ESA-Contract No. 11717/95/NL/CN
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Parameterisation of the Level 0 to 1b Data Processing of the MIPAS-B2 flight No. 6 of 7./8.5.1998

by

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1. Introduction

MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) is a limb viewing interferometer measuring emission spectra of key trace species relevant to ozone chemistry in the mid-infrared spectral region between 4.15 µm and 14.6 µm. A satellite instrument of the MIPAS family will be operated on the ESA/ENVISAT platform and is described in detail in various papers (e.g. [Ende1993]). MIPAS-B2 [Frie1999] may be conceived as a precursor of MIPAS-ENVISAT. The essence of the instrument is a high resolution Fourier transform spectrometer (FTS). In Fourier transform spectroscopy highly sophisticated data analysis methods are required to derive trace gas distributions from raw data obtained by the FTS.
For evaluating and validating the data processing tools similar data to the expected one from the satellite is very valuable. Balloon borne measurements performed by the FTS instrument MIPAS-B2 will be used for this task. The detector optics of MIPAS-B2 has been matched to that of MIPAS-ENVISAT in terms of channel separation and spectral coverage for this purpose.
This draft document is a summary of the document "Level 0 to 1b Data Processing of the MIPAS-B2 balloon borne Fourier Transform Spectrometer ", draft version, 1998 describing the actual processing steps and their parameterisation applied within the level-1b data processing of the MIPAS-B2 data of the 6^{h} flight performed on May 7/8, 1998. A separate technical note has been prepared related to instrument characterisation of MIPAS-B2 [Frie1998]. It is assumed that the reader is familiar with the basic principles of Fourier transform spectroscopy, the MIPAS Experiments and the problems associated with the generation of calibrated spectra from interferograms.

2. Measurement scenario

The processing of the data is linked to the measuring scenario and vice versa. Therefore, the typical constraints on the scenario for the flight of the MIPAS-B2 experiment will be outlined in this chapter.
The measuring scenario is matched to atmospheric conditions in the atmosphere at the time of the flight and the predicted duration of the float. Nevertheless there are some basic principles that normally serve as guideline for every flight:

- At float 1 to 2 complete limb sequences are obtained in a stepwise scanning mode with a typical stepsize of 2 – 3 km. At each elevation angle several interferograms are taken. The number of interferograms on each elevation angle increases with the height of the tangent point to compensate partly for the reduced emitted energy at higher altitudes.
- Calibration measurements consisting of blackbody and so called ‘deep space’ (elevation angle: +20 degree) measurements are taken at the beginning and at the end of each limb scan sequence.

The measurement as performed during the flight of the MIPAS-B2 instrument at Aire sur l’Adour in 1998 is shown below:

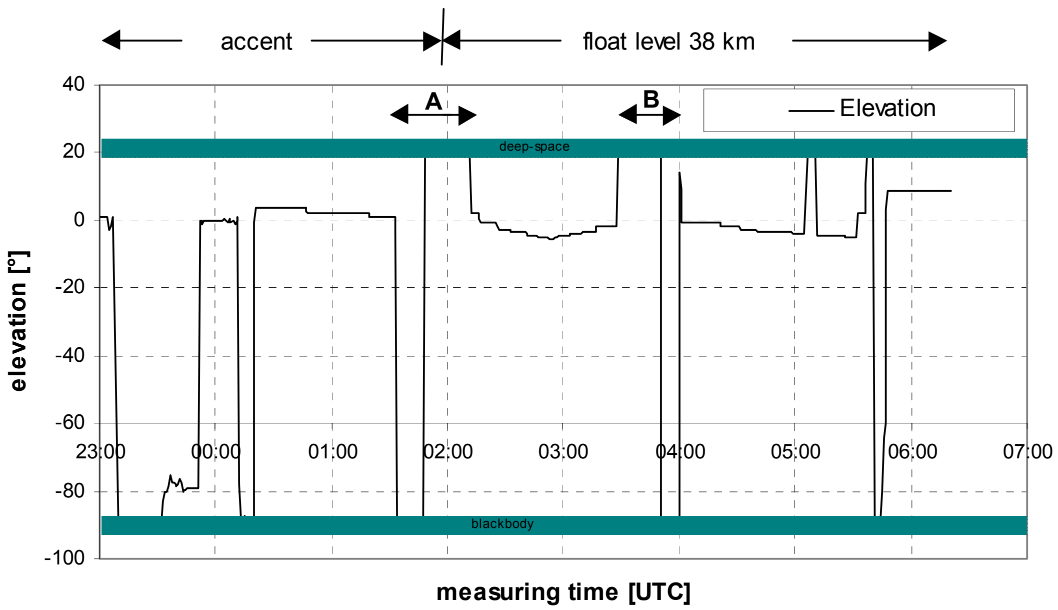

fig. 1: Measuring scenario of the MIPAS-B2 flight on 8.5.1998 at Aire sur l'Adour. The limb sequence is taken between the calibration cycles (A) and (B). The calibration cycles comprises each of a blackbody and deep-space measurements.

The first limb sequence (between the calibration cycles A and B) from MIPAS-B flight No. 6 was selected within the framework of this study. For further information concerning the flight see [Frie1998].

3. Physical description of the processing chain

The interferograms were sampled with the following parameters:

	Channel 1	Channel 2	Channel 3	Channel 4
Sampling distance	9.4948705 µm	5.6969223 µm	10.760853 µm	3.7979482 µm
Spectral range	526.60013 .. 1053.2003 cm^{-1}	877.66688 .. 1755.3338 cm^{-1}	1393.9415 .. 1858.5887 cm^{-1}	1316.5003 .. 2633.0006 cm^{-1}

The interferograms are checked for consistency with respect to sampling errors, spikes, noise elements and stability errors of elevation angle during the scan. Erroneous interferograms are sorted out.
The data processing up to level 1b is concerned with the transformation of the interferograms into calibrated and localised spectra. A dataflow diagram is given in fig. 2 indicating the individual processes and their input/output data products.
The major tasks during the generation of spectra are as follows:

- IFGs recorded for the individual spectral channels are transformed into complex spectra,
- the individual phase of each IFG is calculated,
- the interferograms are corrected by using the phase information,
- the corrected IFGs are transformed into apodised spectra,
- the offset (deep-space) spectra are subtracted from the atmospheric ones and
- the gain calibration is performed by using the blackbody spectra with the associated blackbody temperature and the deep-space spectra.

For calibration purposes three types of spectra are processed (fig. 2):

- the atmospheric raw spectra,
- the blackbody raw spectra for gain calibration and
- the “deep-space” raw spectra for offset calibration.

These three types of spectra are processed differently and therefore will be discussed separately. Co-addition of the spectra or interferograms are performed for blackbody respectively "deep-space" spectra to reduce the noise level. In the following all processes will be briefly described together with their parameterisation in the sequence as they are performed within the processing chain during level 1b data processing. For each of the four MIPAS-B2 channels the sequence of the processes was performed individually.

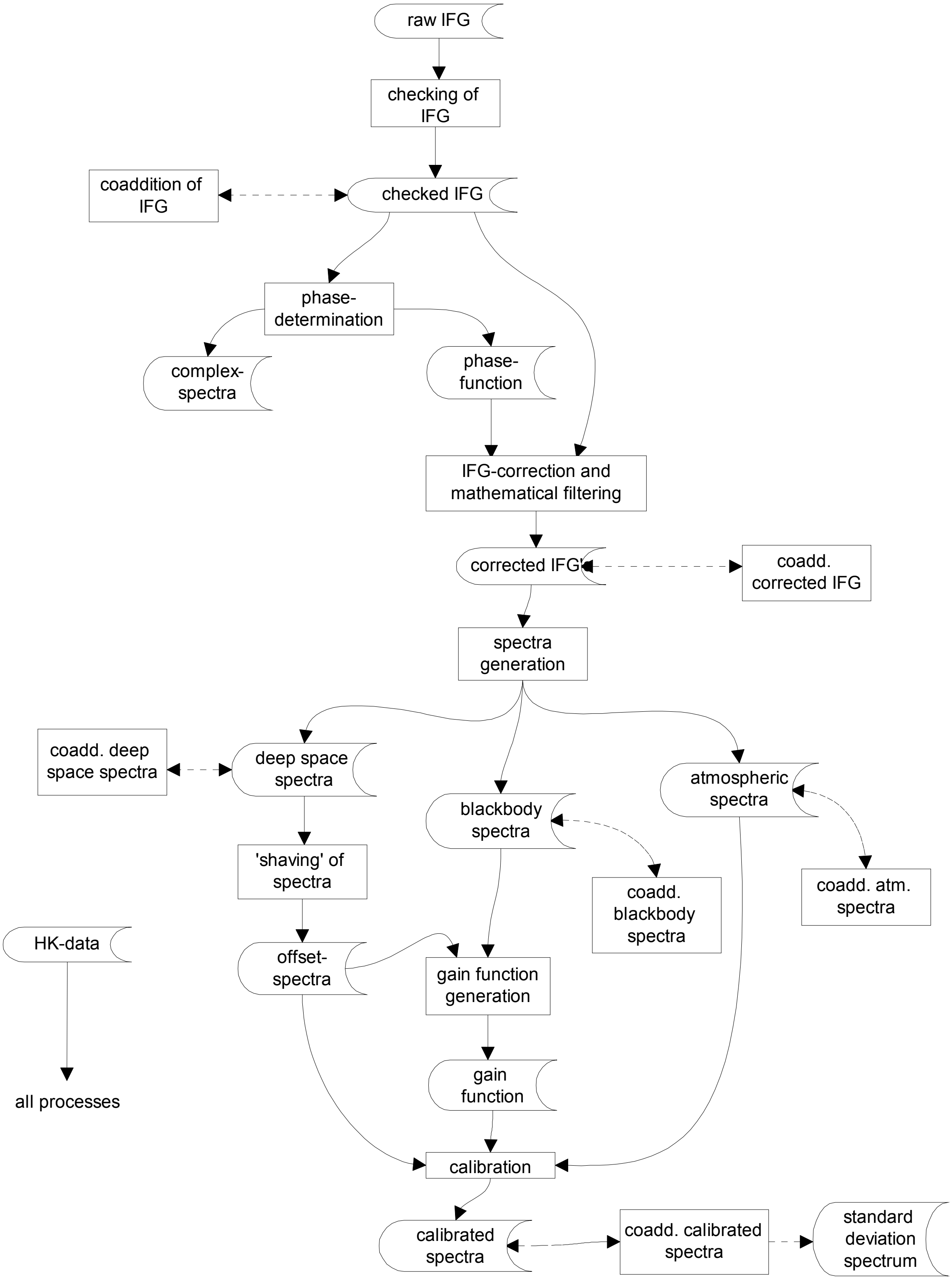

fig. 2: Dataflow diagram of the MIPAS-B2 data processing chain (apodisation is performed during every generation of a spectrum)

3.1. Blackbody spectra

The blackbody spectra are necessary to retrieve the calibration function for radiometric calibration of the atmospheric spectra. Due to the high signal-to-noise ratio these spectra can also be used to determine the instrumental phase.
Two blackbody sequences were analysed: one before (A) and one after (B) the limb sequence.

3.1.1. Phase determination of blackbody interferograms

The phase is obtained by the angle between the real and imaginary part of the complex spectrum S(σ) (classical approach by [Form1966]). The spectrum is derived by a FFT from the interferogram IFG(x) which is degraded by the apodisation function A(x).

$$S(\sigma) = \mathbf{FT}^{+}\left[A(x)\,\mathrm{IFG}(x)\right]$$

$$\phi(\sigma) = \mathbf{arctan}\left[\frac{\mathbf{Im}(S(\sigma))}{\mathbf{Re}(S(\sigma))}\right]$$

Resolution of blackbody spectra	1.0 cm^{-1}
Length of interferogram (OPD) used	+/- 0.5 cm
Apodisation	Norton-strong

The output of this processing step is the “Instrumental phase function” which is used as input for the phase correction of deep space and atmospheric spectra.

3.1.2. Interferogram correction

The phase disturbed interferogram shall be corrected such that the desired spectrum is purely real.

$$\mathrm{IFG}_{corr}(x) = \mathrm{IFG}(x) \otimes \underbrace{\mathbf{FT}^{-}[e^{i\Phi(\sigma)}]}_{k^{*}(x)}$$

The correction kernel k(x) is optimised by the tapering function A(x) to reduce the wiggles of the Gibb’s phenomena. The tapering function can be any apodisation function.

$$k_{(x)} = k^{*}(x)A(x)$$

The corrected IFG is generated by a convolution of the disturbed IFG with the kernel k(x).

$$\mathrm{IFG}_{corr}(x) = \mathrm{IFG}(x) \otimes k(x)$$

Kernel size	2048 points
Tapering function	Norton-strong

3.1.3. Generation of blackbody spectra

The spectrum is derived from a real FFT of the corrected interferogram $IFG_{corr}(x)$ which is tapered by the apodisation function A(x).

$$S(\sigma) = \mathbf{FT}^{+}\left[A(x)\,IFG(x)\right]$$

Resolution of blackbody spectra	0.0345 cm^{-1} (Channel 1+3) 1.0 cm^{-1} (Channel 2+4)
Length of interferogram (OPD) used	+/- 14.5 cm (Channel 1+3) +/- 0.5 cm (Channel 2+4)
Apodisation	Norton-strong (Contract 11717_95_NL_CN) Rectangle (Contract 12078_96_NL_GS)

3.1.4. Co-addition of blackbody spectra

Co-addition in the spectral domain is performed to reduce the noise in the data-product. The result of this procedure is equivalent to the co-addition of the interferograms. The spectra are already based on phase corrected IFGs. Therefore phase instabilities can not degrade the co-added data product. The noise is reduced by the square root of the number of co-added spectra. For co-addition in the spectral domain all spectra have to on the same spectral grid.

Number of co-added spectra (sequence A)	18
Number of co-added spectra (sequence B)	22

3.1.5. Noise reduction in blackbody spectra (only channel 3)

Residual water vapour inside the instrument causes lines in channel 3 blackbody spectra. Therefore, the blackbody spectra could not be processed at lower spectral resolution to reduce the noise in the spectra. To reduce the noise but keeping the lines, the narrow H_2O lines were removed before noise reduction and reinserted afterwards.

A difficulty in the removal process is to distinguish between lines, which have to be removed, and broadband features, which have to remain in the offset spectrum. High altitude spectral lines are sharp and almost purely in the Doppler-broadening regime in the IR. They have an relatively strong gradient at the line wings and a strong curvature at their peaks. The selection of those lines was performed by finding high absolute values of the geometric sum S^d of the first and second derivative of the spectral intensity.

$$S' = \frac{\partial S}{\partial \sigma}\ ,\ S'' = \frac{\partial^2 S}{\partial \sigma^2}$$

$$S^d = \sqrt{\left(\frac{S'}{\mathbf{max}(|S'|)}\right)^2 + \left(\frac{S''}{\mathbf{max}(|S''|)}\right)^2}$$

Another problem is the replacement of these lines selected for removal. Due to the small width of the selected lines, the baseline intensity can be assumed to be linear over the width of the line to remove. This leads to a linear replacement of the selected line. This process will be called "shaving" of spectra.
To reduce the noise in the 'shaved' spectrum and to smooth the edges of the replacement interval, the 'shaved' spectrum is low-pass filtered with an edge-frequency guaranteeing the preservation of the spectral baseline. If channel spectra are present, the low-pass filter is adjusted to the frequency of the channelling effect corresponding to the displacement of the channels from ZOPD in the interferogram.

Resolution of spectrum prior to shaving	0.0345 cm^{-1}
Intermediate resolution after shaving	1.0 cm^{-1}
Resolution of spectrum at line positions after shaving	0.0345 cm^{-1}

3.2. Deep-space spectra

The „deep-space“ spectra are used for offset calibration. With an elevation angle of 20° upwards, broadband emission features from the atmosphere can be neglected. Therefore any broadband feature in the spectrum originates from the instrumental background emission. Lines in the deep-space spectra are due to atmospheric emissions of mainly CO_2 and H_2O. These lines have to be eliminated during calibration.
Two deep-space sequences are analysed: one before (A) and one after (B) the limb sequence.

3.2.1. Co-addition of deep-space interferograms

Co-addition of IFGs is performed to reduce the statistical noise in the interferogram introduced by photon or detector noise. In first order approximation, the noise can be reduced by the square root of the number of co-added IFGs.
Co-addition means an addition of single IFGs on exactly the same OPD grid.This can be guaranteed only if the instrument is working in an absolutely stable mode, i.e. no phase fluctuations occur.
For assigning time to the co-added IFGs the mean value of the measuring time is used. The individual times of the IFGs are taken at ZOPD.

ZOPD-position	Determined by the IFG-Maximum
Number of co-added interferograms (sequence A)	Forward: 28 Backward: 28
Number of co-added interferograms (sequence B)	Forward: 28 Backward: 28

The preceding steps are performed separately for the interferograms taken at forward and backward movement of the interferometer, respectively.

3.2.2. Phase determination of deep-space spectra

The quality of the phase determination is enhanced by applying the following a-priori constraints:

- As already indicated, the total phase-function can be separated into the instrumental part $\Phi^*(\sigma)$ and the linear part $\Delta\Phi(\sigma)$. The second one can be expressed as a straight line with the parameters offset *a* and slope *b*.

$$\Phi(\sigma) = \Phi^*(\sigma) + \Delta\Phi(\sigma) = \Phi(\sigma) + a + b(\sigma - \sigma_0)$$

- the correlation μ between the atmospheric and the beamsplitter spectrum has to vanish:

$$\mu = \mathbf{correl}(\mathbf{Re}(S), \mathbf{Im}(S)) \rightarrow \pm 0$$

  To avoid a correlation between the imaginary and real part of the spectra caused by the spectral response function (due to the Planck- and filter-function), each part is high pass filtered.
- the variance ν of the beamsplitter spectrum has to be minimised. For better convergence the elements of the variance are squared:

$$\frac{d(\nu^2)}{d(\Delta\Phi)} = \frac{d\,\mathbf{variance}\left(\mathbf{Im}^2(S)\right)}{d(\Delta\Phi)} = 0$$

$$= \frac{d\sum_i\left[\mathbf{Im}(S_i) + \mathbf{Re}(S_i)\Delta\Phi\right]^4}{d(\Delta\Phi)}$$

  A solution is found, if:

$$\frac{\partial(\nu^2)}{\partial a} = 0$$

$$\frac{\partial(\nu^2)}{\partial b} = 0$$

The correlation μ is rapidly minimised by variation of the phase-offset *a*. But for the slope *b* the positive line correlation contributions of one side of the spectral band may be compensated by negative line correlation contributions of the other side. On the other hand ν is not a good criterion for the offset *a* but for the slope *b*. A combination at each iteration step of μ for the offset and of ν for the slope *b* results in a good convergence for both parameters.

The complex spectrum used in all steps of this phase determination method is derived by a classical real FFT from the interferogram I(x) which is degraded by the apodisation function A(x).

$$S(\sigma) = \mathbf{FT}^+\left[A(x)\,\mathrm{IFG}(x)\right]$$

The high-pass digital filtering is performed by convolution of the spectrum with a kernel function describing the filter.
The kernel represents the coefficients of a non-recursive, digital filter for evenly spaced data points. The kernel coefficients are Kaiser-weighted. The intensity of the Gibbs phenomenon wiggles are defined in -db; a value of 50 or more should be appropriate.
The resulting vector of coefficients has (2*order + 1) elements.

order of the kernel	20			
reduction of the gibb' phenomena	50 dB			
lower frequency of the filter in fractions of the Nyquist frequency	0.4			
low wavenumber of bandwidth interval	660 cm^{-1}	1000 cm^{-1}	1540 cm^{-1}	1720 cm^{-1}
high wavenumber of bandwidth interval	980 cm^{-1}	1600 cm^{-1}	1800 cm^{-1}	2500 cm^{-1}
Instrumental phase function	As defined in subsection 3.1.1			
Maximum number of iterations	25			

3.2.3. Correction of deep-space interferograms

3.2.4. Generation of deep-space spectra

The same processes are used as described in the section about blackbody spectra, (see subsection 3.1.2 and 3.1.3), but the phase information is taken from the process described in the preceding section. The parameterisation is listed below:

Resolution of deep space spectra	0.0345 cm^{-1}
Length of interferogram (OPD) used	+/- 14.5 cm
Apodisation	Norton-strong (Contract 11717_95_NL_CN) Rectangle (Contract 12078_96_NL_GS)

3.2.5. Shaving of deep-space spectra

The 'shaving' of spectra is necessary to remove any sharp spectral lines formed in the atmosphere above the balloon from the deep space spectra. The "shaving" is performed in the same manner as the "shaving" of blackbody spectra described in subsection 3.1.5.

Resolution of spectrum prior to shaving	0.0345 cm^{-1}
Resolution of spectrum after shaving	1.0 cm^{-1}

3.3. Limb sequence spectra

For the processing of the limb spectra, the first three steps are identical to the processing of deep space spectra, so for

3.3.1. Phase determination of limb sequence spectra

➔ See subsection 3.2.2

3.3.2. Correction of limb sequence interferograms

➔ See subsection 3.1.2

3.3.3. Generation of limb sequence spectra

➔ See subsection 3.2.3

3.4. Calibration

3.4.1. Calibration of limb spectra

The radiometric calibration allows to convert the uncalibrated values into physical units of spectral radiance. A two point calibration is performed. One calibration point is the offset spectrum $S_{instr.}$ which is determined from 'shaved' deep-space spectra. The other calibration 'point' is a spectrum of the relatively 'hot' blackbody (S_{BB}, ~210K). Together with the corresponding Planck-spectrum L_{Planck}, which acts as an ideal spectrum for the blackbody, a gain function can be derived.

$$L_{calib} = \left(S_{atm.} - S_{instr.}\right)\underbrace{\left[\frac{S_{BB} - S_{instr.}}{L_{Planck}}\right]^{-1}}_{\text{Gainfunction}}$$

The calibration is performed by subtraction of the offset spectrum from the atmospheric spectrum and multiplication with the gain function.
Offset and blackbody spectra are interpolated to the time of the measurement.

3.4.2. Interpolation on the ENVISAT spectral grid and spectral calibration

The interpolation on the ENVISAT spectral grid is performed together with the spectral calibration. Spectral calibration has been obtained by retrievals using the HITRAN database.

	Channel 1	Channel 2	Channel 3	Channel 4
Grid interval	0.025 cm^{-1}			
Spectral range	685.0 .. 969.975 cm^{-1}	1020.0 .. 1499.975 cm^{-1}	1570.0 .. 1749.975 cm^{-1}	1820.0 .. 2409.975 cm^{-1}

3.4.3. Calculation of variance respectively the standard deviation

The standard deviation is calculated from consecutive calibrated spectra of subsection 3.4.2 of one elevation angle. The standard deviation corresponds to the overall instrument NESR. The variance, the diagonal elements of the variance/covariance matrix, can be calculated by the square of the standard deviation values.

4. Data exchange for MIPAS-B balloon data between IMK and IROE/Univ. of Bologna

Based on the Memorandum prepared by H. Oelhaf, M. Höpfner, O. Trieschmann (IMK), B. Dinelli (University of Bologna), and M. Ridolfi (IROE-CNR) on 25.9.1998 Referring to WP 6000 of contract 11717/95/NL/CN this memorandum defines the technical interface for the exchange of MIPAS-B balloon data of calibrated spectra and relying housekeeping data between IMK and IROE/University of Bologna.

4.1. Abbreviations

AILS	apodised instrumental line shape
c	character
FOV	field-of-view
i	integer
MPD	maximum optical path difference
r	real

4.2. Definitions and general information

Scan/Sweep/nominal elevation angle
A scan is a limb scanning sequence including spectral measurements at different nominal elevation angles. At each elevation angle several sweeps (spectral measurements) are performed. Therefore, in contrast to MIPAS/ENVISAT more than one sweep can belong to the same nominal elevation angle.

File types
All files are in ASCII format except the calibrated spectra for ESA-Contract No. 12078/96/NL/GS which are stored in the scientific interchange format HDF.

Comment lines of files in ASCII-format
The first character of a comment record is a #. All other records contain data.

4.3. File formats

4.3.1. Channel descriptive data sets (ESA-Contract No. 11717/95/NL/CN and ESA-Contract No. 12078/96/NL/GS)

File name
MIP-B-Vx-Cy
where x is the data version and y the channel number.

Type
ASCII

Typical file size
200 + 62*(number of elevations) + 50*(number of elevations)*(number of spectra per elevation)

Field name	Format	Units	Size	Comments
Data version	i		4	
Channel	i		4	
Boundary of vertical FOV distribution	r	degree	4	The FOV is assumed to extend from -boundary, to +boundary
FOV coefficients	r(9)		72	The FOV is parameterised as a polynomial of 8th order. Negative FOV angles refer to higher elevation
MPD of the measurement	r	cm	8	
Ratio of zerofilling	r		8	
AILS parameters	r(10)		80	
Elevation- a posteriori knowledge	r	arcmin	8	3σ standard deviation
Observer altitude- a posteriori knowledge	r	km	8	3σ standard deviation
Number of nominal elevations	i		4	
Begin nominal elevation 1 ... number of nominal elevations				
Nominal elevation	r	degree	8	
Filename of variance spectrum	c		50	
Number of sweeps	i		4	
Begin sweep 1 ... number of sweeps				
Filename of measured spectrum	c		50	
End sweep 1 ... number of sweeps				
End nominal elevation 1 ... number of nominal elevations				

4.3.2. Spectral data sets (ESA-Contract No. 11717/95/NL/CN)

File name
MIP-B-Vx-Cy-Ez-Sn.ascii
where x is the data version, y the channel number, z the nominal elevation angle, and n the number of the spectrum (as derived in subsection 3.4.2).
n = 0 refers to the standard deviation spectrum (as derived in subsection 3.4.3).

Type
ASCII

Typical file size
100 + 16*(number of spectral grid points)

Field name	Format	Units	Size	Comments
Data version	i		4	
Channel	i		4	
Nominal elevation angle	r	degree	8	
Acquisition date	c		8	given as 'dd.mm.yy'
Acquisition time	c		8	given as 'hh:mm:ss'
Latitude of observer	r	degree	8	
Longitude of observer	r	degree	8	from -180 to +180 with positive eastern longitudes
Altitude of observer	r	km	8	
Elevation angle	r	degree	8	negative angles looking downward
Azimuth angle	r	degree	8	from 0 to 360: N->E->S->W->N
Latitude of tangent point	r	degree	8	includes refraction using initial guess p-T profile
First wavenumber	r	cm^{-1}	8	
Wavenumber grid distance	r	cm^{-1}	8	
Number of grid points	i		4	
Begin grid point 1 ... number of grid points				
wavenumber, intensity	r(2)	cm^{-1}, W/cm^2Srcm^{-1}	16	
End grid point 1 ... number of grid points				

4.3.3. Spectral data sets (ESA-Contract No. 12078/96/NL/GS)

File name
MIP-B-Vx-Cy-Ez-Sn.hdf
where x is the data version, y the channel number, z the nominal elevation angle, and n the number of the spectrum (as derived in subsection 3.4.2).
n = 0 refers to the standard deviation spectrum (as derived in subsection 3.4.3).

Type
HDF

The HDF data format is used for exchange of MIPAS-B2 data between ESA and the contractor. Further information about HDF can be found on the World Wide Web [HDF1999].

The information content is identically to the one described in subsection 4.3.2. The following source code is written in IDL, which condenses the data to the HDF-files:

```
;-----------------------------------------------------------------------------------
; Procedure to construct the HDF files using IDL
;-----------------------------------------------------------------------------------

pro esa_hdf,filename,latitude,longitude,altitude,realelev,azimuth,lattangent

   arr = read_XYfile(strmid(filename,0,21)+'.bin',time=time)
   filename = strmid(filename,0,21)+'.hdf'
   sd_id = HDF_SD_START(filename, /CREATE)
   HDF_DFAN_ADDFDS, filename, 'Spectrum of the MIPAS-B2 Flight from Aire sur
l''Adour,1998 (c) IMK/FZK'
   HDF_SD_ATTRSET, sd_id, 'Filename', filename
   HDF_SD_ATTRSET, sd_id, 'Data version', strmid(filename,7,1)
   HDF_SD_ATTRSET, sd_id, 'Channel', fix(strmid(filename,10,1))
   HDF_SD_ATTRSET, sd_id, 'Nominal elevation angle', loat(strmid(filename,13,5))
   HDF_SD_ATTRSET, sd_id, 'Acquisition date', strmid(time,5,8)
   HDF_SD_ATTRSET, sd_id, 'Acquisition time', strmid(time,14,8)
   HDF_SD_ATTRSET, sd_id, 'Latitude of observer', latitude
   HDF_SD_ATTRSET, sd_id, 'Longitude of observer', longitude
   HDF_SD_ATTRSET, sd_id, 'Altitude of observer', altitude
   HDF_SD_ATTRSET, sd_id, 'Elevation angle', realelev
   HDF_SD_ATTRSET, sd_id, 'Azimuth angle', azimuth
   HDF_SD_ATTRSET, sd_id, 'Latitude of tangent point', lattangent
   HDF_SD_ATTRSET, sd_id, 'First Wavenumber', arr[0,0]
   HDF_SD_ATTRSET, sd_id, 'Wavenumber grid distance', 0.025d0
   sz=size(arr)
   HDF_SD_ATTRSET, sd_id, 'Number of grid points',sz(1)
   if sz(0) eq 0 then return
   sds_id = HDF_SD_CREATE(sd_id, 'Spectrum [Wavenumber,Intensity]', sz(1:sz(0)),
/DOUBLE)
   HDF_SD_ADDDATA, sds_id, arr   ;Write the data into the dataset.
   HDF_SD_ENDACCESS, sds_id      ;End access to any SD IDs.
   HDF_SD_END, sd_id;When finished with the file, close it with a call to

return

end
```

4.3.4. Pressure-temperature initial guess profile (ESA-Contract No. 11717/95/NL/CN and ESA-Contract No. 12078/96/NL/GS)

File name
MIP-B-Vx-PT
where x is the data version.

Type
ASCII

Typical file size
4 + 24*(number of levels)

Field name	Format	Units	Size	Comments
Number of atmospheric levels	i		4	
Altitude of atmospheric levels	r(number of levels)	km	8*number of levels	
Pressure at levels	r(number of levels)	hPa	8*number of levels	
Temperature at levels	r(number of levels)	K	8*number of levels	

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