison between the intensity ratios of all the lines common to the two databases. In this table we give the name of the vibrational band in HITRAN notation, the number of lines common to the two databases, the mean intensity ratio (i.e. the average value of the ratios for all the lines) and the corresponding standard deviation.

One can make the following comments:

- As already stressed a number of bands are present in CDSD and not in HITRAN. In this case a zero value is given for the intensity ratio.
- For a majority of bands the ratios are not very different of unity with a small standard deviation, therefore the two databases are in satisfactory agreement.
- For some bands the ratios are not far from unity but the standard deviation is no longer small: there is a discrepancy between the two databases. For example the R-lines exhibit a ratio larger than unity while the P-lines lead to a ratio smaller than unity, therefore the average is around unity.
- Finally for some bands the average ratio is no longer equal to unity showing a clear disagreement.

Since the two databases are different, it is worthwhile and necessary to check them by simulating ATMOS spectra and making comparisons.

COMPARISON WITH ATMOS SPECTRA

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 CDSD database complemented by the HITRAN line parameters for the isotopomers of CO_2 not accounted for in CDSD.

The results of the simulation of the ATMOS spectra are shown in Tables 1 where a statistical analysis of the residuals was performed comparing CDSD and HITRAN at the three altitudes. As in the case of the analysis of the other species [RD1], 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 and in which the effect of atmospheric continuum was significant. 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 CDSD) give better results, compared with the total number of intervals. From this comparison 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 (CDSD) than with the HITRAN data. A more detailed analysis shows 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.

COMPARISON WITH MIPAS SPECTRA

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 gives the nominal tangent height 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 (CDSD). 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 24km) the new data give better results.

Established the fact that the CDSD 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 CDSD gives better results than HITRAN.

As a conclusion the CO_2 line parameters included in the new version of the MIPAS database are:

- the line parameters of CDSD for the four most abundant isotopic variants of CO_2, namely $^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{16}O^{12}C^{18}O$ and $^{16}O^{12}C^{17}O$, and
- the line parameters of HITRAN for the other isotopic variants of CO_2.

Table 1-a: Comparison of simulated and observed ATMOS spectra using CDSD and **H**ITRAN2K at 15 km

Band	Spectral domain (cm^{-1})	RMS $\cdot 10^{-2}$ CDSD/HITRAN2K	Number of intervals where CDSD give better results
A	925-971	4.62240/4.6593	13 of 16
AB	1065-1092 & 1122-1170		
B	1215-1278 & 1310-1500	2.5182/2.5157	18 of 34
D	1820-2102 & 2111-2201	2.5057/2.5026	24 of 64
Total	-	2.8065/28092	55 of 114

Table 1-b: Comparison of simulated and observed ATMOS spectra using CDSD and HITRAN2K at 27 km

Band	Spectral domain (cm^{-1})	RMS $\cdot 10^{-2}$ CDSD/HITRAN2K	Number of intervals where CDSD give better results
A	704-752 & 826-971	2.6664/2.6561	23 of 47
AB	1065-1092 & 1122-1170	1.3784/1.3800	8 of 30
B	1215-1278 & 1310-1500	2.1366/2.1354	24 of 55
D	1820-2102 & 2111-2201	1.8282/1.8545	71 of 136
Total	-	1.9877/1.9996	126 of 268

Table 1-c: Comparison of simulated and observed ATMOS spectra using CDSD and HITRAN2K at 43 km

Band	Spectral domain (cm^{-1})	RMS $\cdot 10^{-2}$ CDSD/HITRAN2K	Number of intervals where CDSD give better results
A	680-770 & 925-971	2.9032/2.9033	19 of 45
AB	1065-1092 & 1122-1170	1.4803/1.4806	21 of 49
B	1215-1278 & 1310-1500	1.1645/1.1647	10 of 19
D	1820-2102 & 2111-2201	1.4624/1.7548	81 of 128
Total	-	1.7116/1.8670	131 of 241

Table 2 : Average chi-squared values as a function of altitude obtained when retrieving pressure and temperature profiles, using the HITRAN2K and the CDSD database (Orbit 2081 of MIPAS)

ALT (km)	No scans	HITRAN2K	CDSD
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

3.2. Nitric acid HNO_3

In a previous effort the spectral parameters of the hot band $\nu_5 + \nu_9 - \nu_9$ (HIT24-19) were improved using both laboratory spectra and atmospheric spectra recorded by ATMOS ([RD1] and ref[12]) and were included in the MIPAS database (version *hitran_mipas_pf2.0*). However recent **s**imulations of the MIPAS spectra using *hitran_mipas_pf2.0* showed that there is an inconsistency (Figure 1) 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 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 [13] and Table 3 presents a synthesis of available intensity measurements for the 11.2 μm spectral region of HNO_3.

Several comments can be made:

- the total absorption as derived from *hitran_mipas_pf2.0* is in good agreement with the value of Giver et al. [15]. This could be expected since the cold bands of HITRAN2K and hence of *hitran_mipas_pf2.0* were calibrated in absolute using the Giver's value.
- the total absorption measured in ref. [13] is about 14% lower than the *hitran_mipas_pf2.0* value.
- the Hot band Q-branch intensities measured in ref. [12,13] are in good agreement.

If one assumes that the HNO_3 hot band Q-branch is properly measured then the last two points demonstrate that the cold band intensities given in *hitran_mipas_pf2.0* are too high by about 14%, confirming what was found when analyzing the MIPAS spectra (see above).

Now the question to be discussed is the following: should one increase the hot band intensity by about 13% or lower the cold band intensities by the same amount? Our feeling is that the new measurements were carefully done and we then propose to use the new value for the cold bands. Another argument for such a change is that the average value of the low resolution measurements is in agreement with the new total absorption value but we recognize that, given the range of measured values (see Table 3), this argument is not really fully convincing.

In conclusion, it is proposed for the next version (*MIPAS_03*) of the database to multiply the line intensities of the bands ν_5 (HIT18-14), $2\nu_9$ (HIT21-14), ν_3 (HIT27-14)* and ν_4 (HIT17-14)* by the factor 0.879. A HNO_3 retrieval has been performed with this new data and Figure 2 shows the improvement as compared to Figure 1. Moreover, the new data were checked performing systematic retrievals using orbit 2081 of MIPAS and the results are presented in Table 4. The results are given in four columns. The first column gives the nominal tangent height of the retrieved HNO_3 concentration, the second column shows the number of scans for which the averaged chi-squared values are calculated, the third and the fourth columns show the averaged chi-squared values derived from retrievals using on the one hand the previous spectroscopic data (*hitran_mipas_pf2.0*) and on the other hand the new data (*MIPAS_03*). The last row summarizes the total chi-squared averaged over the latitude range for the two databases. It is clear that at all altitudes the new data give better results.

However it is essential to notice that, if it improves noticeably the RMS of the retrievals and hence their precision, this change leads to a systematic increase of the HNO_3 abundances of about 13%.**

** The intensities of these bands have to be multiplied by the same factor as for* ν_5 *and* $2\nu_9$ *since their absolute intensities were calibrated against those of these latter bands.*

*** Increasing the intensity of the hot band by 13% and keeping the intensities of the cold band at their* ***hitran_mipas_pf2.0*** *values would lead to an analogous improvement.*

Table 3: Comparison of measured HNO_3 intensities in the 11.2 µm spectral region

REFERENCES	TOTAL ABSORPTION	HOT BAND Q-BRANCH between 885.418 and 885.437 cm^{-1}
Goldman et al. [14]	585	
Giver et al. [15]	630	
. Massie et al. [16]	483	
Hjorth et al. [17]	541	
Average	560 (10%)	
hitran_mipas_pf2.0	637	
Toth et al. [13]	560 (5%)	
hitran_mipas_pf2.0		2.05
Toth et al. [13]		2.1

The intensities are in units of cm /atm^{-2}.

Table 4: Average chi-squared values as a function of altitude obtained when retrieving HNO_3 profiles, using the *hitran_mipas_pf2.0* and the *MIPAS_03* database (Orbit 2081 of MIPAS)

ALT (km)	No scans	*hitran_mipas_pf2*	*MIPAS_03*
42	54	0.95	0.94
39	54	1.00	1.00
36	54	1.01	1.00
33	54	1.01	1.01
30	54	1.22	1.21
27	54	1.70	1.65
24	53	2.34	2.22
21	51	2.58	2.41
18	48	1.79	1.63
15	48	1.87	1.70
12	48	2.12	1.89
TOTAL		1.51	1.44

Figure 1: Example of **c**omparison between MIPAS spectra and simulations using the *hitran_mipas_pf2.0* database for the microwindow HNO3006 (top panel) . The residual obtained is shown on the bottom panel.

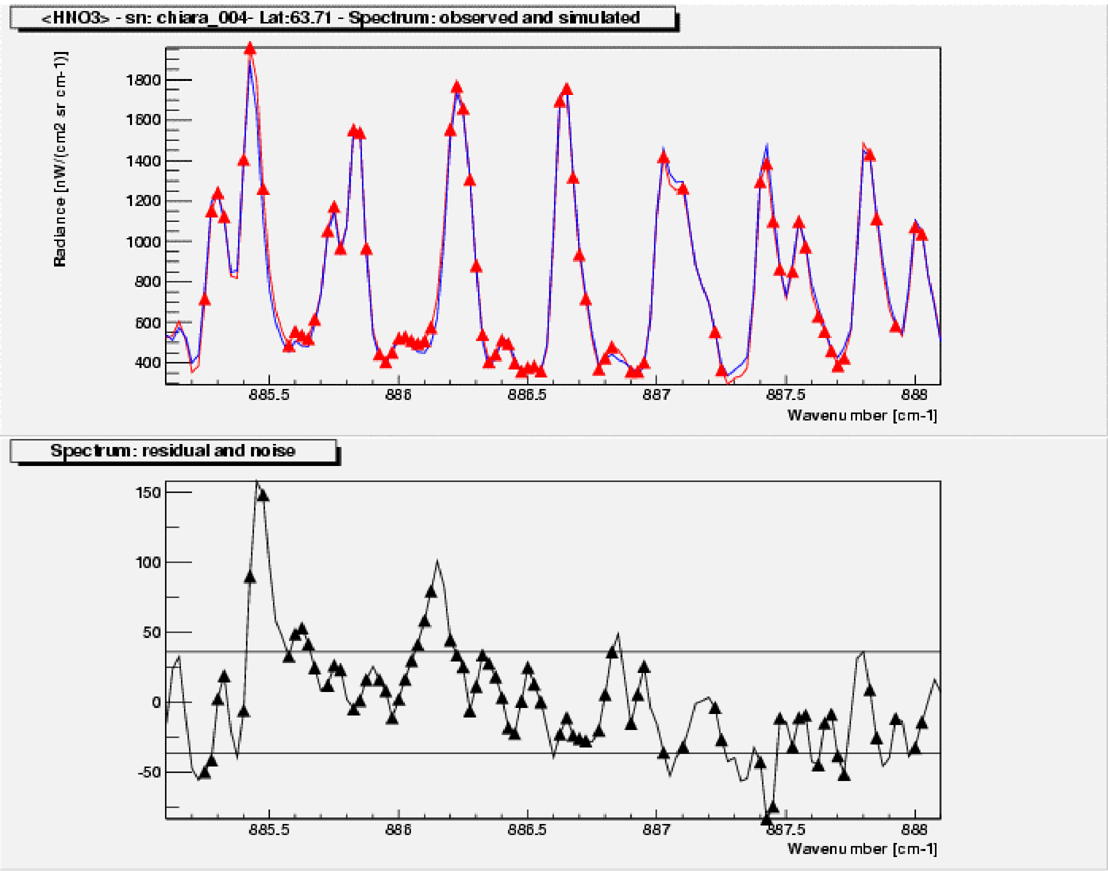
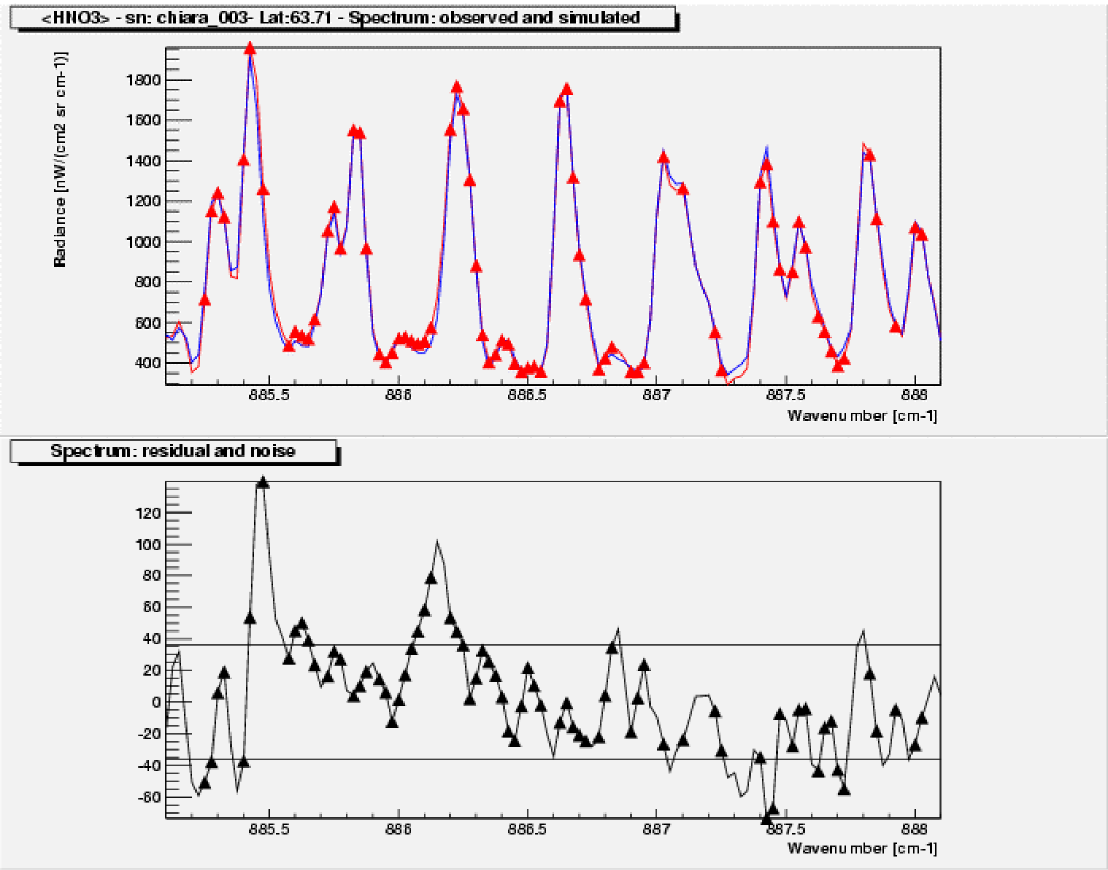


Figure 2: Example of comparison between MIPAS spectra and simulations using the *MIPAS_03* database for the microwindow HNO3006 (top panel) . The residual obtained is shown on the bottom panel.



3.3. Methane $^{12}CH_4$, $^{13}CH_4$, CH_3D

It was shown in [RD1] that the file 06.HIT01.par, which was not included in HITRAN2K, which had been recently updated by L. Brown (JPL, USA) and, which is a total replacement of the 1996 spectroscopic parameters for the three isotopic species of methane, was providing more reliable results than HITRAN96. Accordingly the new data were introduced in *hitran_mipas_pf2.0.*

However recently G. Stiller, N. Glatthor and F. Hase from the IMK group reported that in the 1202 cm^{-1} spectral region the fit quality of ground based FTIR atmospheric spectra was decreasing in terms of spectral residuals when using the updated spectral parameters. A careful analysis by the IMK group showed that, for some lines, there were problems with the new pressure shifts and to a lesser extent with the new pressure broadening coefficients, effects which unfortunately could not be seen using the ATMOS spectra. After discussions with L. Brown it turned out that some of the parameters were inadvertently changed and a new line list was provided.

Using the MIPAS microwindows we have compared retrievals performed using the *hitran_mipas_pf2.0* data and the “corrected” ones. No clear improvement was observed (see Table 5) but, given the findings of the IMK group, we have included the “corrected” data in the new version of the MIPAS database.

Table 5: Comparisons of methane retrievals using *hitran_mipas_pf2.0* and the "corrected" methane data

χ^2	***hitran_mipas_pf2.0***	**New data**
Sequence 8 (2081)	1.083	1.082
Full orbit (2081)	2.25	2.25

3.4. Nitrogen dioxide NO_2

Recently a number of studies have dealt with the line widths of the NO_2 molecule. In particular A. C. Vandaele et al. [18] have performed an overview and a comparison of various papers in order to derive the temperature and pressure dependence of the NO_2 absorption features in the 13200-42000 cm^{-1} range.

Comparing a number of experimental results (see ref. [18] for details) they recommend the values:

$\gamma_{air}(296K) = 0.080(3)\ cm^{-1}/atm, \quad n = 0.8(2)$

These values are to be compared:

* to the values given in HITRAN96 or HITRAN2K:

$\gamma_{air}(296K) = 0.067\ cm^{-1}/atm, \quad n = 0.5$

* or to the values given in HITRAN01:

$\gamma_{air}(296K) = 0.0707^{a}\ cm^{-1}/atm, \quad n = 0.97^{b}$

([a] Mean value calculated from all individual values of Dana et al. [19], [b] value derived from ref. [20-22]).

* or to the values derived from UV spectra in ref. [23]:

$\gamma_{air}(296K) = 0.134(10)\ cm^{-1}/atm, \quad n = 1.03(80)$

noticing that the authors recognize in their paper that the value obtained for γ_{air} is questionable because of line-mixing and resolution problems.

Given these results and the errors associated we suggest, until new experimental or theoretical results are available, to use in the MIPAS database:

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

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

3.5. Ozone O_3

The last versions of the HITRAN database do not include any spectral parameters for the ozone isotopic species in the 4.8 μm when in fact, given their intensities, the corresponding lines appear in atmospheric spectra [24]. Fortunately, recently the bands appearing in this spectral domain ($\nu_1+\nu_3$, $2\nu_1$ and $2\nu_3$) have been studied at high resolution for the $^{16}O^{18}O^{16}O$ and $^{16}O^{16}O^{18}O$ species [25] and the $^{16}O^{17}O^{16}O$ and $^{16}O^{16}O^{17}O$ species [26]. However, before using the corresponding line parameters one should carefully consider the problems and difficulties faced during the spectroscopic analyses.

Line positions

As already said, there are 3 interacting bands, namely $\nu_1+\nu_3$, $2\nu_1$ and $2\nu_3$, absorbing around 4.8 µm. As a consequence the spectroscopic analysis were performed taking into account the vibro-rotational resonances effecting the energy levels and the line intensities. However the main problem was that only the $\nu_1+\nu_3$ band was observed (it is a strong band) whereas the two other bands were not. Accordingly the Hamiltonian constants of these two latter bands were extrapolated constants preventing one to calculate precisely the corresponding line positions.

Line intensities

The line intensity calculations were performed using the transition moments of the main isotopic species $^{16}O_3$. This has two consequences:

- whereas the relative line intensities of the strong $\nu_1+\nu_3$ bands are likely to be more or less correct this is not probably the case for the weak $2\nu_1$ and $2\nu_3$ bands. To emphasize this point Table 6 presents a comparison of the intensities of the three bands of the isotopic species with those of the main isotope. It is obvious that for the strong $\nu_1+\nu_3$ band the mean ratio of the line intensities is in very good agreement with the "normal intensity ratios". On the contrary this is not true for the weak bands. This is not a proof that the intensities of these weak bands are not correctly estimated but it makes them highly questionable.
- as far as absolute intensities are concerned it is extremely difficult to estimate their uncertainties. Indeed, as already stressed, the line intensities of the isotopic species were calculated using the transition moment of the main isotope. Clearly this is theoretically incorrect but, unfortunately, the theory does not allow to transfer properly the transitions moments from $^{16}O_3$ to the other isotopic species (for the bands under study it is the second derivatives of the dipole moment with respect to normal coordinates which are involved). In fact, at this stage, we estimated that the absolute intensities of the $\nu_1+\nu_3$ bands of $^{16}O^{18}O^{16}O$, $^{16}O^{16}O^{18}O$, $^{16}O^{17}O^{16}O$ and $^{16}O^{16}O^{17}O$ are not known to better than 30-40% (conservative estimation).

<u>As a conclusion:</u>

- given the fact that neither $2\nu_1$ nor $2\nu_3$ (which are weak bands) have been observed, which means that the corresponding line positions and intensities are not precise, we do not propose to introduce them in the MIPAS database,
- on the contrary we propose to introduce the line parameters of the strong $\nu_1+\nu_3$ band keeping in mind that their absolute intensities cannot be assumed at this stage to be better known than 30-40%.

As a consequence the corresponding lines can not be used to derive the amount of $^{16}O^{18}O^{16}O$, $^{16}O^{16}O^{18}O$, $^{16}O^{17}O^{16}O$ and $^{16}O^{16}O^{17}O$ in the atmosphere. However they are useful as "interfering" lines.

Table 7 gives a summary of the spectral line parameters that we propose to introduce in the MIPAS database.

TABLE 6
COMPARISON OF THE LINE INTENSITIES OF THE ^{17}O AND ^{18}O OZONE ISOTOPIC SPECIES WITH THOSE OF $^{16}O_3$

^{17}Ozone isotopic species

“Normal intensity ratio”: ~2678

MOLECULE 667

BAND	RATIO	Number of Lines
12-1	2604(17)	18
13-1	2680(265)	1116
14-1	2966(170)	170

MOLECULE 676

BAND	RATIO	Number of Lines
12-1	2886(19)	15
13-1	2758(385)	1039
14-1	2463(1255)	197

^{18}Ozone isotopic species

“Normal intensity ratio”: ~499

MOLECULE 668

BAND	RATIO	Number of Lines
12-1	460(300)	62
13-1	520(96)	1266
14-1	911(933)	159

MOLECULE 686

BAND	RATIO	Number of Lines
12-1	570(55)	159
13-1	507(93)	1496
14-1	634(371)	702

RATIO is the mean ratio between the intensities of the lines of the ozone isotopic species and those of $^{16}O_3$.

TABLE 7
Summary of the isotopic ozone lines

MOLEC = 3, ISOEC = 2, NB LINES = 2571

```
NUM    BAND   XMIN       XMAX      SMIN      SMAX      STOT     NB
  1    13 1  2031.2629 2113.1845 0.120D-24 0.713D-23 0.463D-20 2571
NUM   BAND J1MIN K1MIN J1MAX K1AX J2IN K2IN J2AX K2AX   EMIN   EMAX
  1   13 1    0     0    50   12    0    0   51   12   0.0000 1125.1492
```

MOLEC = 3, ISOEC = 3, NB LINES = 1424

```
NUM    BAND   XMIN       XMAX      SMIN      SMAX      STOT     NB
  1    13 1  1988.4844 2074.4695 0.101D-24 0.689D-23 0.235D-20 1424
NUM   BAND  J1MIN K1MIN J1MAX K1AX J2IN K2IN J2AX K2AX   EMIN   EMAX
  1    13 1   1     0    50   14    0    0   51   14  0.0000  1185.2127
```

MOLEC = 3, ISOEC = 4, NB LINES = 1774

```
NUM    BAND    XMIN       XMAX      SMIN      SMAX      STOT     NB
  1    13 1   2049.9174 2121.4756 0.101D-24 0.132D-23 0.836D-21 1774
NUM   BAND  J1MIN K1MIN J1MAX K1AX J2IN K2IN J2AX K2AX   EMIN   EMAX
  1    13 1   0     0    44   13    0    0   44   13   0.0000  828.2198
```

MOLEC = 3, ISOEC = 5, NB LINES = 861

```
NUM    BAND    XMIN       XMAX      SMIN      SMAX      STOT     NB
  1    13 1   2031.4516 2100.8045 0.100D-24 0.126D-23 0.401D-21  861
NUM   BAND  J1MIN K1MIN J1MAX K1AX J2IN K2IN J2AX K2AX   EMIN   EMAX
  1    13 1   1     0    40   13    0    0   41   13   0.0000 798.6414
```

BAND : Band assignment in HITRAN notation
XMIN,XMAX : Lower and higher line positions
SMIN,SMAX : Lower and higher line intensities
STOT : Total band intensity
NB : Number of lines
J1MIN K1MIN J1MAX K1MAX J2MIN K2MIN J2MAX K2MAX: Lower and higher J and K_a quantum numbers for the upper and lower states of the transitions
EMIN, EMAX : Lower and higher lower states energies for the set of transitions

3.6. COF_2

The COF_2 line parameters in the 5.2 µm spectral region correspond to 3 bands HIT5-1, HIT12-1 and HIT14-1 which are in strong interaction [27]. Among them, the strongest band is the HIT5-1 fundamental band, the two others borrowing their intensities from this band. Indeed since HIT5-1 (ν_1) is a fundamental band and since HIT12-1 ($2\nu_2$) and HIT14-1 ($2\nu_3+\nu_6$) are overtone and combination bands, it is likely that these two latter bands have a much smaller intensity than the fundamental one. Accordingly the relative intensities were partitioned between the three bands assuming a non-zero dipole moment for the ν_1 band and letting the Fermi and Coriolis interactions transfer intensity into the two weaker bands. The total band intensity of the three bands system were scaled using a vibrational partition function of ~1.15 to the best three reported low resolution integrated absorptions [28-30]. In this way a line list was generated [27], the summary of which is given in Table 8.

These data have been compared to the data included in HITRAN2K, the summary of which is given in Table 9. Finally Table 10 gives the comparison of the new data with the HITRAN2K ones.

The following comments can be made:

- the new data have stronger intensities than the HITRAN2K ones. The ratio HIT/CAL is about 0.973 (see Table 10). This is not fully consistent with the ratio of 0.930 obtained when comparing the total intensities of the band systems: 0.568 10^{-16} for the new data (Table 8) versus 0.528 10^{-16} for the HITRAN2K data (Table 9), but can be explained by the fact that the new data have a smaller intensity cut off. Therefore, a lot of weak lines exist which add up to increase the total band intensities.
- the weak HIT14-1 band is not included in HITRAN2K. However, given the weakness of the band, this was not really important for atmospheric retrievals.
- finally it has to be stressed that in HITRAN2K the rotational assignments of the transitions are wrong.

As a conclusion, it is proposed to introduce in the MIPAS database the new data since they are more complete and since the rotational assignments of the transitions are correct. Also, thanks to the better theoretical analysis, the new individual line intensities are likely to be better than the HITRAN2K ones.

TABLE 8

SUMMARY OF THE COF_2 LINES (Ref.[27])

```
IMOLEC= 29
NB OF LINES= 28884
NB OF BANDS=  3

  BAND    XMIN      XMAX       SMIN       SMAX       STOT      NB
 12  1 1856.7303 1984.4377 0.154D-22 0.126D-19 0.137D-16 13083
  5  1 1868.4676 2001.3478 0.157D-22 0.394D-19 0.428D-16 14861
 14  1 1883.8396 1985.3564 0.168D-22 0.187D-19 0.315D-18   940

 BAND    J1MI K1MI J1MA K1MA J2MI K2MI J2MA K2AX   EMIN      EMAX
 12  1    0    0   70   63    0    0   70   63     0.0000 1600.8066
  5  1    0    0   70   69    0    0   70   69     0.0000 1942.8766
 14  1   24    2   70   56   23    1   70   55   112.8008 1427.6216
```

The meaning of the different columns is the same as in Table 7.

TABLE 9

SUMMARY OF THE COF$_2$ LINES (HITRAN2K)

```
IMOLEC= 29
NB OF LINES = 13149
NB OF BANDS=  2

     BAND    XMIN     XMAX      SMIN      SMAX      STOT      NB

       12  1 1879.0245 1968.6326 0.501D-21 0.122D-19 0.122D-16  5211
        5  1 1889.0321 1981.2728 0.501D-21 0.383D-19 0.406D-16  7938

   BAND  J1MI K1MI J1MA K1MA J2MI K2MI J2MA K2MA    EMIN   EMAX

  12  1    1    1   70   47    1    1   70   47     0.5902  960.2829
   5  1    0    0   70   55    0    0   70   55     0.0000 1207.7841
```

The meaning of the different columns is the same as in Table 7.

TABLE 10

COMPARISON BETWEEN COF$_2$ LINES FROM Ref.[27] and HITRAN2K

```
IMOLEC= 29
NB LINES Ref.[27]  = 28884
NB LINES HITRAN2K = 13149
```

BAND HIT12-1

```
NB LINES COMPARED= 5175
 HIT/CAL(MEAN)=    0.97315+-   0.02698
```

BAND HIT5-1

```
NB LINES COMPARED= 7894
 HIT/CAL(MEAN)=    0.97278+-   0.00021
```

4. Conclusions

This technical report described the new version of the spectroscopic database (*MIPAS_03*) compiled starting from hitran_mipas_pf2.0 in order to further improve the actual parameters for the MIPAS experiment. 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$_3$, CH$_4$, HNO$_3$, NO$_2$) and of COF$_2$ using new laboratory spectroscopy or new calculations. Some updates have been validated against ATMOS observations, other using preliminary MIPAS measurements.

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