SCIAMACHY Level 1b-1c Processing
The SciaL1c Command-line Tool
Software User's Manual

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Change Record

Issue	Rev.	Date	Page	Description of Change
1.0		30/01/02	all	completely new, originally provided as document PO-TN-ESA-GS-2307
6.0		10/05/06	all	re-launched as document ENV-SUM-DLR-SCIA-0071
			p.5	Introduction: Comments to de-coupling of tool from EnviView and coupling of tool to the operational software baseline.
			p.6	References: Upgrade of references to current actual issues
			p.8	Document overview: Totally new
			p.16	Table 3-1: Extension by measurement categories 20 through 26

Table of Content

1 Introduction

The extraction and application tool “SciaL1C”shall be used to transform SCIAMACHY level 1b products into a so called 1c products being in general geo-located, calibrated spectral radiance. Since many users had found such a tool useful for their own applications, the tool has also been designed as command-line tool in addition to the provided functionality of EnviView.

In the past this software was available in both, a command line version or imbedded into the EnviView tool, allowing a case by case application supported by a graphical user interface. From a functionality point of view, there was absolutely no difference between both, whereas it is obvious that the command line version is more appropriate for systematic handling of large amount of SCIAMACHY data. During ENVISAT’s mission, the evolution of SCIAMACHY’s calibration algorithm changed substantially the application of calibration data to spectral data in the Level 1b-1c processing step so that the EnviView tool and its sub-tools became out-of-date. For that reason, ESA decided to split the command-line tool functionality from the viewing tool EnviView and presents now the user a stand-alone version of the command-line tool SciaL1c which calibration applications are based on the processor software used in ENVISAT PDS. From that, the user shall recognize to use not longer the SciaL1c tool provided with the EnviView software package.

The operational processing software undergoes in different cycles some upgrades so that the tool SciaL1c is also subject to changes. Note that the now provided version is designed in accordance with the operational Instrument Processing Facility (IPF) version 6.0/6.01. In order to avoid any incompatibilities with products generated with former IPF versions, the SciaL1c has been established downgrade-compatible so that former versions not only readable but can also be used.

In order to allow the users to track the assignment of the User’s Manual, the SciaL1c tool, and the IPF version, the version of SciaL1c and its documentation is kept in accordance to the IPF version for the main version number and version’s first digit, e.g. 6.0.

Note that with this version, the tool is currently available for following platforms:
– Linux
– Sun Solaris

The User’s Manual shall:

- Introduce into the level 1c product structure (including detailed description of data sets, which could be found in the annex).
- Explain the general meaning of the different extraction and calibration options in order to get the user prepared for his specific tasks.
- Give examples for different command lines, which may be used as a starting point for other, user specific extraction/application configurations.

The User’s Manual will not:

- Explain the full level 1b processing principles, which is far beyond the scope of this document. In this case the reader is referred to the ATBD (algorithm theoretical baseline document).

1.1 References

[1] PO-RS-MDA-GS-2009, Is. 3, Rev. C, Date : 16/10/97 “ENVISAT-1 PRODUCTS SPECIFICATIONS, Vol. 5: Product Structures”

[2] PO-RS-MDA-GS-2009, Is. 3, Rev. K, Date : 09/05/06 “ENVISAT-1 PRODUCTS SPECIFICATIONS, Vol. 15: SCIAMACHY products specifications”

[3] ENV-TN-DLR-SCIA-0005 Issue 6.0, 04/04/06 “SCIAMACHY Level 0 to 1b Processing Input/ Output Data Definition”

[4] ENV-TN-DLR-SCIA-0041 Issue 4.0, 19/05/05 “SCIAMACHY Level 0 to 1c Processing: Algorithm Basis Document”

1.2 Abbreviations

ADS	Annotation Data Set
ADSR	Annotation Data Set Record
ASCII	American Standard Code for Information Interchange
ASM	Azimuth Scan Mirror
BSDF	Bi-directional Scattering Distribution Function
BU	Binary Unit
DOAS	Differential Optical Absorption Spectroscopy
DS	Data Set
DSD	Data Set Description
DSR	Data Set Record
ENVISAT	Environmental Satellite
EnviView	Enivisat Viewing Toolbox
ESA	European Space Agency
ESM	Elevation Scan Mirror
ESTEC	European Space Centre of Technology
FPN	Fixed Pattern Noise
GADS	Global Annotation Data Set
GOME	Global Ozone Monitoring Experiment
IECF	Instrument Engineering Calibration Facility
IFE	Institut für Fernerkundung der Universität Bremen
IFOV	Instantaneous Field of View
I/O DD	Input/Output Data Definition
ISP	Instrument Science Packet
IPF	Instrument Processing Facility
LC	Leakage Current
MB	Megabyte
MDS	Measurement Data Set
MDSR	Measurement Data Set Record
MPH	Main Product Header
N/A	not applicable
ND	Neutral Density
NRT	Near Real Time
PCA	Polarisation Correction Algorithm
PDS	Payload Data Segment
PET	Pixel Exposure Time
PMD	Polarisation Measurement Device
PPG	Pixel-to-Pixel Gain
PQF	Product Quality Facility
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
SLS	Spectral Light Source
SGP	SCIAMACHY Ground Processor
SGP_01	SCIAMACHY Ground Processor for Level 0 to 1b Processing
SOS	SCIAMACHY Operations Support
SPH	Specific Product Header
SRON	Space Research Organisation of The Netherlands

SSAG	SCIAMACHY Scientific Advisory Group
SZA	Solar Zenith Angle
TPD	Technisch Physische Dienst
UTC	Universal Time Co-ordinate
WLS	White Light Source

1.3 Document Overview

The document is split in several chapters and an appendix which provides some technical details which are useful for a deeper understanding of the product format and content.

The chapters' content can be summarized to

- *Chapter 1* – is this chapter which provides an introduction including the references, abbrevations, and the document overview;
- *Chapter 2* – provides the user the general product layout and an outline of the tool;
- *Chapter 3* – is dedicated to the data set descriptions of the Level 1c data format;
- *Chapter 4* – introduces the handling of the tool;
- *Chapter 5* – provides some useful examples;
- *Appendix A* – gives an overview over the common data structures of Level 1b and Level 1c products;
- *Appendix B* – describes the data set record structure of the Level 1b product;
- *Appendix C* – adds the specific data set record structures for the Level 1c product; and
- *Appendix D* – is a compilation of parameter tables.

2 The general Scial1c s/w and product layout

SCIAMACHY level 1c products are user specific products, which will have the general ENVISAT data format, i.e. it will be a binary format and not an ASCII format, as still some users might expect.

What makes them so specific is that the user himself decides about its content. In terms of data obtained from the eight science detectors he can look at the data of

- a specific time interval
- a certain geographical area
- a specific measurement type (e.g. all nadir type measurements) or even a measurement categories (e.g. the nadir pointing measurements are a subset of type nadir)
- a specific spectral regions (i.e. clusters)

In terms of data obtained from the polarisation detectors (PMD), he can extract (in combination with filtering for time or geographical area)

- integrated PMD values (32 Hz, synchronised with science detector shortest integration time)
- fractional polarisation values.

Finally, he may decide to copy any further level 1b annotation data set (ADS) into his level 1c product, he may want to use later on for his data analysis.

Notes:

- From an extraction point of view, the smallest extractable unit of measurement data is data of one cluster, which obtained during execution of one specific instrument state, which matches one of the extraction criteria.
- In the remainder of this document, the options above will be referred to as extraction options as they generally select/reduce the amount of 1b data, being transferred to 1c.

Now, on top of that the user can specify how the data, obtained from the 8 science detectors, shall be calibrated. He can choose between

- No calibration
- Memory effect
- Leakage current
- PPG
- Etalon
- Spectral calibration
- Polarisation
- Radiance
- All calibrations

Finally one could say: Any combination of extraction and calibration options is allowed, which means that the user has an enormous freedom to "design" his specific level 1c product. On the other hand not each of the possible combination would be meaningful. E.g. A polarisation correction can only be applied, if spectral calibration was switched on as well.

The general structure of the product is depicted by figure 3.1. As any other ENVISAT data product, it will contain of a main product header (MPH) and a specific product header (SPH), which are just copied over from the level 1b input product. The remaining data sets – so called annotation and measurement data sets (ADS respectively MDS) – all depend on the user's specifications.

The instrument's operational concept (states, being executed in a timeline), is as much as possible reflected by the 1c data structure. This means that most of the data set records (except some of those calibration relevant copies of 1b data sets) contain data, which belong to one state, as it was executed along the orbit.

In more detail, the first column of the three general ADS depicted by figure 1, are basically copies of the level 1b product ADS, but only containing those records (1 record per state) of the extracted states (for details see Annex B). In general they are automatically generated, i.e. they don't have to be specified by the user (see also option –ds section). The "States of the product" ADS is of special importance because it contains mandatory information of state details, like e.g. the cluster definition, the exact duration, integration times etc. The bits and bytes of this data set can be found in annex B of this document.

The second column of figure 1 contains a so called "User Option" GADS. In this automatically generated data set, all selection criteria, the user has applied to the original level 1b product, are summarised in order to trace his work easily and to distinguish between e.g. 1c products, he has derived from the same 1b input. The details of this data set can be found in annex C of this document.

This is followed by the calibration GADS, which are pure copies of the level 1b product. The user might decide himself which of the individual calibration GADS of the 1b he wants to copy into 1c (see recommendations further down the document). Annex B shows the details of each of the data sets, whereas their selection is described in section "-ds option".

Finally, there will be in total 10 measurement data sets possible. Four measurement data sets (MDS) are reserved for nadir, limb, and occultation or monitoring cluster, i.e. science channel data.

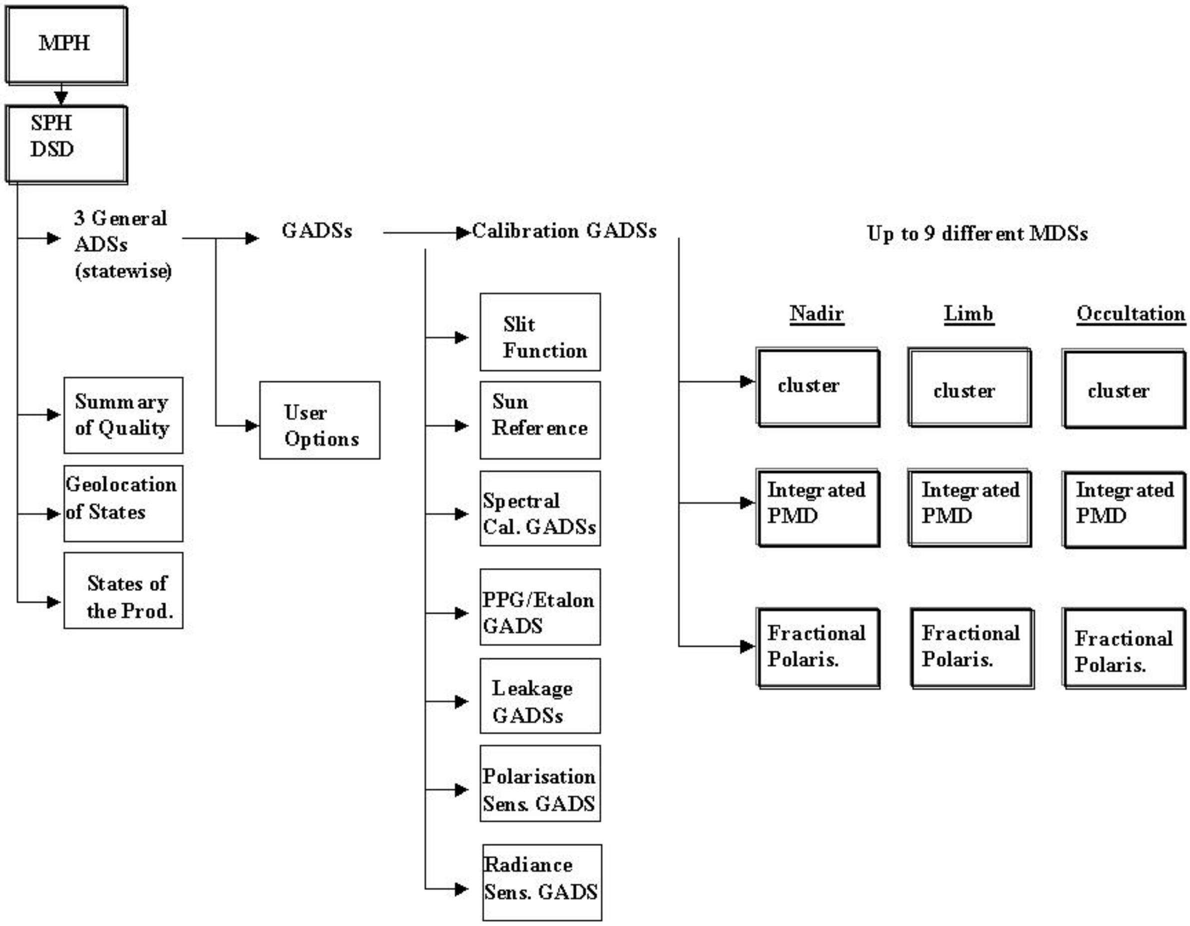

Figure 2-1 The general product structure. Please note that the measurement data set for (calibrated) monitoring data (from science channels) is not depicted in this figure.

Another three sets will contain so called integrated PMD data, again separated by nadir, limb or occultation. Finally, it is also possible to have fractional polarisation values for nadir, limb and occultation. In case of monitoring measurements, no PMD can be extracted. (The level 1b monitoring data sets do not contain integrated respectively fractional polarisation information. Therefore no monitoring related MDS can be foreseen here.)

Finally, the Enviview tool can directly be used to achieve a first may be basic visualisation of the results. Also, the "hdf" conversion capability of Enviview – which is another command line tool – may be used in order to prepare further processing of the 1c data.

3 Level 1c product data sets

In this section some more details of the level 1c data product data sets will be given. To improve the readability of this document, the full details of each data set, which may appear in the level 1c product, are attached in three different annexes.

1. Annex A: Common data structures
2. Annex B: Data sets, copied from the level 1b input product
3. Annex C: Data sets, unique for the level 1c product

The following (sub) chapters will mainly concentrate on the general concepts and ideas of each of the data sets.

3.1 The user options GADS

The user options GADS is basically meant to be a conclusive summary of all extraction and calibration options, the user has applied to the input level 1b product. Therefore the first field directly gives reference to the input level 1b product.

Generally, the various extraction and calibration options are interpreted as flags. They are set to 0, in case the option was disabled, and -1, if it was used.

In case of the geo-location filter was used, start and stop latitude and longitude coordinates will be given explicitly in the GADS in the subsequent fields. Similar it is done for the time filter. Whenever it was used, the selected start and stop times are given in UTC.

All other flags are easy to be interpreted from their names and what they will mean. Details can be found in Annex C.

3.2 Data sets for science channel data

As mentioned before, there can be one MDS for each of the main scientific measurement types which are nadir, limb and occultation. Also, a monitoring MDS may be created.

All MDS are organised in the same way, which should make reading it by other s/w straight forward. Generally, one single record of these MDS will contain data of one cluster which was obtained from execution of one state. The individual cluster readouts (or observations) are put in chronological order. They are followed by the geo-location information for the specific observation, which is a structure of its own (for details of this structures see annex A). Besides ground pixel co-ordinates this structure also hosts solar zenith and azimuth angles and more. The number of (cluster) observations and geo-locations in one record is identical, i.e. for each cluster observation there is exactly the corresponding geo-location attached.[1]

The user is kindly reminded of a general problem with SCIAMACHY level 1 data. Due to the different durations of states, the different cluster lengths and their different integration times, each level 1b and 1c measurement data record is of variable length. For the level 1c product, it

[1] This is a major advantage compared to the level 1b product. There we get geo-location information only on the time grid of the shortest integration time in a state. This is not necessarily the same as the cluster of interest.

was decided to make the record size at least easy computable from just a handful of parameters, which are common to all measurements.

Therefore the user may find each MDS (see Annex C) grouped in four blocks.

Block 1:
Fields 1 to 10: They are identical for all MDS, i.e. they are independent of the type of measurement, the cluster number, etc. They may be even called a fixed record header. They contain information to identify the record and the measurement data it contains, which are in particular field no. 8 (the number of observations) and field no. 9 (the number of pixels in the cluster).

Block 2:
Fields 11 to 13: The second block is composed of fields 11 (pixel ID), 12 (wavelength for pixel) and 13 (wavelength calibration error of pixel). Each field has the size of the cluster, i.e. it can be taken from field no. 9. The pixel/wavelength axis is only written once to each record, as it is common for all cluster readouts, which will follow.

Block 3:
Field 14 to 15: These two fields contain the actual measurement information, i.e. the individual cluster readouts. Their size corresponds to the product of the number of pixels (field no. 9) and the number of observations (field no. 8).

Block 4:
Field no. 16: This field just contains the geo-location information of each of the cluster readouts. Its repetition factor is given by the number of observations (i.e. field no. 9). The details of this structure, which is overtaken from the level 1b product, contains a huge amount of geophysical parameters like the corner coordinates of this specific measurement, the solar zenith and line of sight angles etc. The details are attached to this documents (see annex A)

Important note: The size of one of the geo-location structures is different for nadir, limb/occultation and monitoring measurements (see Annex A).

3.3 Data sets for integrated polarisation values

Integrated PMD data are, in difference to raw PMD data, synchronised with the science detectors. For that purpose they are linked to the shortest possible integration time in a science channel, which is 0.03125 seconds, which corresponds to 32 Hz. These integrated values are used e.g. in the virtual sum algorithm to determine the atmospheric degree of polarisation. Extraction of these values may therefore allow investigating the quality of the polarisation correction, especially when comparing it to fractional polarisation values. Another application of integrated PMD data could be – if normalised to the PMD values of the sun mean reference GADS – some broadband albedo plots.

Note that integrated PMD data sets can be created for only Nadir, Limb or Occultation measurements. In case of monitoring measurements, they are not even in the 1b product and therefore no corresponding monitoring data set can be created.

Similar as for the science data, the integrated PMD data set structure can also comprised to fixed and variable blocks (The detailed structure is given by Annex C). Again, there will be one record per state, which was executed in orbit.

Block 1:

Fields 1 to 9: They are identical for all integrated PMD MDS and contain information to identify the record and the measurement data it contains, which are in particular field no. 8 (the total number of PMD data) and field no. 9 (the number of geo-locations).

Block 2:
Field 10: PMD data is basically written to field no. 10 of the corresponding record structure (see Annex C). The total no. of integrated PMD values (field no. 8), divided by 7 (the number of PMD channels) basically gives the number of individual observations. This means that all 7 PMDs (ordered from 1 to 7) are repeated that many times

Block 3:
Field 11: In difference to the cluster MDS, the geo-location attached to these data sets, is not broken down to the 32 Hz of the integrated PMD data, but repeated with the shortest integration time in the state. Otherwise, the "gelocation overhead" would have been too large. Thanks to the fact that the PMD data is continuously in time, little is to be done on the user's side to find the geo-location values for each individual PMD readout value. The number of geo-locations is specified by field no. 9.

3.4 Data sets for fractional polarisation values

Fractional polarisation values are the atmospheric Stokes parameters itself, which are determined by level 0 to 1b processing for each individual integration time of a state. Values themselves are hidden in the level 1b defined "POLV" structure (see Annex A), which are written into the corresponding MDS records.

All fractional polarisation values, belonging to one integration time, are put in chronological order, starting with the longest integration time in the state.

Similar as for the science data, the fractional polarisation data set structure can also comprised to fixed and variable blocks (The detailed structure is given by Annex C). Again, there will be one record per state, which was executed in orbit.

Block 1:
Fields 1 to 12: They are identical for all integrated PMD MDS and contain information to identify the record and the measurement data it contains, which are in particular field no. 8 (the number of geo-location data), field no. 9 (the total number of fractional polarisation values) as well as field no. 12 (the repetition factors for the individual integration time).

Block 2:
Field 13: Fractional polarisation values are basically written to field no. 13 of the corresponding record structure (see Annex C). The "PolV" structure, containing Stokes vector information for about 12 points (see Annex A), is chronological written first for the longest integration time in the state (which has the lowest repetition factor (field 12), followed by the next shorter one.

Block 3:
Field 14: Geo-location is exactly handled as for integrated PMD records. The number of geo-locations is specified by field no. 8 and corresponds to the shortest integration time in a state. The number of geo-location points therefore automatically matches the number of fractional polarisation values, calculated for the highest repetition factor, which means that for each of these fractional polarisation values there is exactly one Geo-location structure. Consequently the user is forced to combine an appropriate number of Geo-locations whenever he wants to look at data, which belong to longer integration times, i.e. lower repetition factors.

3.5 Data sets copied over from the level 1b input product

Although principally any level 1b data set could be copied one to one into the level 1c product structure (see chapter about the "-ds option", this chapter will only refer to those data sets, which contain necessary annotation information or calibration parameters, which the user might want to extract for additional reference. It should help the user to decide what he needs.

PLEASE LOOK OUT FOR MANDATORY FILES!

As for the previously introduced data sets, the details are given now in appendix B.

Table 3-1 The level 1b calibration GADS. Details are referred to Appendix B.

1b GADS	Content (Summary)	Recommendation/Comments
Sun Mean Reference	Sun mean reference spectra 1 record per different ref. Spectrum Includes also PMD solar reference values	Mandatory for DOAS type trace gas retrieval
PPG/Etalon	PPG correction factor Etalon correction factor Dead/bad pixel mask	Mandatory for DOAS type trace gas retrieval
Slit Function (large Aperture)	Slit function to be applied for further processing of all nadir and limb and lunar occultation type measurements	Mandatory for DOAS type trace gas retrieval
Slit Function (small Aperture)	Slit function to be applied for further processing of all solar occultation measurements	Mandatory (but only) necessary in case of further processing of solar occultation measurements
Radiance Sensitivity Nadir	Full spectrum of nadir radiance response function for various ESM angles	In case a certain calibration application has not been selected, it is always recommended to extract associated 1b GADS as references.
Radiance Sensitivity Limb – Aperture large, ND filter out	Full spectrum of limb radiance response function for various ASM& ESM angles	
Radiance Sensitivity Limb – Aperture small, ND filter in (for Occultation)	Full spectrum of limb radiance response function for various ASM& ESM angles, considering small aperture and ND filter	
Polarisation Sensitivity Nadir	Full spectrum of $\mu_2=(1-\eta/1+\eta)$ Full spectrum of $\mu_3=(1-\zeta/1+\zeta)$ For different elevation mirror positions	
Polarisation Sensitivity Limb Aperture large, ND filter out	Full spectrum of μ2=(1- /1+) Full spectrum of μ3=(1- /1+) For different elevation and azimuth scan mirror positions	
Polarisation Sensitivity Limb – Aperture small, ND filter in (for Occultation)	Full spectrum of μ2=(1- /1+) Full spectrum of μ3=(1- /1+) For different elevation and azimuth scan mirror positions, ND filter in.	
Wavelength Calibration I (polynomial parameters)	Polynomial coefficients per channel	
Wavelength Calibration II (standard calibration)	Precise basis spectral calibration (one wavelength per pixel)	
Leakage current (constant fraction)	All kinds of orbital position independent parameters like fixed pattern noise etc.	
Leakage current (variable fraction)	Orbit dependent leakage parameters like the leakage current itself.	

4 General tool handling

Whenever the user wants to extract/calibrate level 1b data, the command line version “SciaL1C” needs to be called with options, the user wants to apply on the input level 1b product.

The command line would look like:

SciaL1C –option_1 –option_2 … -option_n Path\Inputfilename

The program name SciaL1C is case sensitive!

Options need to be separated by just a blank character from each other. without anyIf the input file is not in the same directory as the SciaL1C software, you have to specify the file including its path. The tool will then produce a level 1c file, having the filename:

Path\Inputfilename.child.

This means that the user has to type in the full product name – a very long name – only once. Additionally, the level 1c filename still allows identifying the product, as it contains start/stop sensing times, orbiting numbers etc. of the 1b input file.

Generally, the user is allowed to produce more than one level 1c file, based on the same level 1b input. E.g. he wants to investigate the input of a specific calibration parameter onto the calibrated signal. Whenever this happens, the tool identifies that automatically and just puts a running number in front of the new filename. In the data directory one would find:

Example:

INPUTFILENAME.child (based on INPUTFILE, but first set of options)
01 INPUTFILENAME.child (based on INPUTFILE, but second set of options)

Whenever the user then later wants to trace back the differences between the two 1c file versions, he can still look up the user options GADS, which contains a summary of all the flags he has set to derive the product. Alternatively, he can store the command line itself (see option “-b”)

4.1 Getting help – Option “-help”

Whenever questions related to syntax or options in general come up, there is some basic help on command line level.

1. SciaL1C –help| more will give a general summary of all and everything.
2. SciaL1C –help –option will give information of the requested option, only.

Of course, this can only be very brief help about handling the tool in general. Questions about e.g. data set records and their structures have to be referred to other documents or the help options of the EnviView tool itself.

4.2 Specifying the output directory – Option “-out”

If the result shall be written into a different directory then the input was, the –out option has to be used to specify the output path.

SciaL1C –option_1 –option_2 … -option_n -out Outputpath path\Inputfilename

4.3 Running in batch mode – Option “-b”

The SciaL1C command line tool is also able to run in batch mode. This shall be possible, if the batch file option (”-b”) is used. The batch file ”batch.bat” , which can be edited by any ASCII editor, may look like

–option_1 –option_2 … -option_n INPUTFILENAME1
–option_1 –option_2 … -option_n INPUTFILENAME2
–option_1 –option_2 … -option_n INPUTFILENAME3
–option_1 –option_2 … -option_n INPUTFILENAME4

In this case, 4 different input files would be processed in a certain way, specified by the options. As said above, the input files need not to be different.
The command line then simplifies to

SciaL1C –b batch.bat

The advantages of this batch operation are obvious. Many products can be treated in one go. Also, once the user has found his favourite extraction/application options, only the input filenames have to be changed.

4.4 Filtering by time – Option “-starttime & -stoptime”

To specify a time window for level 1b data to be selected (and may be calibrated) a start <u>and</u> stoptime has to be entered. Following syntax is applicable:

- -starttime DD-MMM-JJJJ HH:MM:SS.S
- -stoptime DD-MMM-JJJJ HH:MM:SS.S

The selected times can be found back in the user options GADS of the 1c product.

Practical advice:

1. Make sure that selected times are covered by the product (look up the 1b product first with Enviview).

When using only this filter, basically all kinds of measurement data could be extracted. If it is combined with selecting specific clusters, nadir and limb clusters would have to be specified separately. This is due to the different cluster definitions for nadir and limb measurements. See also Annex D respectively the command-line examples in chapter 5.

4.5 Filtering by Geo-location – Option “-topleft & - bottomright”

To specify level 1b data of geographical area of interest, the ”topleft” and ”bottomright” latitude and longitude coordinates have to be entered in degrees.

Longitude range: -180 to + 180
Latitude range: -90 to +90

The applicable syntax, the two coordinates each separated by blanks, would be:

- -topleft Latitude Longitude
- -bottomright Latitude Longitude

Practical advice:

1. Make sure that selected latitude and longitude values are covered by the product (look up the 1b product first with Enviview).
2. When using only this filter, basically all kinds of measurement data could be extracted. If it is combined with selecting specific clusters, nadir and limb clusters would have to be specified separately. This is due to the different cluster definitions for nadir and limb measurements. See also Annex D respectively the command line example section.
3. If the right boundaries are chosen, it is possible to extract a matching pair of nadir and limb measurement. As a decision support, the simple-map view function of enviview, when loading the level 1b input product, shall be used to visualise (on a lat/long map) the state’s corner coordinates.

4.6 Working on specific 1b data type only – Option “-type”

The option ”-type” can be used to specify which type of level 1b data shall be considered for level 1b to 1c processing. One may choose between the items

- Nadir
- Limb
- Occultation
- Monitoring
- All

The syntax to use is: -type item1,item2

The different items have to be separated by comma.

Default: Without applying this option, the default is –type nadir, which means that in this case only level 1b nadir data will be processed. This default will be overruled whenever option ”–cat” is explicitly mentioned as well as the time or geo-location filtering is applied. In this case the default is ‘–type all”.

Practical advice:

1. Selecting e.g. –type limb without any other options will process all data of the level 1b limb MDS. In other words, this would exclude all nadir type measurements.
2. In case, -type nadir was set, there are a couple of different nadir type measurements like nadir large and small swath width but also nadir pointing measurements. If one is interested in only e.g. the pointing states, one would have to combine it with the category option (see below).
3. The option can be combined with time and geo-location options, introduced earlier.
4. ”–type all” processes all level 1b MDS data (nadir, limb, occultation and monitoring). Without any further filter to reduce the amount of data, this is quite a long way to go.

It is also very convenient to combine this option with a specific cluster in order to narrow the spectral bandwidth.

4.7 Working on data of a specific measurement category – Option "-cat"

The "-cat" option is basically a more sensible filter than the "-type", which is explained in Table **Fehler! Kein Text mit angegebener Formatvorlage im Dokument.**-1.

Table Fehler! Kein Text mit angegebener Formatvorlage im Dokument.**-1 Coding of Measurement Categories**

Code #	Measurement Category	Function
1	Nadir	Scientific Measurement
2	Limb	Scientific Measurement
3	Nadir_pointing	Scientific Measurement
4	Solar Occultation, Scanning and Pointing at end of state	Scientific Measurement/Calibration
5	Solar Occultation, Pointing	Scientific Measurement/Calibration
6	Moon Occultation, Pointing	Scientific Measurement/Calibration
7	Moon Scanning	Scientific Measurement/Calibration
8	Sun over Diffuser, Neutral Density Filter out	Calibration
9	Sub Solar Calibration/Pointing	Calibration
10	Spectral Lamp Calibration	Calibration
11	White Lamp Calibration	Calibration
12	Dark current Calibration	Calibration
13	Nadir/Elevation Mirror Calibration, Pointing using the sun	Calibration
14	Nadir/Elevation Mirror Calibration, Scanning, using the moon	Calibration
15	ADC Calibration/ Scanner Maintenance	Calibration/Maintenance
16	Sun over Diffuser, Neutral Density Filter in	Calibration
17	Nadir Eclipse, pointing	Scientific Measurement
18	Nadir Eclipse, scanning	Scientific Measurement
19	White Lamp over Diffuser	Calibration/Monitoring
20	Dark_Current_calibration_HM	Calibration/Monitoring
21	NDF_Monitoring_(ND_OUT)	Monitoring
22	NDF_Monitoring_(ND_IN)	Monitoring
23	Sun_ASM_Diffuser	Calibration/Monitoring
24	Nadir_Pointing_Left	Monitoring
25	Sun_Asm_Diffuser_atmosphere	Monitoring
26	Limb_Mesosphere	Monitoring

Each category basically comprises a group of states or even a single state. They are coded with numbers from 1 to 19.

The syntax to be used is: -cat #1,#2

More than one category can be selected at once. Each category number, as specified by the table above, needs to be separated by comma.

Data will then be written into the corresponding 1c measurement data sets.

Practical advice:

1. Selecting "-cat 5,6,7" would look for only solar, lunar occultation respectively moon scanning data.
2. Data would automatically be written to the level 1c monitoring data set as the –type default nadir is overruled (see previous option).
3. The "-cat" option can of course also be combined with time or geographical filtering, but the probability of finding a granule (i.e. state) which fulfils this request, might not be too high. Therefore it is not recommended.
4. Selecting one or more clusters (see below) is always convenient.

4.8 Extracting spectral cluster – Option "-cluster"

The cluster option is the most powerful tool to get data sets which just contain the spectral information of interest instead of always getting the full SCIAMACHY bandwidth. Although it might be desirable to specify the wavelength interval in nm units directly, this is not the way SciaL1C can support it.

The operational concept took advantage of the fact that within each science detector groups of pixels, all having the same exposure time, may be combined to so called clusters. Each cluster can then be co-added on-board so that this group of pixels gets effectively a different integration time. The latter of course is equivalent to the ground pixel size. The smaller the integration time will be, the smaller the ground pixel, i.e. the higher the spatial resolution.

This clustering concept was introduced for 2 reasons. On the one side, the SCIAMACHY data rate could be regulated; on the other side spectral intervals with high scientific interest could get optimised w.r.t. their spatial resolution.

Now what SciaL1C supports is the selection of individual clusters, which can be addressed via an identifier in the range from 1 to 64. For details please look at annex D, where the definitions in terms of identifiers, pixel and wavelength range is laid out.

The syntax to be used is either

1. -clus 1,2,3….64:
2. -nadirclus 1,2,3…64
3. -limbclus 1,2,3…64
4. -occclus 1,2,3,….64
5. -monclus 1,2,3….64
6. –noclus

Practical Advice

Due to the fact that the cluster definition, i.e. the allocations of pixels to cluster identifiers is different at least for nadir or limb measurements, careful usage of the above mentioned options is recommended.

1. The default of the cluster options is of course to select all clusters. I.e. that would be the result if no cluster is specifically selected.

2. Whenever it is clear that only data of one type (which is having the same cluster definition for all states involved) it is sufficient to use "-clus"
3. Whenever time or geo-location filters are planned to be used in parallel, the selected data may be of different type and therefore using different cluster definitions. In these cases it is recommended to specify something like: -starttime utc_start –stoptime utc_stop –nadircluster 5,6 –limbcluster 3. This means that whenever nadir data is found in the 1b, only cluster 5 and 6 will be selected, but for limb data, cluster 3 will be taken only.
4. Cluster definitions (as given by annex D) are written to be in agreement with testdata. The definition (i.e. which cluster with identifier ID covers which wavelength range) has changed already and will change in future, probably. According support tables will be updated then in order to allow decision which cluster to select.
5. Finally there is also the option –noclus, which basically avoids to create cluster data related MDS at all. This may be practical for a user, who just wants to extract integrated PMD data or fractional polarisation values.

4.9 Copying level 1b data sets – Option "-ds"

This option is foreseen to select level 1b data sets, which shall be copied into the level 1c data. If it is not specified, the following level 1b data sets will be automatically in the 1c product:

- States of the product ADS
- Geo-location of States ADS
- Product Quality ADS
- PPG/Etalon GADS
- Sun mean reference GADS
- Slit function large aperture GADS

This default setting is defined for a level 1 user, who is preparing for his level 2 processing. Therefore those annotation data sets, which are mandatory for that purpose (see above) will extracted by default. It presumes that he does not need other calibration relevant GADS.

Whenever other data sets shall be extracted, the "-ds" option needs to be activated. The syntax is

-ds no1,no.2…no.n

Each 1b data set may be addressed via an identifier, which can be looked up in Annex D.

Alternatively, help on command line level can be ordered via

SciaL1C –list inputfilename |more

Practical advice

1. Whenever the –ds option is activated, the default (see above) <u>will no longer</u> be extracted automatically. This means that each data set, which shall go into the level 1c product, needs explicit mentioning.
2. The option may be most interesting for a level 1 user who is investigating the quality of the various calibration/correction parameters (or their impact on level 2 retrieval).

4.10 Extracting integrated PMD data – Option “-pmd”

Whenever integrated PMD values (see previous section) shall be in the 1c product, the user has to actively order them. I.e. by default, he won’t get this data.

The command syntax is as simple as

- pmd

Practical advice:

1. In case of monitoring states, no integrated PMD data are available. Be aware of this when setting the extraction options.
2. The integrated pmd values are probably of biggest use if the Sun mean reference GADS is extracted in parallel. If –ds is used, make sure to extract that GADS.

4.11 Extracting fractional polarisation values – Option “-fracpol”

Whenever fractional polarisation values (see previous section) shall be in the 1c product, the user has to actively order them. I.e. by default, he won’t get this data.

The command syntax is as simple as

-fracpol

Practical advice:

1. In case of monitoring states, no integrated PMD data are available. Be aware of this when setting the extraction options.

4.12 Calibrating the data – Option “-cal”

In this section the different corrections and calibration, which can be applied to SCIAMACHY science detector data, will be described. Principally one can choose to apply:

0. Memory Effect
1. Leakage current
2. pixel to pixel gain (ppg)
3. etalon
4. Straylight
5. Spectral calibration
6. Polarisation
7. Radiance
8. allcal

The syntax to be used is

-cal option1,option2…(options separated by comma)
-cal allcal

The idea is to let the user decide about which calibrations/corrections he might want to apply. Especially in the beginning this will be a very helpful thing because we first have to find out about the "quality" of the corrections, to be applied. Therefore one might want to compare same 1b input under different configurations of the calibration options, to learn about the absolute value of correction first and secondly to see the influence on a level 2 product, which is based on differently calibrated level 1c. (see examples section).

Practical advice

1. For the moment the default of the calibration options is set to no calibration, which might change in the future. Therefore one should not forget to specify the calibrations one wants to apply.
2. Calibrations 0 to 4 are all wavelength independent, no 6 and 7 are. This means they cannot be applied without a wavelength calibration being applied before.
3. Monitoring states cannot be calibrated for polarisation (because the 1b processor does not calculate fractional polarisation values for monitoring states). Therefore make sure that whenever "-cal allcal" is chosen, the selected data (i.e. selected by time, geo-location etc.) does not contain monitoring data, to avoid errors.
4. Radiance calibration for monitoring measurements is not supported.
5. Whenever a specific calibration/correction was not switched on, it is recommended to extract at least the calibration parameter related GADS values for further reference, if it is not contained in the "-ds" option anyway. Consider practical advice of this option as well.

5 Command line examples

In the following, some typical configurations for the extraction/applications will be discussed. They may be used as starting point for own configurations of the SciaL1C command line tool.

5.1 Extracting and calibrating level 1b data for further level 2 processing

A user who wants to do his own trace gas retrieval requires geo-loated spectral radiance, resulting from either nadir, limb or occultation measurements. He may want to do his analysis over the full orbit, considering all measurements of one category, e.g. all nadir states. As he wants to do a retrieval for a specific trace gas, he only needs limited spectral information, i.e. he will probably specify only one or a few spectral clusters.

For his purpose he needs (not necessarily) fully calibrated data. This means that he has to apply all calibrations or only a part of it. The Sun Mean Reference GADS, the PPG/Etalon GADS, containing the dead and bad pixel mask, and finally the Slitfunction GADS will be automatically in his product, unless he does not use the „-ds" option.

Integrated PMD data as well as fractional polarisation values are not necessarily needed for his retrieval and might therefore not be considered for extraction.

The command line (excluding product name and path) would look like

-type nadir –nadircluster 3,4,9,16 –allcal

- All nadir type measurements (so including eclipse scanning/pointing states) will be treated.
- Only clusters 3,4,9,16 will be in the product.
- If the 1b input product would contain e.g. 30 nadir type states, the 1b product would contain 120 records, each containing one cluster for one complete state.
- The ordering of records would be by time. I.e. The first record would be cluster 3 for nadir state 1 of the 1b product, the second record would be cluster 4 for nadir state 1 etc.
- All calibrations will be applied.
- Besides the MDS, the 1c product will contain all default data sets, which are necessary for further 1 to 2 processing.

-cat 1 –nadircluster 3,4,9,16 –cal 0,1,2,3,4,5,7 –ds 1,2,6,9,10,17,19

- All, but only nadir scanning, large swath width would be processed by applying this category filter (see previous sections).
- Same clusters extracted as under previous example.
- Same ordering of records as for previous example.
- All calibrations, except polarisation were applied.
- -ds option was used to get polarisation sensitivity GADS nadir (10) on top of the default (which is 1,2,6,9,17,19).

5.2 Extraction/calibration of 1b data for radiance verification/validation

This user wants to investigate the general quality of the level 1b product and its associated calibration GADS.

He most probably will restrict on data of one measurement (i.e. one state of either nadir, limb or occultation), selected via either time or geo-location of the measurement. The measurement he decides to take either corresponds to a certain atmospheric scenario he has references for. Another opportunity would be to take data with „known“ radiance targets like e.g. deserts.

In difference to user 1, he most probably will not narrow the spectral range. Calibrations he wants to apply step by step, starting from „no calibration“ applied to „full calibration“ , so that in the end he will derive different level 1c products from one and the same 1b input data, in order to estimate the different calibration impacts. In this case he might find it helpful to extract the 1b calibration GADS completely, in order to check their correct application.

For additional verification, he will not only investigate the science channels, but also the PMD channels – both, integrated values as well as atmospheric polarisation might be relevant. „ applicaton“ described above, would look like described below. No input filename as well as output path is specified.

Start and stoptimes (utc, see above) are just abbreviated to t1 and t2. This filter could of course be replaced by „topleft/bottomright“.

Below a typical batch file following the descripiton above, is written down.

```
-startime „t1“ –stoptime „t2“ –ds 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,31 –pmd –fracpol
-startime „t1“ –stoptime „t2“ –ds 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,31 –pmd –fracpol –cal 0
-startime „t1“ –stoptime „t2“ –ds 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,31 –pmd –fracpol –cal 0,1
-startime „t1“ –stoptime „t2“ –ds 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,31 –pmd –fracpol –cal 0,1,2
-startime „t1“ –stoptime „t2“ –ds 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,31 –pmd –fracpol –cal 0,1,2,3
-startime „t1“ –stoptime „t2“ –ds 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,31 –pmd –fracpol –cal 0,1,2,3,4
-startime „t1“ –stoptime „t2“ –ds 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,31 –pmd –fracpol –cal 0,1,2,3,4,5
-startime „t1“ –stoptime „t2“ –ds 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,31 –pmd –fracpol –cal 0,1,2,3,4,5,6
-startime „t1“ –stoptime „t2“ –ds 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,31 –pmd –fracpol –cal 0,1,2,3,4,5,6,7
```

For calling up this batch file, please look under „option –b“.

5.3 Extraction/calibration of 1b data for level 2 sensitivity studies

This user wants to investigate the impact of the various calibrations on the quality of a trace gas retrieval. Motivation of this exercise might result from validation activities. E.g. he tries to validate a SCIAMACHY ozone vertical column against a ground based value. In case he finds systematic deviations between the two columns he has to find out step by step, what might have gone wrong with the Sciamachy product – presuming of course his validation reference being the „truth“.

Therefore his demands will be very similar to those of user type 2, except that he will most probably limit his investigations on a small spectral window, which is relevant for his trace gas retrieval.

Calibrations he wants to in different combinations, so that in the end he will derive different level 1c products from one and the same 1b input data. These will be the input for his further trace gas retrieval, where he can investigate the impact of different calibrations on the trace gas product quality.

Below a typical batch file following the descripiton above, is written down.

```
-startime „t1“ –stoptime „t2“ –clus 16 –cal 0,1,2,3 –ds  a,b,c,d
-startime „t1“ –stoptime „t2“ –clus 16 –cal 0,1,2,3,4 –ds  a,b,c
-startime „t1“ –stoptime „t2“ –clus 16 –cal 0,1,2,3,4,5 –ds a,b
-startime „t1“ –stoptime „t2“ –clus 16 –cal 0,1,2,3,4,5,6 –ds a
-startime „t1“ –stoptime „t2“ –clus 16 –cal 0,1,2,3,4,5,6,7
```

Comments:

- By using just –clus 16, he would always get cluster 16 extracted, which has a different definition for nadir and limb in terms of allocated pixel, i.e. wavelengths. The user better makes sure that the time window (or alternative geo-location window) contains just one type of measurement data. Alternatively he has to specify nadir and limb clusters differently (see above).
- Of course, the impact of calibration effects on the level 2 processing can directly be tested along a full orbit, just specifying all nadir or all limb measurements. This can also be done and processed in one batch.
- Whatever the combination of filters would be, the output would always be a number of 1c files, all based on the same level 1b input file. They may turn up in all the same directory – this was not explicitly mentioned in this command line example. Files can easily be distinguished by a running number, indexed at the beginning of the output file names. This is done by SciaL1C automatically.

A COMMON 1B/1C DATA STRUCTURES

Annex A Table	Content
A.1	Data types used in 1b/1c data record tables
A.2	Predefined Structures of level 1b and 1c data products
A.3	The cluster configuration structure
A.4	Level 1b Signal values without co-adding (i.e. co-adding factor =1) – given for completeness only, as this structure is not used anymore in the level 1c
A.5	Level 1b Signal values with co-adding (i.e. co-adding factor unequal to 1) – given for completeness only, as this structure is not used anymore in the level 1c
A.6	Structure for fractional polarisation values
A.7	"Coord" structure
A.8	Geo-location – Limb/occultation structure
A.9	Geo-location – nadir structure
A.10	Geo-location – monitoring structure
A.11	Modified Julian date

A.1 Data types used in the following tables.

Notation	***Description***
sc	signed character: -128 to 127
uc	unsigned character: 0 to 255
ss	signed short (2-byte integer): -32768 to 32767
us	unsigned short (2-byte integer): 0 to 65535
sl	signed long (4-byte integer): -2.147.483.648 to 2.147.483.647
ul	unsigned long (4-byte integer): 0 to 4.294.967.295
sd	signed long long (8-byte integer): -9.223.372.036.854.775.808 to 9.223.372.036.854.775.807
du	unsigned long long (8-byte integer): 0 to 18.446.744.073.709.551.615
fl	float (4-byte real number): 3.40282347e+38 maximum absolute value to 1.17549435e-38 minimum absolute value
do	double (8-byte real number): 1.79e+308 maximum absolute value to 2.22e-308 minimum absolute value
tx	Text field
b	binary field (e.g. flags, detailed description in the remarks column)
<acronym>	two or more of the above (e.g. combined in structures)

A.2 Predefined structures which will be used in the following tables

Notation	***Description***
Clcon	Cluster configuration
Coord	Geographical co-ordinate (ISO 6709)
Flags	Quality Flags
GeoL	Geo-location for limb measurements
GeoN	Geo-location for nadir measurements
GeoCal	Geo-location for calibration and monitoring measurements
MJD	Modified Julian Date for the year 2000
PolV	Fractional polarisation values
Rsig	RETICON detector signal, memory effect correction and straylight record not co-added
Rsigc	RETICON detector signal, memory effect correction and straylight record co-added
Esig	EPITAXX detector signal and straylight record not co-added
ESigc	EPITAXX detector signal and straylight record co-added

A.3: The cluster configuration structure, as it appears in the States of the product ADS.

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Cluster ID (1-64 are valid entries for an existing cluster, the first cluster ID being '0' notifies the end of the cluster ID list)	-	uc	1	1
2	Channel Number (1-8)	-	uc	1	1
3	Start pixel number (inclusive, 0-1023)	-	us	1	2
4	Cluster length (1-1024)	-	us	1	2
5	Pixel Exposure Time (PET)	s	fl	1	4
6	Integration Time	$^1/_{16}$ s	us	1	2
7	Co-adding factor	-	us	1	2
8	Number of cluster readouts per DSR	-	us	1	2
9	Cluster data type (Rsig = 1, Rsigc = 2, ESig = 3, ESigc = 4)	-	uc	1	1
Size of compound Type:					*17*

Field no.9 distinguishes between the different science detector type (Rsig(c) stands for the reticon detectors without or with coadding, Esig(c) represents the Epitaxx detectors without or with coadding. This information is only needed in case of reading pure level 1b data. Their details can be found for completeness, below.

RETICON and Epitaxx detector signal with memory effect correction and straylight not co-added
Notation: Rsig respectively Esig

A.4: Reticon signal (i.e. science channel 1 to 5) without coadding

Field	*Comments*	*Unit*	*Type*	#	*Size*
1	Memory effect correction	BU	sc	1	1
2	Signal value of one detector element	BU	us	1	2
3	Straylight[2]	$^1/_{10}$ BU	uc	1	1
Size of compound Type:					*4*

Note: Co-adding factor equal to 1. In case of the epitaxx structure (Esig) the location for memory effect is reserved for non-linearity correction. For IPF versions below 6.0, this location is spare for epitaxx structure.

RETICON and Epitaxx detector signal with memory effect correction and stray-light co-added
Notation: Rsigc respectively Esigc

A.5: Reticon signal (i.e. science channel 1 to 5) with co-adding

Field	*Comments*	*Unit*	*Type*	#	*Size*
1	Signal value of one detector element and memory effect correction coded into one unsigned long value(the signal value is given in the lower 24 bits in BU, the memory effect correction is given in the upper 8 bits as signed character in BU)	BU	ul	1	4
2	Straylight	$^1/_{10}$ BU	uc	1	1
Size of compound Type:					*5*

Note that the co-adding factor is unequal to 1. In case of the epitaxx structure (Esigc) the location for memory effect is reserved for non-linearity correction. For IPF versions below 6.0, this location is spare for epitaxx structures.

Structure of field 1:

Rsigc

MSB			*LSB*
8 bit (sc)	*24 bit*		
Mem effect corr		Signal value	

[2] To yield the actual straylight the value for straylight given here and in the following data types has to be multiplied with the scale factor given in the States ADS for each state and channel.

Fractional polarisation values
Notation: PolV

A.6: The PolV structure, as it is used for the level 1c fractional polarisation data set.

Field	*Comments*	*Unit*	*Type*	#	*Size*
1	Fractional polarisation values Q (6 values derived from the PMDs, 5 values derived from the over-lapping regions and one model value below 300 nm)	-	fl	12	48
2	Errors on Q values	-	fl	12	48
3	Fractional polarisation values U (6 values derived from the PMDs and one model value below 300 nm)	-	fl	12	48
4	Errors on the U values	-	fl	12	48
5	Representing wavelength for the fractional polarisation values and the 45° PMD	nm	fl	13	52
6	GDF parameters	-	fl	3	12
Size of compound Type:					*256*

Some explanation to field 1 respectively 3: First 6 values, derived from the PMDs are given in ascending wavelength. Note that only 6 PMDs of different wavelength ranges are available. PMD 7, also called the 45 degree sensor, has the same throughput as PMD 4. These 6 values are followed by those parameters, derived from the 5 science channel overlaps, again sorted in ascending wavelength order. Overlaps are between channels 1&2, 2&3, 3&4, 4&5, 5&6.

Geographical co-ordinate (ISO 6709)

Notation: Coord

A.7: Structure Coord as it is used in geo-location records and structures.

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Latitude (-90 to 90, -90 is the south pole, 90 the north pole, 0 the equator)	10^{-6} deg	sl	1	4
2	Longitude (-180 to 180, meridian is '0' and minus is going to West)	10^{-6} deg	sl	1	4
Size of compound Type:					*8*

Geo-location for limb measurements

Notation: GeoL

A.8: The geo-location structure for limb measurement, as it appears in the level 1c measurement data set for limb and occultation measurements.

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Position of ESM compared to zero position	degree	fl	1	4
2	Position of ASM compared to zero position	degree	fl	1	4
3	Solar zenith angles of the start, middle and end of the integration time at TOA	degree	fl	3	12
4	Solar azimuth angles of the start, middle and end of the integration time at TOA.	degree	fl	3	12
5	Line-of-sight zenith angles of start, middle and end of the integration time at TOA.	degree	fl	3	12
6	Line-of-sight azimuth angles of start, middle and end of the integration time at TOA.	degree	fl	3	12
7	Satellite Height at the middle of the integration time	km	fl	1	4
8	Earth radius at the middle of the integration time	km	fl	1	4
9	Sub-satellite point at the middle of the integration time	-	Coord	1	8
10	Co-ordinates of tangent ground point of the start, middle and end of the integration time	-	Coord	3	24
11	Tangent height of the start, middle and end of the integration time	km	fl	3	12
12	Doppler shift at 500 nm at the middle of the integration time	nm	fl	1	4
Size of compound Type:					*112*

Geo-location for nadir measurements
Notation: GeoN

A.9: The geo-location structure for nadir measurements, as it appears in the level 1c measurement data set for nadir measurements.

Field	*Comments*	*Unit*	*Type*	#	*Size*
1	Position of ESM compared to zero position	degree	fl	1	4
2	Solar zenith angles of the start, middle and end of the integration time at TOA	degree	fl	3	12
3	Solar azimuth angles of the start, middle and end of the integration time at TOA	degree	fl	3	12
4	Line-of-sight zenith angles of start, middle and end of the integration time at TOA	degree	fl	3	12
5	Line-of-sight azimuth angles of start, middle and end of the integration time at TOA	degree	fl	3	12
6	Satellite Height at the middle of the integration time	km	fl	1	4
7	Earth radius at the middle of the integration time	km	fl	1	4
8	Sub-satellite point at the middle of the integration time	-	Coord	1	8
9	4 corner co-ordinates of the nadir ground pixel(the first co-ordinate is the one which is the first in time and flight direction, the second the first in time and last in flight direction, the third the last in time and first in flight direction and the fourth the last in time and flight direction)	-	Coord	4	32
10	Centre co-ordinate of the nadir ground pixel	-	Coord	1	8
Size of compound Type:					*108*

Geo-location for calibration and monitoring measurements
Notation: GeoCal

A.10: The geo-location structure for monitoring measurement, as it appears in the level 1c.

Field	*Comments*	*Unit*	*Type*	#	*Size*
1	Position of ESM compared to zero position	degree	fl	1	4
2	Position of ASM compared to zero position	degree	fl	1	4
3	Solar zenith angle at the middle of the integration time	degree	fl	1	4
4	Sub-satellite point at the middle of the integration time	-	Coord	1	8
Size of compound Type:					*20*

Modified Julian Date for the year 2000

Notation: MJD

A.11: The MJD structure as it is used in almost every 1b respectively 1c data record to notify the start time of measurement.

Field	***Comments***	***Unit***	***Type***	**#**	***Size***
1	Number of days elapsed since the 1.1.2000 at 00:00 hour (this may be negative before that date)	day	sl	1	4
2	Seconds elapsed since the beginning of the day	s	ul	1	4
3	Number of microseconds elapsed since the last second	us	ul	1	4
Size of compound Type:					*12*

B LEVEL 1B DATA SET RECORD STRUCTURES

Annex B Table	Content	Component Type	-DS FILTER IDENTIFIER
B.1	*Main Product Header*	*MPH*	
B.1	*Specific Product Header*	*SPH*	
B.1	*Data Set Descriptor*	*DSD*	
B.2	*Summary of Quality Flags*	*SQADS*	*1*
B.3	*Geo-location of the State*	*LADS*	*2*
B.4	*Static Instrument Parameters*	*GADS*	*3*
B.5	*Leakage Current Parameters (constant fraction)*	*GADS*	*4*
B.6	*Leakage Current Parameters (variable fraction)*	*GADS*	*5*
B.7	*PPG/Etalon Parameters*	*GADS*	*6*
B.8	*Precise Basis Array of Spectral Calibration*	*GADS*	*7*
B.9	*Spectral Calibration Parameters*	*GADS*	*8*
B.10	*Sun Reference Spectrum*	*GADS*	*9*
B.11	*Polarisation Sensitivity Parameters Nadir*	*GADS*	*10*
B.12	*Polarisation Sensitivity Parameters Limb/Occultation without ND*	*GADS*	*11*
B.13	*Polarisation Sensitivity Parameters Limb/Occultation with ND*	*GADS*	*12*
B.14	*Radiance Sensitivity Parameters Nadir*	*GADS*	*13*
B.15	*Radiance Sensitivity Parameters Limb/Occultation without ND*	*GADS*	*14*
B.16	*Radiance Sensitivity Parameters Limb/Occultation with ND*	*GADS*	*15*
B.17	*Errors on Key Data*	*GADS*	*16*
B.18	*Slit Function Parameters*	*GADS*	*17*
B.19	*Small Aperture Slit Function Parameters*	*GADS*	*18*
B.20	*States of the Product*	*ADS*	*19*
B.21	*PMD Data Packets*	*ADS*	*20*
B.22	*Auxiliary Data Packets*	*ADS*	*21*
B.23	*Leakage Current Parameters (newly measured*	*ADS*	*22*

Annex B Table	Content	Component Type	-DS FILTER IDENTIFIER
	parts)		
B.24	*Average of the Dark Measurements per State*	*ADS*	*23*
B.25	*PPG/Etalon Parameters, newly measured*	*ADS*	*24*
B.26	*Spectral Calibration Parameters, newly measured*	*ADS*	*25*
B.27	*Surn Reference Spectrum, newly measured*	*ADS*	*26*

Component: **Main Product Header**
Component Type: MPH No of Records: 1 Record Size: 1247

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	The Main Product Header is described in Ref. [1]	-	m	1	1247
				Size of Component:	*1247*

Component: **Specific Product Header of Level 1b Product**
Component Type: SPH No of Records: 1 Record Size: 693

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	The Specific Product Header is described in Ref. [2]	-	m	1	693
				Size of Component:	*693*

Component: **Data Set Descriptor Record**
Component Type: DSD No of Records: 36 Record Size: 280

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Data Set Descriptor Record, as described in Ref. [1]	-	m	36	280
Size of Component (all 36 DSDs):					*10080*

B.1: References for Main & Specific product headers as well as data set descriptors.

Component: **Summary of Quality Flags per State**
Component Type: SQADS No of Records: variable Record Size: 182

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Start time of the scan phase of the state	-	MJD	1	12
2	Flag indicating if MDS DSRs are attached to the current ADS DSR	-	uc	1	1
3	Mean value of the wavelength differences of Fraunhofer lines compared to the wavelength calibration parameters (per channel)	nm	fl	8	32
4	Standard deviation of the wavelength differences from field 3	nm	fl	8	32
5	Spare (Number of missing readouts in state)	-	us	1	2
6	Mean difference of leakage current or offset per channel and PMD (this field is only valid for limb states; channel 1 to 8, general PMD A to F and the 45° PMD)	%	fl	15	60
7	Sun glint region flag	-	uc	1	1
8	Rainbow region flag	-	uc	1	1
9	SAA region flag	-	uc	1	1
10	Number of hot pixel per channel and PMD (order: 1 to 8 and A to F and 45°)	-	us	30	30
11	Spare for additional flags	-	uc	10	10
Size of Component:					*182*

B.2: Summary of Quality flags from level 1b product (-ds 1).

Component: **Geo-location of the States**
Component Type: LADS No of Records: variable Record Size: 45

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Start time of the scan phase of the state	-	MJD	1	12
2	Flag indicating if MDS DSRs are attached to the current ADS DSR	-	uc	1	1
3	4 corner co-ordinates of the ground scene which is covered by the state (the first co-ordinate is the one which is the first in time and flight direction, the second the first in time and last in flight direction, the third the last in time and first in flight direction and the fourth the last in time and flight direction)	-	Coord	4	32
Size of Component:					*45*

B.3: Geo-location of States from level 1b (-ds 2). For “Coord” structure can be look up annex A.

Component: **Static Instrument Parameters**
Component Type: GADS No of Records: 1 Record Size: 382

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	n_lc_min	-	uc	1	1
2	ds_n_phases (~12)	-	uc	1	1
3	ds_phase_boundaries (# = ds_n_phase + 1)	-	fl	13	52
4	lc_stray_index	-	fl	2	8
5	lc_harm_order	-	uc	1	1
6	ds_poly_order	-	uc	1	1
7	do_var_lc_cha (3 times 4 characters per EPITAXX channel)	-	tx	12	12
8	do_stray_lc_cha (8 times 4 characters per channel)	-	tx	32	32
9	do_var_lc_pmd (2 times 4 characters per IR PMDs)	-	tx	8	8
10	do_stray_lc_pmd (7 times 4 characters per PMD)	-	tx	28	28
11	electrons_bu (per channel)	1/BU	fl	8	32
12	ppg_error	-	fl	1	4
13	stray_error	-	fl	1	4
14	sp_n_phases (~12)	-	uc	1	1
15	sp_phase_boundaries (# = sp_n_phase + 1)	-	fl	13	52
16	startpix_6+	-	us	1	2
17	startpix_8+	-	us	1	2
18	h_toa	m	fl	1	4
19	lambda_end_gdf	nm	fl	1	4
20	do_pol_point ("t" for true and "f" for false)	-	tx	12	12
21	sat_level	BU	us	8	16
22	pmd_saturation_limit	BU	us	1	2
23	do_use_limb_dark ("t" for true and "f" for false)	-	tx	1	1
24	do_pixelwise ("t" for true and "f" for false)	-	tx	8	8
25	alpha0_asm	degree	fl	1	4
26	alpha0_esm	degree	fl	1	4
27	do_fraunhofer (8 times 5 characters per channel)	-	tx	40	40
28	do_etalon (8 times 3 characters per channel)	-	tx	24	24
29	do_IB_SD_ETN ("t" for true and "f" for false)	-	tx	7	7
30	do_IB_OC_ETN ("t" for true and "f" for false)	-	tx	7	7
31	level_2_SMR	-	uc	8	8
Size of Component:					*382*

B.4 Static instrument parameters from level 1b (-ds 3). This data set basically contains essential summary of the level 0 to 1b initialisation file.

Component: **Leakage Current Parameters (constant fraction)**
Component Type: GADS No of Records: 1 Record Size: 163952

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Constant fraction of the fixed pattern noise (FPN) for each detector element of all eight channels (intersect of leakage current straight line)	BU	fl	8192	32768
2	Error on constant fraction of FPN	BU	fl	8192	32768
3	Constant fraction of the leakage current for each detector element of all eight channels (slope of leakage current straight line)	BU/s	fl	8192	32768
4	Error on constant fraction of LC	BU/s	fl	8192	32768
5	Constant fraction of the PMD dark offset of all 7 PMDs, for amplifier A and B (given as 1A, 1B, 2A, etc.)	BU	fl	14	56
6	Error on constant fraction of PMD offset	BU	fl	14	56
7	Mean noise (mean value of standard deviations per detector element)	BU	fl	8192	32768
Size of Component:					*163952*

B.5 Leakage current constant part from level 1b (-ds 4). It is a copy of the leakage current constant part GADS of the leakage current auxiliary file, as determined from the IECF.

Component: **Leakage Current Parameters (variable fraction)**
Component Type: GADS No of Records: appr. 12 Record Size: 90228

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Orbit phase after eclipse (range: 0-1)	-	fl	1	4
2	OBM (near radiator), detector (channels 6-8) and PMD temperatures	K	fl	10	40
3	Variable fraction of the leakage current on top of the constant fraction (field 1 and 3) for channels 6 to 8	BU/s	fl	3072	12288
4	Error of variable fraction of LC	BU/s	fl	3072	12288
5	Solar straylight scattered from the azimuth mirror	BU/s	fl	8192	32768
6	Error on the solar straylight	BU/s	fl	8192	32768
7	Straylight offset for PMDs	BU	fl	7	28
8	Error on straylight offset for PMDs	BU	fl	7	28
9	Variable fraction of the PMD dark offset on top of the constant fraction (field 5) for PMD 5 and 6	BU	fl	2	8
10	Error on the variable fraction of PMD offset	BU	fl	2	8
Size of Component (in case of 12 records):					*1082736*

B.6 Leakage current variable part from level 1b (-ds 5). It is a copy of the leakage current variable part GADS of the leakage current auxiliary file, as determined from the IECF. The number of orbital regions, i.e. the number of records is defined by the initialisation file (see B.3). The number of 12 is just a starting value for begin of life and will be verified (and probably adapted) during commissioning phase).

Component: **PPG/Etalon Parameters**
Component Type: GADS No of Records: 1 Record Size: 139264

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Pixel-to-pixel gain factor	-	fl	8192	32768
2	Etalon Correction Factor	-	fl	8192	32768
3	Etalon Residual	-	fl	8192	32768
4	WLS degradation factor	-	fl	8192	32768
5	Bad pixel mask	-	uc	8192	8192
Size of Component:					*139264*

B.7 PPG/Etalon GADS from level 1b (-ds 6). It is a copy of the ppg/etalon auxiliary file, as determined from the IECF. Especially field no. 5, the bad pixel mask is of importance for further level 2 retrievals. If no “ds” option is used, this data set will be automatically in the level 1c output product.

Component: **Precise Basis of the Spectral Calibration Parameters**
Component Type: GADS No of Records: 1 Record Size: 32768

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Wavelength of detector pixel	-	fl	8192	32768
Size of Component:					*32768*

B.8 Precise Bais of the spectral Calibration Parameters from level 1b (-ds 7). This data set can be seen as the best guess assignment between pixel and wavelength. All deviations from this basic assignment are covered by the second spectral calibration set, which is then based on (maily) oboard SLS measurements along the orbit.

Component: **Spectral Calibration Parameters**
Component Type: GADS No of Records: 12 Record Size: 372

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Orbit phase after eclipse (range: 0-1)	-	fl	1	4
2	Coefficients of the 4th order polynomial for each detector array (channel)	-	do	40	320
3	Number of used lines per channel	-	us	8	16
4	Wavelength calibration error per channel	-	fl	8	32
Size of Component:					*4464*

B.9 Precise Bais of the spectral Calibration Parameters from level 1b (-ds 8). Orbit analysis has been performed by the IECF, first which gives this information bakc as the spectral calibration auxiliary file.

Component: **Sun Reference Spectrum**
Component Type: GADS No of Records: variable Record Size: 163942

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Sun spectrum identifier ("Dn" for sun diffuser , "O∅" for occultation, "S∅" for sub-solar; "n" may indicate various diffuser angles)	-	tx	2	2
2	Wavelength of the sun measurement	nm	fl	8192	32768
3	Mean sun reference spectrum	photons/ $m^2 \cdot nm \cdot s$	fl	8192	32768
4	Radiometric precision of the mean sun reference spectrum		fl	8192	32768
5	Radiometric accuracy of the mean sun reference spectrum	-	fl	8192	32768
6	Diffuser/Small Aperture Etalon	-	fl	8192	32768
7	Average azimuth mirror position	degree	fl	1	4
8	Average elevation mirror position (diffuser)	degree	fl	1	4
9	Average solar elevation angle	degree	fl	1	4
10	Mean value of the corresponding PMD measurements	BU	fl	7	28
11	PMD out-of-band signal with ND out	BU	fl	7	28
12	PMD out-of-band signal with ND in	BU	fl	7	28
13	Doppler shift at 500 nm	nm	fl	1	4
Size of Component:					*163942*

B.10 Sun mean reference GADS Parameters from level 1b (-ds 9). It is a copy of the sun mean reference auxiliary file, as determined from the IECF. If no “ds” option is used, this data set will be automatically in the level 1c output product. This data set may contain more than one record, each containing a reference spectrum from different source (e.g. old diffuser, new diffuser, via azimuth and elevation mirror (occultation) or via elevation mirror only (subsolar). May be, there will be even old diffuser measurements under different then regular angles, which are just optimised for normalisation of single spectral channels. Commissioning will hopefully show that. The important thing about this data set is that the level 1c user, if he wants to do his own level 2 processing, can decide himself which spectrum he wants to take for normalisation.

Component: **Polarisation Sensitivity Parameters Nadir**
Component Type: GADS No of Records: 10 Record Size: 65540

Field	*Comments*	*Unit*	*Type*	#	*Size*
1	Elevation mirror position	degree	fl	1	4
2	μ_2 nadir for the elevation mirror position of field 1	-	fl	8192	32768
3	μ_3 nadir for the elevation mirror position of field 1	-	fl	8192	32768
Size of Component (of 10 records):					*655400*

B.11: Polarisation sensitivity parameters nadir from 1b product (ds -10). $\mu 2$ respectively $\mu 3$ are calculated from keyparamters η and ζ. $\mu 2 = (1-\eta)/(1+\eta)$. $\mu 3 = (1-\zeta)/(1+\zeta)$. They are on the same spectral grid as the sun mean reference GADS. Both parameters are part of the nadir polarisation correction factor.

Component: **Polarisation Sensitivity Parameters Limb/Occultation without ND**
Component Type: GADS No of Records: 20 Record Size: 65544

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Elevation mirror position	degree	fl	1	4
2	Azimuth mirror position	degree	fl	1	4
3	μ_2 limb for the elevation and azimuth mirror position of field 1 and 2	-	fl	8192	32768
4	μ_3 limb for the elevation and azimuth mirror position of field 1 and 2	-	fl	8192	32768
Size of Component:					*65544*

B.12: Polarisation sensitivity parameters limb from 1b product (ds -11). μ2 respectively μ3 are calculated from keyparamters η and ζ. μ2 = (1-η)/(1+η). μ3 = (1-ζ)/(1+ζ). (the limb ones). They are on the same spectral grid as the sun mean reference GADS. Both parameters are part of the limb polarisation correction factor. They have to be looked for polarisation correction of regular limb measurements. The related data set below is strictly spoken only applicable for occultation measurements, as there are indications that the instrument eta function is changed by the neutral density filter, which is used for these measurements to reduce the signal in channels 3 to 6.

Component: **Polarisation Sensitivity Parameters Limb/Occultation with ND**
Component Type: GADS No of Records: 20 Record Size: 65544

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Elevation mirror position	degree	fl	1	4
2	Azimuth mirror position	degree	fl	1	4
3	μ_2 limb for the elevation and azimuth mirror position of field 1 and 2	-	fl	8192	32768
4	μ_3 limb for the elevation and azimuth mirror position of field 1 and 2	-	fl	8192	32768
Size of Component:					*65544*

B.13: Polarisation sensitivity parameters limb from 1b product (ds -12). Both parameters are part of the occultation polarisation correction factor (see comments above). Mirror positions are different from limb.

Component: **Radiance Sensitivity Parameters Limb/Occultation with ND**
Component Type: GADS No of Records: 100 Record Size: 32772

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Elevation mirror position	degree	fl	1	4
2	Radiance sensitivity for the elevation and azimuth mirror position of field 1 and 2	(BU/s)/ (photons/ m^2·nm·sr·s)	fl	8192	32768
Size of Component (of 100 records):					*3277200*

B.14: Radiance sensitivity parameters nadir from 1b product (ds -13). It is on the same spectral grid as the sun mean reference GADS. The number of angular grid points is defined in the level 0 to 1b initialisation file.

Component: **Radiance Sensitivity Parameters Limb/Occultation without ND**
Component Type: GADS No of Records: 100 Record Size: 32776

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Elevation mirror position	degree	fl	1	4
2	Azimuth mirror position	degree	fl	1	4
3	Radiance sensitivity for the elevation and azimuth mirror position of field 1 and 2	(BU/s)/ (photons/ m^2·nm·sr·s)	fl	8192	32768
Size of Component (of 100 records):					*3277600*

B.15: Radiance sensitivity parameters limb from 1b product (ds -14). It is on the same spectral grid as the sun mean reference GADS. The number of angular grid points is defined in the level 0 to 1b initialisation file.

Component: **Radiance Sensitivity Parameters Limb/Occultation with ND**
Component Type: GADS No of Records: 100 Record Size: 32776

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Elevation mirror position	degree	fl	1	4
2	Azimuth mirror position	degree	fl	1	4
3	Radiance sensitivity for the elevation and azimuth mirror position of field 1 and 2	(BU/s)/(photons/ m^2·nm·sr·s)	fl	8192	32768
Size of Component (of 100 records):					*3277600*

B.16: Radiance sensitivity parameters occultation from 1b product (ds -15). It is on the same spectral grid as the sun mean reference GADS. The number of angular grid points is defined in the level 0 to 1b initialisation file. The main difference to the previous data set are basically the elevation and azimuth mirror positions, which are in this case only covering the solar occultation observational range.

Component: **Errors on Key Data**
Component Type: GADS No of Records: 1 Record Size: 294912

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Error on μ_2 nadir	-	fl	8192	32768
2	Error on μ_3 nadir	-	fl	8192	32768
3	Error on μ_2 limb	-	fl	8192	32768
4	Error on μ_3 limb	-	fl	8192	32768
5	Error on the radiance sensitivity for the optical bench only	(BU/s)/(photons/m^2·nm·sr·s)	fl	8192	32768
6	Error on radiance sensitivity for elevation mirror only (nadir viewing)	-	fl	8192	32768
7	Error on radiance sensitivity for elevation and azimuth mirror (limb viewing)	-	fl	8192	32768
8	Error on radiance sensitivity for diffuser and azimuth mirror (sun diffuser measurement)	-	fl	8192	32768
9	Error on BSDF	-	fl	8192	32768
Size of Component:					*294912*

B.17: Errors on Keydata from 1b product (ds -16). It is on the same spectral grid as the sun mean reference GADS.

Component: **Slit Function Parameters**
Component Type: GADS No of Records: 40 Record Size: 11

Field	***Comments***	***Unit***	***Type***	**#**	***Size***
1	Pixel position for which the slit function is given (0-8191)	-	us	1	2
2	Type of slit function (1 = gauss, 2 = single hyperbolic, 3 = voigt)	-	uc	1	1
3	FWHM of slit function [pixel]	-	fl	1	4
4	For voigt: FWHM of Lorenzian part [pixel]	-	fl	1	4
Size of Component:					*440*

B.18: Slit function parameters – large aperture from level 1b product(-ds 17). This data set is mandatory for level 2 processing and will be part of the 1c default extracted data, i.e. if the –ds option is not applied.

Component: **Small Aperture Slit Function Parameters**
Component Type: GADS No of Records: 40 Record Size: 11

Field	***Comments***	***Unit***	***Type***	**#**	***Size***
1	Pixel position for which the slit function is given (0-8191)	-	us	1	2
2	Type of slit function (1 = gauss, 2 = single hyperbolic, 3 = voigt)	-	uc	1	1
3	FWHM of slit function [pixel], for voigt: Lorenzian part	-	fl	1	4
4	For voigt only: FWHM of Gaussian part [pixel]	-	fl	1	4
Size of Component:					*440*

B.19: Slit function parameters – small aperture from level 1b product(-ds 18). This data set is mandatory for level 2 processing only in those cases measurements with small aperture (sun occultation) shall be processed. This data set will not be part of the default 1c data sets and has to be selected via –ds 18, anyway.

Component: **States of the Product**

Component Type: ADS No of Records: variable Record Size: 1387

Field	*Comments*	*Unit*	*Type*	#	*Size*
1	Start time of scan phase of the state	-	MJD	1	12
2	Flag indicating if MDS DSRs are attached to the current ADS DSR (1: no, 0: yes)	-	uc	1	1
3	Reason code if the attachment flag is set to '1' 0: MDS DSRs are not attached, because this type measurement is not intended to be in the level 1b product (dark measurements) 1: the measurement state was corrupted	-	uc	1	1
4	Orbit phase after eclipse of the state (range: 0-1)	-	fl	1	4
5	Measurement Category	-	us	1	2
6	State ID	-	us	1	2
7	Duration of scan phase of the state	$^1/_{16}$ s	us	1	2
8	Longest integration time	$^1/_{16}$ s	us	1	2
9	Number of clusters	-	us	1	2
10	Cluster Configuration	-	Clcon	64	1088
11	MDS for this state (1 = nadir, 2 = limb, 3 = occultation, 4 = monitoring)	-	uc	1	1
12	Number of repeated geo-location and level 0 headers	-	us	1	2
13	Number of integrated PMD values	-	us	1	2
14	Number of different integration times in all clusters	-	us	1	2
15	Various integration times in this state	$^1/_{16}$ s	us	64	128
16	Number of fractional polarisation values per different integration time	-	us	64	128
17	Total number of fractional polarisation values	-	us	1	2
18	Number of DSRs	-	us	1	2
19	Length of DSR	-	ul	1	4
Size of Component:					*1387*

B.20: States of the product ADS from level 1b product(-ds 19). This data set, which is present for each state, which has been executed, is part of the 1c default extracted data, i.e. if the –ds option is not applied. It contains state execution parameters which are generally helpful to interpret the 1b respectively 1c data. Again, as soon as the –ds option is activated, one should not forget to explicitly extract this data set.

Component: **PMD Data Packets**
Component Type: ADS No of Records: variable Record Size: 6833

Field	***Comments***	***Unit***	***Type***	***#***	***Size***
1	Start time of the PMD data packet	-	MJD	1	12
2	Flag indicating if MDS DSRs are attached to the current ADS DSR	-	uc	1	1
3	PMD data packet of the level 0 data	-	b	6820	6820
Size of Component:					*6833*

B.21: PMD Data Packets ADS from 1b product (-ds 20). This data set basically contains the raw PMD data which is still at 40 Hz, i.e. not synchronised with the science detectors. It is totally uncalibrated and still in level 0 format (field 3). So this data set may be interesting only for some specialist who are able to read level 0 data and who just want to extract the raw PMD data. Most scientific applications would better take the sychronised and calibrated „integrated PMD values" (see Annex C).

Component: **Auxiliary Data Packets**
Component Type: ADS No of Records: 780 Record Size: 1679

Field	***Comments***	***Unit***	***Type***	***#***	***Size***
1	Start time of the auxiliary data packet	-	MJD	1	12
2	Flag indicating if MDS DSRs are attachedto the current ADS DSR	-	uc	1	1
3	Auxiliary data packet of the level 0 data	-	b	1666	1666
Size of Component:					*1309620*

B.22: Auxiliary Data Packets ADS from 1b product (-ds 21). This data set basically contains the raw, i.e. level 0 formatted auxiliary data packets (field no. 3). This data set may be interesting only for some specialist who are able to read level 0 data and who just want to extract this auxiliary data.

Component: **Leakage Current Parameters (newly calculated partial set)**
Component Type: ADS No of Records: ~12 Record Size: 164021

Field	***Comments***	***Unit***	***Type***	***#***	***Size***
1	Start time of the first dark measurement state which was used to calculate this ADSR	-	MJD	1	12
2	Flag indicating if MDSRs are attached to the current ADSR (always set to 1, because these parameters are not directly related to a MDS)	-	uc	1	1
3	Start time of the last dark measurement state which was used to calculate this ADSR	-	MJD	1	12
4	Orbit phase after eclipse (range: 0-1)	-	fl	1	4
5	OBM (near radiator), detector (8x) and PMD temperatures	BU	fl	10	40
6	Fixed pattern noise for channels 1 to 8	BU	fl	8192	32768
7	Error on the FPN	BU	fl	8192	32768
8	Leakage current for channels 1 to 8	BU/s	fl	8192	32768
9	Error on the LC	BU/s	fl	8192	32768
10	Mean noise (mean value of standard deviations per detector element)	BU	fl	8192	32768
11	PMD dark offset for all PMDs for the amplifier A and B (1A, 1B, 2A, etc.)	BU	fl	14	56
12	Error on the PMD offset	BU	fl	14	56
Size of Component:					*164021*

B.23: Leakage current (newly measured) ADS from 1b product (-ds 22). This data set basically contains the input for the IECF, which is doing an orbital analysis of it before it gives it back to the processing in form of an auxiliary file. This data set may be extracted and used as reference/point of comparison against the corresponding GADS. But note that this is NOT THE LEAKAGE CURRENT WHICH IS USED FOR LEAKAGE CURRENT CALIBRATION. THIS IS ALWAYS TAKEN FROM THE GADS.

Component: **Average of the Dark Measurements per State**
Component Type: ADS No of Records: variable Record Size: 131253

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Start time of the dark measurement state which was used to calculate this ADSR	-	MJD	1	12
2	Flag indicating if MDSRs are attached to the current ADSR (always set to 1, because these parameters are not directly related to a MDS)	-	uc	1	1
3	Average dark measurement spectrum	BU	fl	8192	32768
4	Standard deviation of the dark measurement spectrum	BU	fl	8192	32768
5	PMD dark offset for all PMDs for the amplifier A and B (1A, 1B, 2A, etc.)	BU	fl	14	56
6	Error on the PMD offset	BU	fl	14	56
7	Solar straylight scattered from the azimuth mirror	BU/s	fl	8192	32768
8	Error on the solar straylight	BU/s	fl	8192	32768
9	Straylight offset for PMDs	BU	fl	7	28
10	Error on the PMD straylight offset	BU	fl	7	28
Size of Component:					*131253*

B.24: Leakage current (average) ADS from 1b product (-ds 23). This data set basically contains the second input for the IECF, which is doing an orbital analysis of it before it gives it back to the processing in form of an auxiliary file. This data set may be extracted and used as reference/point of comparison against the corresponding GADS. It might be of particular interest during early phases of the mission, as the avarage dark measurement spectrum (field no. 3) is basically the raw dark current data of a dark current state (but just averaged over the dark current state duration).

But also note that this is NOT THE LEAKAGE CURRENT WHICH IS USED FOR LEAKAGE CURRENT CALIBRATION. THIS IS ALWAYS TAKEN FROM THE GADS.

Component: **PPG/Etalon Parameters**
Component Type: ADS No of Records: 1 Record Size: 172045

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Start time of the WLS measurement state which was used to calculate this ADSR	-	MJD	1	12
2	Flag indicating if MDSRs are attached to the current ADSR (yes, in the Monitoring MDS)	-	uc	1	1
3	Pixel-to-pixel gain factor	-	fl	8192	32768
4	Etalon Correction Factor	-	fl	8192	32768
5	Etalon Residual	-	fl	8192	32768
6	Average WLS spectrum which has been used for the determination of PPG and Etalon	BU	fl	8192	32768
7	Standard deviation of the WLS spectrum	BU	fl	8192	32768
8	Bad pixel mask	-	uc	8192	8192
Size of Component:					*172045*

B.25: PPG/Etalon (nefwly measured) ADS from 1b product (-ds 24). This data set basically contains the input for the IEC, which is doing a quality\ analysis of it before it gives it back to the processing in form of an auxiliary file. Especially the bad pixel mask – here it contains values, determined by the 0/1b processor, which are dead/bad on top of the already known ones – are first set back to the keydata values, unless confidence is given that a specific pixel is really dead/bad. This will not be decided without integrated a number of detector experts.

This data set may be extracted and used as reference/point of comparison against the corresponding GADS. It might be of particular interest during early phases of the mission.

But also note that this is NOT THE PPG/ETALON VALUES WHICH ARE USED FOR PPG & ETALON CALIBRATION. THEY ARE ALWAYS TAKEN FROM THE GADS.

Component: **Spectral Calibration Parameters**
Component Type: ADS No of Records: variable Record Size: 33257

Field	***Comments***	***Unit***	***Type***	**#**	***Size***
1	Start time of the SLS or sun measurement state which was used to calculate this ADSR	-	MJD	1	12
2	Flag indicating if MDSRs are attached to the current ADSR (yes, in the Monitoring MDS)	-	uc	1	1
3	Orbit phase after eclipse (range: the absolute value is between '0' and '1')	-	fl	1	4
4	Coefficients of the 4th order polynomial for each detector array (channel)	-	do	40	320
5	Source of spectral calibration parameters (0=SLS, 1=sun)	-	uc	8	8
6	Number of used lines per channel	-	us	8	16
7	Wavelength calibration error per channel	-	fl	8	32
8	Average SLS or solar spectrum which has been used for the determination of spectral calibration parameters	BU	fl	8192	32768
9	Selected line positions for 3 lines per channel	nm	fl	24	96
Size of Component:					*33257*

B.26: Spectral Calibration Parameters (nefwly measured) ADS from 1b product (-ds 25). This data set basically contains the input for the IEC, which is doing orbital analysis of it before it gives it back to the processing in form of an auxiliary file.

This data set may be extracted and used as reference/point of comparison against the corresponding GADS, which is in fact the copy of the auxiliary file, which was produced by the IECF. It might be of particular interest during early phases of the mission.

But also note that this is NOT THE SPECTRAL CALIBRATION PARAMETERS WHICH ARE USED FOR SPECTRAL CALIBRATION. THEY ARE ALWAYS TAKEN FROM THE GADS.

Component: **Sun Reference Spectrum**
Component Type: ADS No of Records: variable Record Size: 163928

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	Start time of the sun diffuser measurement state which was used to calculate this ADSR	-	MJD	1	12
2	Flag indicating if MDSRs are attached to the current ADSR (yes, in the Monitoring MDS)	-	uc	1	1
3	Sun spectrum identifier ("D∅" for sun diffuser, "O∅" for occultation, "S∅" for sub-solar)	-	tx	2	2
4	Neutral density filter flag	-	uc	1	1
5	Wavelength of the sun spectrum	nm	fl	8192	32768
6	Mean sun reference spectrum	photons/ m^2·nm·s	fl	8192	32768
7	Relative radiometric precision of the mean sun reference spectrum	-	fl	8192	32768
8	Relative radiometric accuracy of the mean sun reference spectrum	-	fl	8192	32768
9	Diffuser/Small Aperture Etalon	-	fl	8192	32768
10	Average azimuth mirror position	degree	fl	1	4
11	Average elevation mirror position (diffuser)	degree	fl	1	4
12	Average solar elevation angle	degree	fl	1	4
13	Mean value of the corresponding PMD measurements	BU	fl	7	28
14	PMD out-of-band signal	BU	fl	7	28
15	Doppler shift at 500 nm	nm	fl	1	4
Size of Component:					*163928*

B.27: Sun mean reference spectrum (newly measured) ADS from 1b product (-ds 26). This data set basically contains the input for the IECF, which copies the new records into the corresponding auxiliary file, which is then given back to the processing. The IECF just overwrites the auxiliary file records, which belong to the same type as the newly measured input.

This data set may be extracted and used as reference/point of comparison against the corresponding GADS, which is in fact the copy of the auxiliary file, which was produced by the IECF. It might be of particular interest during early phases of the mission.

But also note that this is NOT THE SUN REFERENCE DATA SET WHICH IS USED FOR DOAS TYPE RETRIEVALS IN THE LEVEL 1B TO 2 NRT PROCESSOR. THIS IS AWAYS TAKEN FROM THE GADS.

C LEVEL 1C SPECIFIC DATA RECORD STRUCTURES

Annex C Table	**Content**
C.1	The level 1c MDS structure (science channel data)
C.2	The integrated PMD MDS record structure
C.3	The fractional polarisation record structure

C.4	The user options GADS record structure

Component: **1c MDS structure**
Component Type: MDS No of Records: variable Record Size: variable

Field	*Comments*	*Unit*	*Type*	#	*Size*
1	Start time of scan phase of the state	-	MJD	1	12
2	DSR length	-	fl	1	4
3	Quality flag -1 for blank record, 0 otherwise	-	sc	1	1
4	Orbit phase after eclipse (range: 0-1)	-	fl	1	4
5	Measurement Category	-	us	1	2
6	State ID	-	us	1	2
7	Cluster ID of selected Cluster in the state (can have a value between 1 and 64, according to the number of defined clusters per nadir respectively limb/occ/monitoring state)	-	us	1	2
8	Number of observations for selected cluster Nobs.	-	us	1	2
9	Number of pixels in selected cluster Npixels	-	us	1	2
10	Unit flag for following fields (0: BU, -1: radiance units)	-	us	1	
11	Pixel ID for cluster	-	uc	Npixels	Npixels*2
12	Wavelength for pixels in cluster n	nm	fl	Npixels	Npixels*4
13	Wavelength calibration error for pixels in cluster n	nm	fl	Npixels	Npixels*4
14	Signal value for one detector element of the selected cluster	Depends on Flag field 10	fl	Npixels *Nobs	Npixels*Nobs*4
15	Signal error for one detector element of the selected cluster	Depends on Flag field 10	fl	Npixels *Nobs	Npixels*Nobs*4
16	Geo-locations for selected cluster	-	GeonN or GeoL or Geocal	Nobs	Nobs*108 (Nadir) Nobs*112 (Limb/Occ) Nobs*20 (monitoring)

C.1: The level 1c MDS structure. There are no architectural differences between the different types of MDS (nadir, limb, occultation or monitoring). Depending on the type of MDS (i.e. whether it contains nadir, limb, occultation or monitoring data), corresponding geo-location structures are used in field 16. Their definition can be found in Annex A.

Component: **1c integrated PMD MDS structure**
Component Type: MDS No of Records: variable Record Size: variable

Field	***Comments***	***Unit***	***Type***	**#**	***Size***
1	Start time of scan phase of the state	-	MJD	1	12
2	DSR length		fl	1	4
3	Quality flag		sc	1	1
4	Orbit phase after eclipse	-	fl	1	4
5	Measurement Category	-	us	1	2
6	State ID	-	us	1	2
7	Duration of scan phase	1/16 s	us	1	2
8	Total no. of integrated PMD values in this state "Num_pmd"	-	us	1	2
9	No. of Geo-locations "Ngeo"	-	us	1	2
10	Integrated PMD values	BU	fl	Num_pmd	Num_pmd*4
11	Geo-location	-	GeoN GeoL/Occ	NGeo	Ngeo*108 (Nadir) Ngeo*112 (Limb/occ)

C.2: The integrated PMD MDS record structure. The data in filed 10 is ordered from PMD 1 to 7. Note that PMD 7 is the 45 degree sensor, which covers approximately the same wavelength as PMD 4.

Component: **1c integrated PMD MDS structure**
Component Type: MDS No of Records: variable Record Size: variable

Field	***Comments***	***Unit***	***Type***	**#**	***Size***
1	Start time of scan phase of the state	-	MJD	1	12
2	DSR length	-	fl	1	4
3	Quality flag	-	sc	1	1
4	Orbit phase after eclipse	-	fl	1	4
5	Measurement Category	-	us	1	2
6	State ID	-	us	1	2
7	Duration of Scan phase	1/16 s	us	1	2
8	No. of Geo-locations "num_geo"	-	us	1	2
9	Total number of fractional polarisation values		us	1	2
10	Number of different integration times		us	1	2
11	Integration times, ordered from longest to shortest	-	us	64	128
12	Repetition factors, ordered from lowest to highest, one per integration time	-	us	64	128
13	Fractional polarisation values	-	Polv	Field[9]	Field[9]*256
14	Geo-location	-	GeoN GeoL/Occ	Field[8]	Field[8]*108 (Nadir) Field[8]*112 (Limb/occ)

Table C.3: The fractional polarisation record structure. The fractional polarisation values, given by field no. 13 have a predefined, level 1b structure, which is explained in annex A.

Component: **1c user options GADS**
Component Type: GADS No of Records: 1 Record Size: variable 400

Field	*Comments*	*Unit*	*Type*	*#*	*Size*
1	L1b product name	-	ASCII	1	62
2	Geofilter flag (0 not used, -1 used)	-	sc	1	1
3	Start latitude	10-6 deg	fl	1	4
4	Start longitude	10-6 deg	fl	1	4
5	End latitude	10-6 deg	fl	1	4
6	End longitude	10-6 deg	fl	1	4
7	Time filter flag (0 not used, -1 used)	-	sc	1	1
8	Start time	MJD	UTC		12
9	Stop time	MJD	UTC	1	12
10	category filter flag (0 not used, -1 used)	-	sc	1	1
11	Category (up to 5 selected categories possible)	-	us	5	10
12	Nadir MDS filter flag (0 not used, -1 used)	-	sc	1	1
13	Limb MDS filter flag (0 not used, -1 used)	-	sc	1	1
14	Occultation MDS filter flag (0 not used, -1 used)	-	sc	1	1
15	Monitoring MDS filter flag (0 not used, -1 used)	-	sc	1	1
16	Integrated PMD MDS filter flag (0 not used, -1 used)	-	sc	1	1
17	Fractional Polarisation MDS filter flag (0 not used, -1 used)	-	sc	1	1
18	Slit function GADS (-1 copied, 0 not copied)	-	sc	1	1
19	Sun mean reference GADS	-	sc	1	1
20	Leakage current GADS	-	sc	1	1
21	Spectral calibration GADS	-	sc	1	1
22	Polarisation sensitivity GADS	-	sc	1	1
23	Radiance sensitivity GADS	-	sc	1	1
24	Ppg/etalon GADS	-	sc	1	1
25	Number of seleceted nadir cluster	-	us	1	2
26	Number of seleceted limb cluster	-	us	1	2
27	Number of seleceted occultation cluster	-	us	1	2
28	Number of seleceted monitoring cluster	-	us	1	2
29	Nadir cluster flag	-	sc	64	64
30	Limb cluster flag	-	sc	64	64
31	Occultation cluster flag	-	sc	64	64
32	Monitoring cluster flag	-	sc	64	64
33	Memory effect calibration flag (-1 applied, 0 not applied)	-	sc	1	1
34	Leakage current calibration flag	-	sc	1	1
35	Straylight calibration flag	-	sc	1	1
36	Ppg calibration flag	-	sc	1	1
37	Etalon calibration flag	-	sc	1	1
38	Spectral calibration flag	-	sc	1	1
39	Polarisation calibration flag	-	sc	1	1
40	Radiance calibration flag	-	sc	1	1

C.4: The level 1c user options GADS. It can be used to trace back the filters/applications which were applied to the original level 1b input.

D PARAMETER TABLES

Annex D Table	**Content**
D.1	Cluster definition nadir
D.2	Cluster definition limb
D.3	Data set id's for option "-ds"

Index	Ch.	Start pixel	End pixel	Approximate Wavelength [nm]	Purpose
1	1a	0	4	-	Blinded pixel
2	1a	216	743	240.00 – 305.99	Virtual channel 1a
3	1b	744	767	306.11 – 308.99	Virtual channel 1b
4	1b	768	807	309.12 – 314.00	Overlap region
5	1b	1019	1023	-	Blinded pixel
6	2b	1024	1028	-	Blinded pixel
7	2b	1119	1215	405.00 – 394.06	Overlap region
8	2b	1215	1857	319.94 – 314.06	Virtual channel 2b
9	2a	1858	1909	313.95 – 309.00	Virtual channel 2a
10	2a	1910	1953	-	Overlap region
11	2a	2043	2047	-	Blinded pixel
12	3	2048	2052	-	Blinded pixel
13	3	2094	2139	394.00 – 404.95	Overlap region
14	3	2140	2221	405.19 – 424.90	-
15	3	2222	2324	425.14 – 449.95	NO2
16	3	2325	2529	450.20 – 499.82	O3
17	3	2530	2735	500.07 – 549.94	-
18	3	2736	2776	550.18 – 559.91	Aerosol
19	3	2777	2957	560.16 – 603.94	-
20	3	2958	3023	604.19 – 620.00	Overlap region
21	3	3067	3071	-	Blinded pixel
22	4	3072	3076	-	Blinded pixel
23	4	3118	3192	604.00 – 619.99	Overlap region
24	4	3193	3349	620.21 – 653.93	-
25	4	3350	3395	654.14 – 663.87	Aerosol
26	4	3396	3816	664.08 – 754.86	-
27	4	3817	3932	755.07 – 779.93	Clouds
28	4	3933	3955	780.15 – 784.90	-
29	4	3956	4047	785.12 – 804.78	Overlap region
30	4	4091	4095	-	Blinded pixel
31	5	4096	4100		Blinded pixel
32	5	4150	4218	785.00 – 804.74	Overlap region
33	5	4219	4409	805.03 – 860.18	-
34	5	4410	4442	860.47 – 869.75	Aerosol
35	5	4443	4856	870.04 – 989.92	-
36	5	4857	4890	990.21 – 999.79	Aerosol
37	5	4891	4925	1000.08 – 1009.95	-
38	5	4926	5063	1010.24 – 1050.00	Overlap region
39	5	5115	5119	-	Blinded pixel
40	6	5120	5129	-	Blinded pixel
41	6	5177	5227	1009.66 – 1049.89	Overlap region
42	6	5228	5457	1050.70 – 1234.98	-
43	6	5458	5481	1235.78 – 1254.29	Aerosol
44	6	5482	5649	1255.10 – 1389.48	-
45	6	5650	5674	1390.29 – 1409.60	Water vapour
46	6	5675	5848	1410.41 – 1549.62	-
47	6	5849	5910	1550.43 – 1599.52	Water/Ice
48	6	5911	6034	1600.32 – 1699.30	Water/Ice
49	6	6035	6097	1700.11 – 1750.00	Water/Ice

50	6	6134	6143	-	Blinded pixel
51	7	6144	6153	-	Blinded pixel
52	7	6217	7093	1940.00 – 2040.00	-
53	7	7158	7167	-	Blinded pixel
54	8	7168	7177	-	Blinded pixel
55	8	7241	8118	2265.00 – 2380.00	
56	8	8182	8191	-	Blinded pixel

D.1: Cluster definitions for Nadir measurements. Definition according to existing test products.

Index	Ch.	Start pixel	End pixel	Approximate Wavelength [nm]	Purpose
1	1a	0	4	-	Blinded pixel
2	1a	5	14	-	Straylight
3	1a	216	743	240.00 – 305.99	Virtual channel 1a
4	1b	744	807	306.11 – 314.00	Virtual channel 1b
5	1b	1009	1018	-	Straylight
6	1b	1019	1023	-	Blinded pixel
7	2b	1024	1028	-	Blinded pixel
8	2b	1119	1857	405.00 – 320.05	Virtual channel 2b
9	2a	1858	1953	319.94 – 309.00	Virtual channel 2a
10	2a	2033	2042	-	Straylight
11	2a	2043	2047	-	Blinded pixel
12	3	2048	2052	-	Blinded pixel
13	3	2094	3024	394.00 – 620.00	Channel 3
14	3	3067	3071	-	Blinded pixel
15	4	3072	3076	-	Blinded pixel
16	4	3118	4048	604.00 – 805.00	Channel 4
17	4	4091	4095	-	Blinded pixel
18	5	4096	4100	-	Blinded pixel
19	5	4150	5063	785.00 – 1050.00	Channel 5
20	5	5115	5119	-	Blinded pixel
21	6	5120	5129	-	Blinded pixel
22	6	5165	6097	1000.00 – 1750.00	Channel 6
23	6	6134	6143	-	Blinded pixel
24	7	6144	6153	-	Blinded pixel
25	7	6217	7093	1940.00 – 2040.00	Channel 7
26	7	7158	7167	-	Blinded pixel
27	8	7168	7177	-	Blinded pixel
28	8	7241	8091	2265.00 – 2380.00	Channel 8
29	8	8182	8191	-	Blinded pixel

D.2: Cluster Definitions for limb and occultation measurements. Definition according to existing test products. Has changed already and will probably change again during commissioning. It will be updated accordingly.

Id	Product Components	Component Type
	Main Product Header	*MPH*
	Specific Product Header	*SPH*
	Data Set Descriptor	*DSD*
1	*Summary of Quality Flags*	*SQADS*
2	*Geo-location of the State*	*LADS*
3	*Static Instrument Parameters*	*GADS*
4	*Leakage Current Parameters (constant fraction)*	*GADS*
5	*Leakage Current Parameters (variable fraction)*	*GADS*
6	*PPG/Etalon Parameters*	*GADS*
7	*Precise Basis Array of Spectral Calibration*	*GADS*
8	*Spectral Calibration Parameters*	*GADS*
9	*Sun Reference Spectrum*	*GADS*
10	*Polarisation Sensitivity Parameters Nadir*	*GADS*
11	*Polarisation Sensitivity Parameters Limb/Occultation without ND*	*GADS*
12	*Polarisation Sensitivity Parameters Limb/Occultation with ND*	*GADS*
13	*Radiance Sensitivity Parameters Nadir*	*GADS*
14	*Radiance Sensitivity Parameters Limb/Occultation without ND*	*GADS*
15	*Radiance Sensitivity Parameters Limb/Occultation with ND*	*GADS*
16	*Errors on Key Data*	*GADS*
17	*Slit Function Parameters*	*GADS*
18	*Small Aperture Slit Function Parameters*	*GADS*
19	*States of the Product*	*ADS*
20	*PMD Data Packets*	*ADS*
21	*Auxiliary Data Packets*	*ADS*
22	*Leakage Current Parameters (newly calculated parts)*	*ADS*
23	*Average of the Dark Measurements per State*	*ADS*
24	*PPG/Etalon Parameters, newly calculated*	*ADS*
25	*Spectral Calibration Parameters, newly calculated*	*ADS*
26	*Sun Reference Spectrum, newly calculated*	*ADS*

D.3 Data set id’s to be used for option “-ds” . Note that the 1b measurement data sets (which would have identifiers 27 to 30) cannot be copied in 1b format into the 1c product. If this would be intention, other command line tools have to be used.