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TITLE: ENVISAT-1 PRODUCTS SPECIFICATIONS
VOLUME 15: SCIAMACHY PRODUCTS SPECIFICATIONS

Abstract: The present document identified by version number 3/M details the formats of the SCIAMACHY Level 1b version 8 and Level 2 version 6 products and related auxiliary files.

Written by: Gabriele Brizzi

Approval: Massimo Cardaci

Accepted: ESA – Angelika.Dehn

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AMENDMENT POLICY

The document is amended by releasing a new issue.

The Amendment Record Sheet below records changes of the document. For an overview of the history of this document, the user is invited to check the previous version (3L).

AMENDMENT RECORD SHEET

ISSUE	REVISION	DATE	CHANGE STATUS	ORIGIN
3	M	30 April 2016	Document entirely revised Aligned to mission phase F Fixed typos and inconsistencies Fixed error for Polarization Sensitivity Parameters Limb and Occultation GADS and for Radiance Sensitivity Parameters Limb and Occultation GADS. Added references to Calibration Initialization File, Calibration Database and Reference in-flight auxiliary files. Revised Auxiliary File section	R-1

REFERENCED DOCUMENTS

RD.1 SCIAMACHY Level 0 to 1b Processing - Input / Output Data Definition, ENV-TN-DLR-SCIA-0005, Issue 8, 2014.

RD.2 SCIAMACHY Level 1b to 2 Off-line Processing Input / Output Data Definition, ENV-ID-DLR-SCI-2200-4, Issue 6, 2015.

RD.3 ENVISAT-1 PRODUCTS SPECIFICATIONS, VOLUME 5: PRODUCTS STRUCTURES, PO-RS-MDA-GS-2009, issue 3E.

RD.4 ENVISAT-1 PRODUCTS SPECIFICATIONS, VOLUME 16: AUXILIARY DATA FILES, PO-RS-MDA-GS-2009, issue 3G.

RD.5 ENVISAT-1 PRODUCTS SPECIFICATIONS, ANNEX A: PRODUCT DATA CONVENTIONS, PO-RS-MDA-GS-2009, 2005.

RD.6 ENVISAT-1 PRODUCTS SPECIFICATIONS, VOLUME 6: LEVEL 0 PRODUCTS SPECIFICATION, PO-RS-MDA-GS-2009, 1998, issue 3C.

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15. SCIAMACHY PRODUCTS SPECIFICATIONS

15.1 INSTRUMENT OVERVIEW

The Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (SCIAMACHY) instrument provided spectra measured from light transmitted, back scattered or reflected in the atmosphere. The instrument was designed for global measurement of trace gases in the Troposphere and Stratosphere by means of a spectrometer scanning the atmosphere either at nadir or in limb view. The instrument recorded radiation in the range 0.24 µm to 2.4 µm with eight detector modules.

SCIAMACHY on board of the Environmental Satellite ENVISAT-1 (2002-2012) made spectral measurements in passive limb and nadir looking geometries, permitting ground based computation of atmospheric constituents. The mission goal was detection of small optical absorptions (as small as 2E-4 in some regions of the spectrum). SCIAMACHY measured the global distribution of trace gases, aerosols and clouds in both the Troposphere and the Stratosphere. The targeted species include

- for the Troposphere: O_3, O_4, N_2O, NO_2, CH_4, CO, CO_2, H_2O, HCHO, CHOCHO and aerosols and, in polluted conditions, SO_2
- for the Stratosphere: O_3, O_2, O_2*, O_4, NO, NO_2, BrO, N_2O, CO, CO_2, H_2O, CH_4 plus under volcanic eruption SO2, plus under ozone hole conditions OClO and ClO.

The present document (version 3/M) details the formats of the SCIAMACHY Level 1b version 8 and Level 2 version 6 products. The Level 2 sections are currently only drafted, awaiting for the final data release.

Table 15.1-1 - SCIAMACHY Instrument Characteristics	
GEOMETRY	Nadir viewing IFOV: 0.045 deg (across track) * 1.8 deg (along track) Max Swath width: 960 km Typical footprint: 30 km (along track) * 60 km (across track) Limb viewing 0.045 deg (elevation) * 1.8 deg (azimuth) 0 to 100 km at typically 34 steps and 3 km resolution The maximum azimuth range was +/- 44 deg. relative to satellite velocity and was adjusted in order to cover the same atmospheric volume as for nadir measurements within 5 minutes.
SPECTRAL	Eight detector modules operated in the 0.24−2.4 µm spectral region. Channel 1 = 240 - 314 nm, Channel 2 = 307 - 405 nm, Channel 3 = 391 - 605 nm, Channel 4 = 598 - 809 nm, Channel 5 = 776 - 1051 nm, Channel 6 = 1033 - 1765 nm, Channel 7 = 1938 - 2043 nm, Channel 8 = 2259 - 2383 nm. Polarization Measurement Devices (PMD) Polarization was measured in several channels: PMD A = 302 -385 nm, PMD B = 441 - 527 nm, PMD C = 602 - 707 nm, PMD D = 785 - 913 nm, PMD E = 1447 - 1641 nm, PMD F = 2262 - 2380 nm, PMD 45° detector = 800 - 912 nm.

15.2 PRODUCTS OVERVIEW

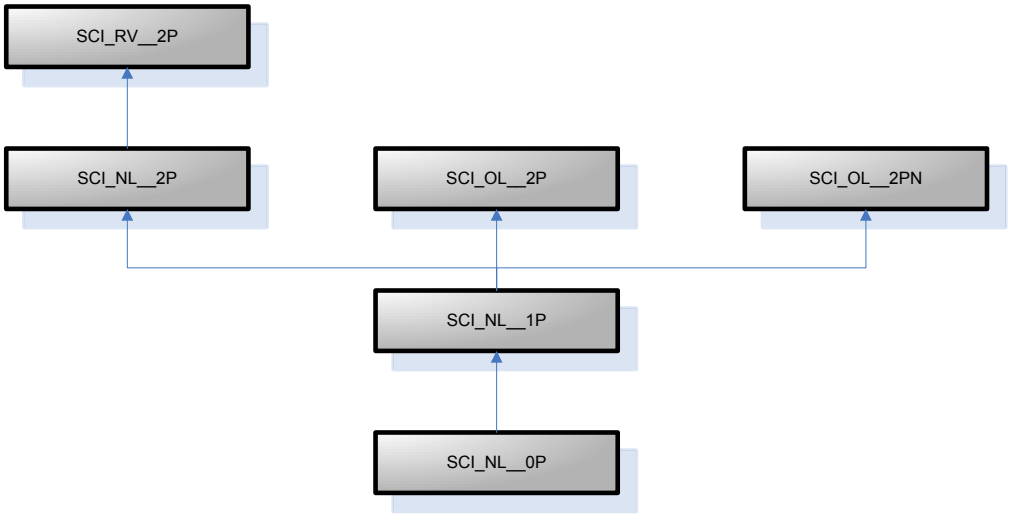
SCIAMACHY products may be classified as Level 0, Level 1b, or Level 2.

The characteristics of each product are summarized in Table 15.2-1 and Figure 15.2-1.

Table 15.2-1- SCIAMACHY Products

Product ID	Description
SCI_NL__0P	SCIAMACHY Level 0
SCI_NL__1P	SCIAMACHY Level 1b Geolocated, Radiometrically and Spectrally Calibrated radiance spectra for Nadir, Limb, and Occultation measurements. The Level 1b product is the lowest level of SCIAMACHY data delivered to the general user.
SCI_NL__2P	SCIAMACHY Level 2 Geolocated vertical column amounts. Processing suspended in May 2006.
SCI_OL__2P	SCIAMACHY consolidated Level 2 Geolocated vertical column amounts anf profiles from trace gas species, cloud-top pressure, cloud fractional cover and aerosols parameters.
SCI_RV__2P	SCIAMACHY Level 2 Selected vertical column amounts. Processing suspended in May 2006.
SCI_OL__2PN	SCIAMACHY fast-delivered Level 2 For Level 2 SGP version 5, the Fast Delivery operational processing chain was activated, generating products within 24 hours from acquisition.

Figure 15.2-1 - SCIAMACHY Product Tree



15.2.1 Product Specific Notations

The following notations are used in the description of SCIAMACHY products.

Table 15.2.1-1 - SCIAMACHY Notations

Notation	Description
%	Percent
(BU/s)*sr	Binary units per second of a solid angle
(BU/s) / (photons/cm2 * nm * s)	Binary units per second per radiance
-	No unit
1/16 s (1)	Time of BCPS (62.5 ms)[2]
BU	Binary units of signal read-outs
BU/s	Binary units per second
cm	Centimetre
day	Day
degree	General Angle (360 per circle)
keyword	A keyword in the format definition
km	Kilometre
Lat/Long	Geographical Co-ordinate
m	metre

[2] *The readout of the clusters was synchronised via a clock that every 1/16-second sent a Broadcast Pulse Signal (BCPS); hence all detector exposure times are multiples of 1/16 second.*

m/s	metre per second
mbar	Millibar (Pressure)
mol/cm2	Column density
mol/cm3	Number Density
ms	Millisecond
nm	Nanometre (Wavelength)
photons / (cm2 * nm * sr * s)	Radiance
ppV	Volume mixing ratio; parts per Volume
Rel. fraction	Relative fraction
s	Second
sr	Steradian
terminator	Terminator of fields
µs	Microsecond

The following acronyms are used to describe combined data structures in the products. A detailed description of the structure of these fields is given in Section 15.4.1.7.1.

Table 15.2.1-2 - SCIAMACHY Combined Data Structures

Notation	Description
Clcon	Cluster configuration
Coord	Geographical coordinate
GeoL	Geolocation for limb measurements
GeoN	Geolocation for nadir measurements
GeoCal	Geolocation for calibration measurements
PolV	Fractional polarisation values
L0Hdr	Level 0 header structure

The following table reports the notation used in this document to specify the basic data types of the different data sets.

Table 15.2.1-3 – Data Types

Symbol	Type	Bytes
uc	Unsigned char	1
us	Unsigned short integer	2
ul	Unsigned long integer	4

Symbol	Type	Bytes
fl	Single precision floating point	4
do	Double precision floating point	8
sc	Signed char	1
sl	Signed long integer	4
ac	Single ASCII character (SXXX)	4
al	ASCII characters (SXXXXXXXXXX)	11
mjd	Modified Julian Date	12
dsd	Dataset descriptor	280

15.3 LEVEL 0 PRODUCTS

There is one Level 0 product corresponding to the main SCIAMACHY measurement mode.

15.3.1 SCIAMACHY Level 0

SCIAMACHY Level 0 products are composed of time ordered and annotated Instrument Source Packets (ISPs, in instrument data units) with main and specific product ASCII headers. There are three different types of instrument source packets: Detector, PMD, and Auxiliary Data Packets.

The SCIAMACHY Level 0 product is the basis of all data processing to create higher-level SCIAMACHY products.

During operations, the Level 0 products were produced systematically in two versions: as near-real-time (NRT) and off-line (OFL, fully consolidated) products. The NRT product was available from the PDHS 3 hours after data acquisition. The off-line product was available from the PAC 1-2 weeks after data acquisition.

15.3.1.1 Input Data

Annotated Instrument Source Packets as received from the Front End Processor (FEP), plus auxiliary data as indicated below.

15.3.1.2 Auxiliary Data Used

The Level 0 product requires the following auxiliary information:

- Phase, cycle and orbit number data,
- ID of systems and subsystem that collect and process the data,
- ENVISAT orbital state vectors,
- Processor Configuration file, which includes PCD threshold values,
- SBT to UTC conversion data.

15.3.1.3 Processing Performed

Determination of the satellite position and conversion of Satellite Binary Time (SBT) to Universal Time Co-ordinates (UTC) is accomplished using ESA software.

15.3.1.4 Product Structure

The Level 0 product structur is defined in R-6.

Table 15.3.1-1 - SCIAMACHY Level 0 PRODUCT SUMMARY SHEETS

SCIAMACHY Level 0	
PRODUCT ID	SCI_NL__0P
PRODUCT NAME	SCIAMACHY Level 0
DESCRIPTION	This data consists of time ordered AISPs containing spectra measured from light transmitted, backscattered or reflected by trace gases in the atmosphere.
APPLICATIONS	Archived product forming basis for all higher level processing
DELIVERY TIME	NRT version available from PDHS within 3 hours from data acquisition. Off-line (fully consolidated) version available from the LRAC starting 1-2 weeks after data acquisition.
COVERAGE	Full orbit, all measurement types
THROUGHPUT	One product per orbit (100 minutes) 400 kbps instrument data rate.
PRODUCT SIZE	Maximum 230 MB per orbit
AUXILIARY DATA	Orbit State Vectors; SBT/UTC Time conversion parameters
ALGORITHMS USED	Satellite positioning, UTC time conversion
NOTES	Produced systematically during operations

15.4 LEVEL 1b PRODUCTS

According to the PDGS architecture rules, there is only one output product resulting from the Level 0 to 1b processing of SCIAMACHY measured signals: the SCIAMACHY Level 1b product. Information regarding this product type is extracted from the SCIAMACHY Level 0 to 1b IODD [R-1].

15.4.1 SCIAMACHY Level 1b

SCIAMACHY Level 1 products are geolocated spectra, with radiometric and spectral calibration information from nadir, limb, and sun/moon occultation geometries. The Level 1b product is the foundation for further processing.

Level 1b products were produced systematically during mission operations. The near-real-time (NRT) version of the product was available from the PDHS 3 hours after data acquisition. The Level 1b off-line (OFL) products, containing fully consolidated spectra, were generated at D-PAC 1-2 weeks after acquisition. During mission phase F, only consolidated products are generated by ESA with dedicated reprocessing campaigns and distributed to the users.

15.4.1.1 Input Data

Level 0 product plus auxiliary data as indicated below.

15.4.1.2 Auxiliary Data Used

The sources of auxiliary data required for the Level 0 to 1b processing with baseline version 8 are listed in the table below. In-flight calibration parameters, previously extracted from LK1, SU1, SP1, and PE1 auxiliary data files, are now derived from a calibration database. Auxiliary files are described in R-4.

Table 15.4.1.2-1 - Auxiliary Information for SCIAMACHY Level 0-1b processing

Source	Auxiliary File ID
Calibration Database of in-flight parameters	N/A
Reference Leakage Current Parameters file	SCI_LK1_AX
Reference PPG/Etalon Parameters file	SCI_PE1_AX
Reference Spectral Calibration Parameters file	SCI_SP1_AX
Reference Sun Spectrum file	SCI_SU1_AX
Initialization file	SCI_LI1_AX
Key Data file (Instrument Characterization file)	SCI_KD1_AX
M-Factor file (Key Data correction factors) version 8	SCI_MF1_AX[3]
Calibration Initialization file	SCI_LIC_AX

[3] Starting from the Level 1 baseline version 8, SCI_MF1_AX files are used for the Level 0 to 1b processing step. M-factors are provided by the University of Bremen.

Source	Auxiliary File ID
Envisat-1 Restituded Attitude Data file	AUX_FRA_AX
Orbit state vector file	DOR_VOR_AX

15.4.1.3 Processing Performed

Please note that this is not the applicable document for algorithm details.

The following is a high-level overview of the processing performed for Level 1b product generation:

- Extraction of Level 0 data and processing of PCD data;
- Extraction / processing / calibration of auxiliary data;
- Validation / monitoring of critical instrument parameters through analysis of auxiliary and measurement data;
- Processing of orbit / geometry data;
- Spectral and radiometric calibration of scene data;
- Straylight correction;
- Polarization correction;
- Processing of spectral covariance data (noise assessment);
- Processing of Level 1b annotation data;
- Generation of Level 1b product file and related output data.

Table 15.4.1-1 - SCIAMACHY Level 1b PRODUCT SUMMARY SHEETS

SCIAMACHY Level 1b	
PRODUCT ID	SCI_NL__1P
PRODUCT NAME	SCIAMACHY Geolocated and Calibrated Spectra
DESCRIPTION	This is the base level 1b product for SCIAMACHY and includes calibrated spectra, calibration and housekeeping information. Calibration data is extracted from the raw data stream and is stored separately in the instrument specific header. Additional geolocation information is also associated with each measurement. The spectra themselves have been calibrated from on-board auxiliary data.
APPLICATIONS	Calibrated product is basis for Level 2 generation
DELIVERY TIME	NRT version available from PDHS within 3 hours from data acquisition. Off-line (fully consolidated) version available from the D-PAC starting 1-2 weeks after data acquisition (LRAC processing stopped since December 2004)
COVERAGE	Full orbit, all measurement types
THROUGHPUT	One product per orbit
PRODUCT SIZE	Max. size approx 400 MBytes per orbit
ALGORITHMS USED	Extraction / processing / calibration of auxiliary data; Validation/monitoring of critical instrument parameters through analysis of auxiliary and measurement data; Processing or orbit/ geometry data; Spectral and radiometric calibration of scene data, straylight correction; Polarization correction; Processing of spectral covariance data (noise assessment)
NOTES	Produced systematically during operations from Level 0 data

15.4.1.4 Product Structure

The high level structure of the SCIAMACHY Level 1b product is shown below:

Table 15.4.1.4-1 - SCIAMACHY Level 1b Product Structure

MPH
SPH (including DSDs)
Summary Quality ADS (SQADS)
Geolocation ADS (LADS)
Static Instrument Parameters GADS
Leakage Current Parameters (constant fraction) GADS
Leakage Current Parameters (variable fraction) GADS

PPG/Etalon Parameters GADS
Precise Basic Array of Spectral Calibration GADS
Spectral Calibration Parameters GADS
Sun Reference Spectrum GADS
Polarization Sensitivity Parameters Nadir GADS
Polarization Sensitivity Parameters Limb GADS
Polarization Sensitivity Parameters Occultation GADS
Radiance Sensitivity Parameters Nadir GADS
Radiance Sensitivity Parameters Limb GADS
Radiance Sensitivity Parameters Occultation GADS
Errors on Key Data GADS
Slit Function Parameters GADS
Small Aperture Slit Function Parameters GADS
States of the Product ADS
PMD Data Packets ADS
Auxiliary Data Packets ADS
Leakage Current (newly calculated parts) ADS
Average of the Dark Measurement per State ADS
PPG/Etalon (newly calculated) ADS
Spectral Calibration (newly calculated) ADS
Sun Reference Spectrum (newly calculated) ADS
Nadir MDS
Limb MDS
Occultation MDS
Monitoring MDS

Note that the presence of some data sets in the Level 1b product depends on the corresponding measurement timeline, in case the specific measurements (calibration or monitoring type) were executed.

The following sections present the detailed definition of the components listed above.

15.4.1.5Main Product Header

The Main Product Header (MPH) is described in the Product Specifications R-3. MPF record size is 1247 bytes.

15.4.1.6Specific Product Header

The Specific Product Header (SPH) conforms to the ASCII conventions defined in R-3. The symbol Ø indicates the position within a record of an ASCII blank space character.

Table 15.4.1.6-1 - Specific Product Header of Level 1b Product

#	Description	Units	Byte Length	Data Type	Dim.
1	**SPH_DESCRIPTOR=**	keyword	15	uc	15
	quotation mark (“)	-	1	uc	1
	SPH descriptor Set to “SCI_NL__1PØSPECIFIC HEADERØØ”	-	28	uc	28
	quotation mark (“)	-	1	uc	1

Table 15.4.1.6-1 - Specific Product Header of Level 1b Product

#	Description	Units	Byte Length	Data Type	Dim.
	newline character	terminator	1	uc	1
2	**STRIPLINE_CONTINUITY_INDICATOR=**	keyword	31	uc	31
	Value: +000 (No stripline continuity) in case the product is a complete segment. Other: Stripline Counter	-	4	ac	1
	newline character	terminator	1	uc	1
3	**SLICE_POSITION=**	keyword	15	uc	15
	Value: from +001 to NUM_SLICES Default value if no stripline continuity = +001	-	4	ac	1
	newline character	terminator	1	uc	1
4	**NUM_SLICES=**	keyword	11	uc	11
	Number of slices in this stripline Default value if no continuity = +001	-	4	ac	1
	newline character	terminator	1	uc	1
Product Location Information					
5	**START_TIME=**	keyword	11	uc	11
	quotation mark (“)	-	1	uc	1
	Start time of the measurement data in the product, UTC time of first MDSR	utc	27	uc	27
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
6	**STOP_TIME=**	keyword	10	uc	10
	quotation mark (“)	-	1	uc	1
	Time of the end of the measurement data in the product ,UTC time of last MDSR (start time of last state + duration)	utc	27	uc	27
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
7	**START_LAT=**	keyword	10	uc	10
	Latitude of the satellite nadir at START_TIME WGS84 latitude, positive = North Example: +0048000000 for 48º North	10-6 deg	11	al	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
8	**START_LONG=**	keyword	11	uc	11
	Longitude of the satellite nadir at START_TIME WGS84 longitude, positive = East, 0 = Greenwich Example: -0120000000 for 120º West	10-6 deg	11	al	1
	<10-6degE>	units	10	uc	10
	newline character	terminator	1	uc	1
9	**STOP_LAT=**	keyword	9	uc	9
	Latitude of the satellite nadir at STOP_TIME WGS84 latitude, positive = North	10-6 deg	11	al	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
10	**STOP_LONG=**	keyword	10	uc	10

Table 15.4.1.6-1 - Specific Product Header of Level 1b Product

#	Description	Units	Byte Length	Data Type	Dim.
	Longitude of the satellite nadir at STOP_TIME WGS84 longitude, positive = East, 0 = Greenwich	10-6 deg	11	al	1
	<10-6degE>	units	10	uc	10
	newline character	terminator	1	uc	1
11	The first 33 characters of this record provide initialisation file version and decontamination flag: INIT_VERSION=xxxxØDECONT=ddddddddd with d='n' or 'y' for each channel. Example:INIT_VERSION= 500 DECONT=nnnnnyyy	-	50	uc	50
	newline character	terminator	1	uc	1
Data version information					
	KEY_DATA_VERSION=	keyword	17	uc	17
	quotation mark (")	-	1	uc	1
12	Data version (pattern XX.XX, e.g. 01.25)	-	5	uc	5
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
	M_FACTOR_VERSION=	keyword	17	uc	17
	quotation mark (")	-	1	uc	1
13	Data version (pattern XX.XX, e.g. 01.25)	-	5	uc	5
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
Product Quality Information					
	SPECTRAL_CAL_CHECK_SUM=	keyword	23	uc	23
	quotation mark (")	-	1	uc	1
14	Quality flag for range of spectral calibration error (ε): "GOOD" if ε <= 0.02 "FAIR" if 0.02 < ε <= 0.05 "BADØ" if ε > 0.05	-	4	uc	4
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
	SATURATED_PIXEL=	keyword	16	uc	16
	quotation mark (")	-	1	uc	1
15	Quality flag for number of saturated detector pixels (n): "GOOD" if n = 0 "FAIR" if 0 < n <= 100 "BADØ" if n > 100	-	4	uc	4
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
16	**DEAD_PIXEL=**	keyword	11	uc	11
	quotation mark (")	-	1	uc	1

Table 15.4.1.6-1 - Specific Product Header of Level 1b Product

#	Description	Units	Byte Length	Data Type	Dim.
	Quality flag for number of dead detector pixels (n): "GOOD" if n = 0 "FAIR" if 0 < n <= 10 "BADØ" if n > 10	-	4	uc	4
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
17	**DARK_CHECK_SUM=**	keyword	15	uc	15
	quotation mark (")	-	1	uc	1
	Quality flag for the difference between measurement and calibrated dark signal: "GOOD" "FAIR" "BADØ"	-	4	uc	4
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
18	**NO_OF_NADIR_STATES=**	keyword	19	uc	19
	Number of Nadir states where MDSRs have been stored. Example: +025	-	4	ac	1
	newline character	terminator	1	uc	1
19	**NO_OF_LIMB_STATES=**	keyword	18	uc	18
	Number of Limb states where MDSRs have been stored. Example: +025	-	4	ac	1
	newline character	terminator	1	uc	1
20	**NO_OF_OCCULTATION_STATES=**	keyword	25	uc	25
	Number of Occultation states where MDSRs have been stored. Example: +025	-	4	ac	1
	newline character	terminator	1	uc	1
21	**NO_OF_MONI_STATES=**	keyword	18	uc	18
	Number of Monitoring measurement states (WLS, SLS, and sun diffuser states) where MDSRs have been stored. Example: +025	-	4	ac	1
	newline character	terminator	1	uc	1
22	**NO_OF_NOPROC_STATES=**	keyword	20	uc	20
	Number of states present in the processing time window applied to the Level 0 product but not processed to the Level 1b product. Example: +025	-	4	ac	1
	newline character	terminator	1	uc	1
23	**COMP_DARK_STATES=**	keyword	17	uc	17
	Number of processed complete dark states	-	4	ac	1
	newline character	terminator	1	uc	1
24	**INCOMP_DARK_STATES=**	keyword	19	uc	19
	Number of incomplete dark states	-	4	ac	1
	newline character	terminator	1	uc	1
25	**Spare (blank characters (Ø))**	-	4	uc	4
	newline character	terminator	1	uc	1
DSDs for Attached Data Sets					
26	*DSD (A) for the Summary Quality ADS*	-	280	dsd	1

Table 15.4.1.6-1 - Specific Product Header of Level 1b Product

#	Description	Units	Byte Length	Data Type	Dim.
27	*DSD (A) for the Geolocation ADS (LADS)*	-	280	dsd	1
28	*DSD (A) for Instrument Parameters GADS*	-	280	dsd	1
29	*DSD (G) for the Leakage Current (constant part) GADS*	-	280	dsd	1
30	*DSD (G) for the Leakage Current (variable part) GADS*	-	280	dsd	1
31	*DSD (G) PPG/Etalon Parameters GADS*	-	280	dsd	1
32	*DSD (G) for the Precise Basis Array of Spectral Calibration GADS*	-	280	dsd	1
33	*DSD (G) for the Spectral Calibration Parameters GADS*	-	280	dsd	1
34	*DSD (G) for the Sun Reference Spectrum GADS*	-	280	dsd	1
35	*DSD (G) for the Polarization Sensitivity Nadir GADS*	-	280	dsd	1
36	*DSD (G) for the Polarization Sensitivity Limb GADS*	-	280	dsd	1
37	*DSD (G) for the Polarization Sensitivity Occultation GADS*	-	280	dsd	1
38	*DSD (G) for the Radiance Sensitivity Parameters Nadir GADS*	-	280	dsd	1
39	*DSD (G) for the Radiance Sensitivity Parameters Limb GADS*	-	280	dsd	1
40	*DSD (G) for the Radiance Sensitivity Parameters Occultation GADS*	-	280	dsd	1
41	*DSD (G) Errors on Key Data GADS*	-	280	dsd	1
42	*DSD (G) for the Slit Function Parameters GADS*	-	280	dsd	1
43	*DSD (G) for the Small Aperture Slit Function Parameters GADS*	-	280	dsd	1
44	*DSD (A) for the States of the Product ADS*	-	280	dsd	1
45	*DSD (A) for the PMD Data Packets ADS*	-	280	dsd	1
46	*DSD (A) for the Auxiliary Data Packets ADS*	-	280	dsd	1
47	*DSD (A) for the Leakage Current (newly calculated parts) ADS. If not used for this product, set to NOT USED as defined in R-3.*	-	280	dsd	1
48	*DSD (A) for the Average of the Dark Measurement per State ADS. If not used for this product, set to NOT USED as defined in R-3.*	-	280	dsd	1
49	*DSD (A) PPG/Etalon Parameters (newly calculated) ADS. If not used for this product, set to NOT USED as defined in R-3.*	-	280	dsd	1
50	*DSD (A) for the Spectral Calibration (newly calculated) ADS. If not used for this product, set to NOT USED as defined in R-3.*	-	280	dsd	1
51	*DSD (A) for the Sun Reference Spectrum (newly calculated) ADS. If not used for this product, set to NOT USED as defined in R-3.*	-	280	dsd	1

Table 15.4.1.6-1 - Specific Product Header of Level 1b Product

#	Description	Units	Byte Length	Data Type	Dim.
52	*DSDs (M) for the Nadir MDS. If not used for this product, set to NOT USED as defined in R-3.*	-	280	dsd	1
53	*DSDs (M) for the Limb MDS. If not used for this product, set to NOT USED as defined in R-3.*	-	280	dsd	1
54	*DSDs (M) for the Occultation MDS. If not used for this product, set to NOT USED as defined in R-3.*	-	280	dsd	1
55	*DSDs (M) for the Monitoring MDS. If not used for this product, set to NOT USED as defined in R-3.*	-	280	dsd	1
	DSDs for reference files				
56	*DSD (R) for the Level 0 product*	-	280	dsd	1
57	*DSD (R) for the Key Data file (Instrument Characterization file)*	-	280	dsd	1
58	*DSD (R) for the M-factor file*	-	280	dsd	1
59	*DSD (R) for the Initialisation file*	-	280	dsd	1
60	*DSD (R) for the Calibration Initialization file*	-	280	dsd	1
61	*DSD (R) for the Orbit State Vector File used*	-	280	dsd	1
62	*DSD (R) for the Attitude Data File used*	-	280	dsd	1
63	*DSD (R) for the Calibration database Leakage Current (constant part)*	-	280	dsd	1
64	*DSD (R) for the Calibration database Leakage Current (variable part)*	-	280	dsd	1
65	*DSD (R) for the Calibration database Sun Reference Spectrum D0*	-	280	dsd	1
66	*DSD (R) for the Calibration database Sun Reference Spectrum E0*	-	280	dsd	1
67	*DSD (R) for the Calibration database Sun Reference Spectrum D1*	-	280	dsd	1
68	*DSD (R) for the Calibration database Sun Reference Spectrum E1*	-	280	dsd	1
69	*DSD (R) for the Calibration database Sun Reference Spectrum D2*	-	280	dsd	1
70	*DSD (R) for the Calibration database Sun Reference Spectrum A0*	-	280	dsd	1
71	*DSD (R) for the Calibration database Spectral Averages*	-	280	dsd	1
72	*DSD (R) for the Calibration database PPG and Etalon*	-	280	dsd	1
73	*DSD (R) for the Calibration database Bad Pixel Mask*	-	280	dsd	1
74	*DSD Spare (279 blank space characters followed by one newline character)*	-	280	dsd	1

Table 15.4.1.6-1 - Specific Product Header of Level 1b Product

#	Description	Units	Byte Length	Data Type	Dim.
Size (in bytes)			**variable**		

The sum of fields 18 to 22 equals the total number of states in the processing time window.

The value for the KEY_DATA_VERSION field of Level 1b products version 8 is 03.30.
The value for the M_FACTOR_VERSION field of Level 1b products version 8 is 08.31.

The Data Set Descriptor records are logically part of the SPH.

With product version 8, the number of DSD records has been modified and is now fixed to a maximum of 49. This number results from the sum of the four possible measurement state types, plus a maximum of 26 records which are given by the number of ADSs (GADS, SQADS, LADS, and others), 18 records for the description of the external reference inputs, and one spare record.

The field DS_NAME in the DSDs are filled as specified in the table below:

Table 15.4.1.6-2 – SPH DS_NAME fields for DSDs

DSD	DS_NAME
DSD (A) for the SQ ADS	SUMMARY_QUALITY
DSD (A) for the Geolocation ADS (L ADS)	GEOLOCATION
Static instrument parameters (GADS)	INSTRUMENT_PARAMS
DSD (G) for the Leakage Current (constant part) GADS	LEAKAGE_CONSTANT
DSD (G) for the Leakage Current (variable part) GADS	LEAKAGE_VARIABLE
DSD (G) PPG/Etalon Parameters GADS	PPG_ETALON
DSD (G) for the Precise Basis Array of Spectral Calibration GADS	SPECTRAL_BASE
DSD (G) for the Spectral Calibration GADS	SPECTRAL_CALIBRATION
DSD (G) for the Sun Reference Spectrum GADS	SUN_REFERENCE
DSD (G) Polarization Sensitivity Nadir GADS	POL_SENS_NADIR
DSD (G) Polarization Sensitivity Limb GADS	POL_SENS_LIMB
DSD (G) Polarization Sensitivity Occultation GADS	POL_SENS_OCC
DSD (G) for the Radiance Sensitivity Nadir GADS	RAD_SENS_NADIR

Table 15.4.1.6-2 – SPH DS_NAME fields for DSDs	
DSD	**DS_NAME**
DSD (G) for the Radiance Sensitivity Limb GADS	RAD_SENS_LIMB
DSD (G) for the Radiance Sensitivity Occultation GADS	RAD_SENS_OCC
DSD (G) for the Errors on Key Data	ERRORS_ON_KEY_DATA
DSD (G) for the Slit Function Parameters GADS	SLIT_FUNCTION
DSD (G) for the Small Aperture Slit Function Parameters GADS	SMALL_AP_SLIT_FUNCTION
DSD (A) for the States ADS	STATES
DSD (A) for the PMD Data Packets ADS	PMD_PACKETS
DSD (A) for the Auxiliary Data Packets ADS	AUXILIARY_PACKETS
DSD (A) for the Leakage Current (newly calculated parts) ADS	NEW_LEAKAGE
DSD (A) for the Average of the Dark Measurement per State ADS.	DARK_AVERAGE
DSD (A) PPG/Etalon Parameters (newly calculated) ADS	NEW_PPG_ETALON
DSD (A) for the Spectral Calibration (newly calculated) ADS	NEW_SPECTRAL_CALIBRATION
DSD (A) for the Sun Reference Spectrum (newly calculated) ADS	NEW_SUN_REFERENCE
DSD for the Nadir MDS. If not used for this product, set to NOT USED as defined in R-3.	NADIR
DSD for the Limb MDS. If not used for this product, set to NOT USED as defined in R-3.	LIMB
DSD for the Occultation MDS. If not used for this product, set to NOT USED as defined in R-3.	OCCULTATION
DSD for the Monitoring MDS. If not used for this product, set to NOT USED as defined in R-3.	MONITORING
DSD (R) for the Level 0 product	LEVEL_0_PRODUCT
DSD (R) for the Key Data file (Instrument Characterization file)	KEY_DATA_FILE
DSD (R) for the M-factor file	M_FACTOR_FILE
DSD (R) for the Initialisation file	INIT_FILE
DSD (R) for the Calibration Initialization file	CAL_INIT_FILE
DSD (R) for the Orbit State Vector file	ORBIT_FILE
DSD (R) for the Attitude Data File	ATTITUDE_FILE
DSD (R) for the Calibration database Leakage Current (constant part)	scia_****_leakageconstant
DSD (R) for the Calibration database Leakage Current (variable part)	scia_****_leakagevariable
DSD (R) for the Calibration database Sun Reference Spectrum D0	scia_****_sunreference_D0
DSD (R) for the Calibration database	scia_****_sunreference_E0

Table 15.4.1.6-2 – SPH DS_NAME fields for DSDs	
DSD	**DS_NAME**
Sun Reference Spectrum E0	
DSD (R) for the Calibration database Sun Reference Spectrum D1	scia_****_sunreference_D1
DSD (R) for the Calibration database Sun Reference Spectrum E1	scia_****_sunreference_E1
DSD (R) for the Calibration database Sun Reference Spectrum D2	scia_****_sunreference_D2
DSD (R) for the Calibration database Sun Reference Spectrum A0	scia_****_sunreference_A0
DSD (R) for the Calibration database Spectral Averages	scia_****_spectralaverages
DSD (R) for the Calibration database PPG and Etalon	scia_****_ppgetalon
DSD (R) for the Calibration database Bad Pixel Mask	*scia_****_badpixelmask*
Spare DSD	

In Level 1b product version 8, the DSDs for the in-flight auxiliary data files were removed as usage of real auxiliary files were discontinued for the in-flight parameters; the corresponding calibrations are now extracted from a calibration database. Eleven new DSDs for the calibration database tables have been inserted.

15.4.1.7 Data Sets

The following sub-sections describe the individual data sets, which together form the Level 1b product. Data sets are in mixed-binary format. ASCII strings may be included within the data sets, but the string is not surrounded by quotation marks as for the MPH and SPH structures.

15.4.1.7.1 Compound Data Structures

The following structures are used in the descriptions of the Level 1b products.

Table 15.4.1.7.1-1 – Geographical Coordinate (Coord) Structure						
#	**Description**		**Units**	**Byte Length**	**Data Type**	**Dim.**
1	**Latitude**	**(convention defined in R-5)**	10-6 deg	4	sl	1
2	**Longitude**	**(convention defined in R-5)**	10-6 deg	4	sl	1
Size (in bytes)				**8**		

The Coordinate Structure is used in the Geolocation ADS.
Latitude values from -90 to 90 (-90 is the South Pole, 90 the North Pole, 0 the Equator).
Longitude values from -180 to 180 (meridian is 0 and minus is going to West).

Table 15.4.1.7.1-2 - Cluster configuration (Clcon) Structure					
#	Description	Units	Byte Length	Data Type	Dim.
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	-	1	uc	1
2	Detector channel number (1-8)	-	1	uc	1
3	Start pixel number (inclusive, 0-1023)	-	2	us	1
4	Cluster length (1-1024)	-	2	us	1
5	Pixel Exposure time (PET)	s	4	fl	1
6	Integration time	1/16s	2	us	1
7	Co-adding factor	-	2	us	1
8	Number of cluster readouts per DSR	-	2	us	1
9	Cluster Data Type Value defining the cluster data structure: 1= Rsig (Reticon detector, straylight not co-added) 2= Rsigc (Reticon detector, straylight co-added) 3 = Esig (Epitax detector, straylight not co-added) 4 = Esigc (Epitax detector, straylight co-added)	-	1	uc	1
Size (in bytes)			**17**		

The Cluster Configuration Structure is used in the States ADS.

Table 15.4.1.7.1-3 - Rsig Structure RETICON detector signal with memory effect correction and straylight not co-added					
#	Description	Units	Byte Length	Data Type	Dim.
1	Memory effect correction	BU	1	sc	1
2	Signal value of one detector element	BU	2	us	1
3	Straylight[4]	1/10 BU	1	uc	1
Size (in bytes)			**4**		

Table 15.4.1.7.1-4 - Rsigc Structure RETICON detector signal with memory effect correction and straylight co-added					
#	Description	Units	Byte Length	Data Type	Dim.
1	Signal value of one detector element and memory effect correction coded into one unsigned long value (the signal is given in the lower 24 bits (LSBs) in BU, the memory effect correction is given in the upper 8 bits (MSBs) as signed character in BU)	BU	4	ul	1
2	Straylight	1/10 BU	1	uc	1

[4] To yield the actual straylight the value given here must be multiplied by the scale factor given in the States ADS for each state and channel.

Table 15.4.1.7.1-4 - Rsigc Structure RETICON detector signal with memory effect correction and straylight co-added		
Size (in bytes)	**5**	

Table 15.4.1.7.1-5 - Esig Structure EPITAXX detector signal with straylight not co-added					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Memory effect correction	BU	1	sc	1
2	Signal value of one detector element	BU	2	us	1
3	Straylight	1/10 BU	1	uc	1
Size (in bytes)			**4**		

Remark: Esig is equal to data type Rsig. The location for memory effect is used for non-linearity correction.

Table 15.4.1.7.1-6 - Esigc Structure EPITAXX detector signal with straylight co-added					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Signal value of one detector element and memory effect correction coded into one unsigned long value (the signal is given in the lower 24 bits (LSBs) in BU, the memory effect correction is given in the upper 8 bits (MSBs) as signed character in BU)	BU	4	ul	1
2	Straylight	1/10 BU	1	uc	1
Size (in bytes)			**5**		

Remark: Esigc is equal to data type Rsigc. The location for memory effect is used for non-linearity correction.

Table 15.4.1.7.1-7 - Fractional polarization values (PolV) Structure					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	**Fractional polarization values Q** (6 values derived from PMDs, 5 values derived from the overlapping regions, and one model value below 300 nm)	-	48	fl	12
2	**Errors on Q values**	-	48	fl	12
3	**Fractional polarization values U** (6 values derived from PMDs, 5 values derived from the overlapping regions, and one model value below 300 nm)	-	48	fl	12
4	**Errors on the U values**	-	48	fl	12
5	**Representing wavelength for the fractional polarisation values and the 45 degree PMD**	nm	52	fl	13
6	**GDF parameters**	-	12	fl	3
Size (in bytes)			**256**		

Table 15.4.1.7.1-8 - Geolocation for limb measurements (GeoL) Structure

#	Description	Units	Byte Length	Data Type	Dim.
1	Position of ESM compared to zero position	degrees	4	fl	1
2	Position of ASM compared to zero position	degrees	4	fl	1
3	Solar zenith angles of start, middle, and end of the integration time at TOA	degrees	12	fl	3
4	Solar azimuth angles of start, middle, and end of the integration time at TOA	degrees	12	fl	3
5	Line of sight nadir angles of start, middle, and end of the integration time at TOA	degrees	12	fl	3
6	Line of sight azimuth angles of start, middle, and end of the integration time at TOA	degrees	12	fl	3
7	Satellite height at the middle of the integration time	km	4	fl	1
8	Earth radius at the middle of the integration time	km	4	fl	1
9	Sub-satellite point at the middle of the integration time	-	8	Coord	1
10	Co-ordinates of tangent ground point of the start, middle, and end of the integration time	-	24	Coord	3
11	Tangent height of the start, middle, and end of the integration time	km	12	fl	3
12	Doppler shift at 500 nm at the middle of the integration time	nm	4	fl	1
Size (in bytes)			**112**		

Table 15.4.1.7.1-9 - Geolocation for nadir measurements (GeoN) Structure

#	Description	Units	Byte Length	Data Type	Dim.
1	Position of ESM compared to zero position	degrees	4	fl	1
2	Solar zenith angles of start, middle, and end of the integration time at TOA	degrees	12	fl	3
3	Solar azimuth angles of start, middle, and end of the integration time at TOA	degrees	12	fl	3
4	Line of sight nadir angles of start, middle, and end of the integration time at TOA	degrees	12	fl	3
5	Line of sight azimuth angles of start, middle, and end of the integration time at TOA	degrees	12	fl	3
6	Satellite height at the middle of the integration time	km	4	fl	1
7	Earth radius at the middle of the integration time	km	4	fl	1
8	Sub-satellite point at the middle of the integration time	-	8	Coord	1
9	4 corner coordinates 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)	-	32	Coord	4
10	Center co-ordinate of the nadir ground pixel	-	8	Coord	1
Size (in bytes)			**108**		

Table 15.4.1.7.1-10 - Geolocation for calibration and monitoring measurements (GeoCal) Structure

#	Description	Units	Byte Length	Data Type	Dim.
1	Position of ESM compared to zero position	degrees	4	fl	1
2	Position of ASM compared to zero position	degrees	4	fl	1
3	Solar zenith angle at the middle of the integration time	degrees	4	fl	1
4	Sub-satellite point at the middle of the integration time	-	8	Coord	1
Size (in bytes)			**20**		

Table 15.4.1.7.1-11 - Level 0 Data Header of the Detector Module ISPs (L0Hdr) Structure within State MDS

#	Description	Units	Byte Length	Data Type	Dim.
1	Consists of a Packet header (6 bytes) and a Data field Header (66 bytes).	-	72	uc	72
Size (in bytes)			**72**		

15.4.1.7.2 Summary Quality ADS

To support the Product Quality Facility (PQF), a summary of all quality flags for each state is given in the Summary Quality ADS. There are several ADSRs in this ADS. The format of the ADSR is shown below.

Table 15.4.1.7.2-1 - Summary Quality ADSR

#	Description	Units	Byte Length	Data Type	Dim.
1	Start time of the scan phase of the state	-	12	mjd	1
2	Flag indicating if MDSRs are attached to the current ADSR (1 = no MDSRs, 0 = otherwise)	-	1	uc	1
3	Mean value of the wavelength differences of Fraunhofer lines compared to the wavelength calibration parameters (per channel). Set to zero in the case of a corrupted state or an unprocessed state.	nm	32	fl	8
4	Standard deviation of the wavelength differences from field 3. Set to zero in the case of a corrupted state or an unprocessed state.	nm	32	fl	8
5	Spare (Number of missing readouts in state)	-	2	us	1
6	Mean difference of leakage current or offset per channel and PMD (this field is only valid for limb states). The ordering is Channels 1 to 8, followed by PMDs 1 to 6, followed by the 45 degree PMD. Set to zero in the case of a corrupted state or an unprocessed state.	%	60	fl	15

Table 15.4.1.7.2-1 - Summary Quality ADSR					
7	**Sun glint region flag** 0 = no sun glint or corrupted / unprocessed state 1 = sun glint	-	1	uc	1
8	**Rainbow region flag** 0 = no rainbow or corrupted / unprocessed state 1 = rainbow	-	1	uc	1
9	**South Atlantic Anomaly (SAA) region flag** 0 = state outside SAA region 1 = state above SAA region	-	1	uc	1
10	**Number of hot pixel per channel and PMD** (order: 1 to 8 and A to F and 45°)	-	30	us	15
11	Spare for additional flags	-	10	uc	10
Size (in bytes)			**182**		

An ADSR occurs for states that are not processed but appear in the processing time window applied to the Level 0 product. This is the case for the presence of incomplete dark states (i.e., one or two states appearing rather than the required three).

Sun glint is a phenomenon that does not invalidate the Level 1b data, but it hampers the calculation of the air mass factors in the Level 1b to 2 processing. A flag is therefore provided for the entire state. A similar indication is also provided for each cluster readout in the observational MDSs.

15.4.1.7.3 Geolocation of the States ADS

To support the extraction of SCIAMACHY data according to a given geolocation, the Geolocation ADS gives the geolocation (4 corner co-ordinates) of the scene on-ground covered by each state. There are several ADSRs for this ADS. The format of each ADSR is shown below.

Table 15.4.1.7.3-1 - Geolocation of the States ADSR					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Start time of the scan phase of the state	-	12	mjd	1
2	Flag indicating if MDSRs are attached to the current ADSR 1= no MDSRs, 0 otherwise	-	1	uc	1

Table 15.4.1.7.3-1 - Geolocation of the States ADSR					
3	For Nadir: 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) For Limb: The first coordinate corresponds to the first geolocation start of integration time, the second the first geolocation end of integration time, the third the last geolocation start of integration time, and the fourth the last geolocation end of integration time. For Occultation: The first two coordinates are the tangent ground point of the middle of the integration time for the first geolocation and the second two coordinates are the tangent ground point of the middle of the integration time for the last geolocation. For all other states: The first two coordinates are the sub-satellite point of the middle of the integration time for the first geolocation and the second two coordinates are the sub-satellite point of the middle of the integration time for the last geolocation. If a state is corrupted, values are set to zero.	-	32	Coord	4
Size (in bytes)			**45**		

An ADSR occurs for states that are not processed but appear in the processing time window applied to the Level 0 product. This is the case for the presence of incomplete dark states (i.e., one or two states appearing rather than the required three).

For Limb and Occultation measurements, the coordinates are representing the tangent ground point of the beginning and the end of the state, while for all other measurements (calibration and monitoring) these coordinates shall be filled with the sub-satellite point at the beginning and at the end of the state. In these cases the first and the second, as well as the third and fourth co-ordinates, have the same values.

15.4.1.7.4 Static Instrument Parameters GADS

This GADS contains some instrument specific parameters from the initialisation file, which shall be available to the Level 1b application program SciaL1c, and Level 2 retrieval processing chain. The format of the Static Instrument Parameters GADS is defined in the table below.

Table 15.4.1.7.4-1 - Static Instrument Parameters

#	Description	Units	Byte Length	Data Type	Dim.
1	n_lc_min	-	1	uc	1
2	ds_n_phases (~12)	-	1	uc	1
3	ds_phase_boundaries (# = ds_n_phase +1)	-	52	fl	13
4	lc_stray_index	-	8	fl	2
5	lc_harm_order	-	1	uc	1
6	ds_poly_order	-	1	uc	1
7	do_var_lc_cha (3 times 4 characters per EPITAXX channel)	-	12	uc	12
8	do_var_lc_cha (8 times 4 characters per channel)	-	32	uc	32
9	do_var_lc_pmd (2 times 4 characters per IR PMD)	-	8	uc	8
10	do_var_lc_pmd (7 times 4 characters per PMD)	-	28	uc	28
11	electrons_BU (per channel)	1/BU	32	fl	8
12	ppg_error	-	4	fl	1
13	stray_error	-	4	fl	1
14	sp_n_phases (~12)	-	1	uc	1
15	sp_phase_boundaries (# = sp_n_phase +1)	-	52	fl	13
16	startpix_6+	-	2	us	1
17	startpix_8+	-	2	us	1
18	h_toa	m	4	fl	1
19	lambda_end_gdf	nm	4	fl	1
20	do_pol_point (“t” for true and “f” for false)	-	12	uc	12
21	sat_level	BU	16	us	8
22	pmd_saturation_limit	BU	2	us	1

Table 15.4.1.7.4-1 - Static Instrument Parameters					
23	do_use_limb_dark (“t” for true and “f” for false)	-	1	uc	1
24	do_pixelwise (“t” for true and “f” for false)	-	8	uc	8
25	alpha0_asm	degree	4	fl	1
26	alpha0_esm	degree	4	fl	1
27	do_fraunhofer (8 times 5 characters per channel)	-	40	uc	40
28	do_etalon (8 times 3 characters per channel)	-	24	uc	24
29	do_IB_SD_ETN (“t” for true and “f” for false)	-	7	uc	7
30	do_IB_OC_ETN (“t” for true and “f” for false)	-	7	uc	7
31	level_2_SMR	-	8	uc	8
Size (in bytes)			**382**		

15.4.1.7.5 Leakage Current Parameters (constant fraction) GADS

The format of this GADS is defined in the table below. There is only one record.

Table 15.4.1.7.5-1 - Leakage Current Parameters (constant fraction)					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	**Constant fraction of the fixed pattern noise (FPN) for each detector element of all eight channels** (intersect of leakage current straight line)	BU	32768	fl	8192
2	**Error on constant fraction of FPN**	BU	32768	fl	8192
3	**Constant fraction of the leakage current (LC) for each detector element of all eight channels** (slope of leakage current straight line)	BU/s	32768	fl	8192
4	**Error on constant fraction of LC**	BU/s	32768	fl	8192
5	**Constant fraction of the PMD dark offset** of all 7 PMDs, for amplifier A and B (given as 1A, 1B, 2A, etc.)	BU	56	fl	14
6	**Error on constant fraction of PMD offset**	BU	56	fl	14
7	**Mean noise** (mean value of standard deviations per detector element)	BU	32768	fl	8192
Size (in bytes)			**163952**		

15.4.1.7.6 Leakage Current Parameters (variable fraction) GADS

This GADS consists of 12 records of the type shown below.

Table 15.4.1.7.6-1 - Leakage Current Parameters (variable fraction) GADSR					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Orbit phase after eclipse (range: 0-1)	-	4	fl	1
2	OBM (near radiator), detector (channels 6-8) and PMD temperatures	K	40	fl	10
3	Variable fraction of the leakage current on top of the constant fraction for channels 6 to 8	BU/s	12288	fl	3x1024
4	Error of variable fraction of the leakage current	BU/s	12288	fl	3x1024
5	Solar straylight scattered from the azimuth mirror	BU/s	32768	fl	8192
6	Error on the solar straylight	BU/s	32768	fl	8192
7	Straylight offset for PMDs	BU	28	fl	7
8	Error on straylight offset for PMDs	BU	28	fl	7
9	Variable fraction of the PMD dark offset on top of the constant fraction for PMDs 5 and 6	BU	8	fl	2
10	Error on the variable fraction of PMD offset	BU	8	fl	2
Size (in bytes)			**90228**		

Both types of detector used for the eight channels of SCIAMACHY resulted affected by the existence of leakage current. The detectors used for channels 1 to 5 were random access linear photo-diode arrays, and were not expected to be sensitive to the temperature fluctuations foreseen in SCIAMACHY. Therefore, it was expected that a monthly update of the leakage current parameters was sufficient for an appropriate leakage current correction for these channels. Channels 6 to 8 were measuring in the near infrared, which required a different type of detector material. These detectors were very sensitive to temperature fluctuations of the surrounding material (mainly the optical bench) and themselves. Therefore, two types of leakage current parameters were required:

- The default leakage current pattern (for all orbital positions and all integration or exposure times) is valid for channels 1 to 5 and PMDs 1 to 4 and 7 (45° sensor). These parameters serve as a basis for the other detectors.

- A set of differences in leakage current corresponding to the orbital position, which may be interpolated for a certain orbital position before applying it to the default leakage current pattern of channels 6 to 8 and PMDs 5 and 6.

There is one additional parameter over orbit position which is the solar straylight scattered from the azimuth mirror. This parameter is valid for all eight detector arrays,

but only for limb measurements. The parameter has obviously nothing to do with leakage current, but it is determined using the calculation of the leakage current parameters and therefore placed into the variable fraction of the leakage current.

The 'Orbit phase after eclipse' field of the variable fraction leakage current parameters has a range between 0 and 1. 0 represents the moment when the sub-satellite point on the ground is entering eclipse in the southern hemisphere (SZA = -90 degrees) and then it runs proportional to time until it reaches 1 after one orbit (approx. 100 minutes). It is given for the start of a region in which the calibration parameters are valid. The number of regions required for appropriate determination of the leakage current parameters (12) was determined during the satellite-commissioning phase.

The sequence of PMD dark and straylight offsets is given for the regular PMDs from 1 to 6 with the last value being the one for the 45° PMD detector.

15.4.1.7.7 PPG/Etalon Parameters GADS

The format of the GADS is defined in the table below. There is only one record.
Coded into the PPG parameters, existence and identity of dead pixels is mentioned.

Table 15.4.1.7.7-1 - PPG/Etalon Parameters GADS

#	Description	Units	Byte Length	Data Type	Dim.
1	Pixel-to-pixel gain factor	-	32768	fl	8192
2	Etalon Correction Factor	-	32768	fl	8192
3	Etalon Residual	-	32768	fl	8192
4	WLS degradation factor		32768	fl	8192
5	Bad Pixel Mask[5]	-	8192	uc	8192
Size (in bytes)			**139264**		

[5] *The bad pixel mask indicates the position of dead or otherwise harmed pixels, which may not be used for further processing. The possible values are: 0 = OK, or 1 = bad pixel*

15.4.1.7.8 Precise Basis of the Spectral Calibration Parameters GADS

The format of the GADS is defined in the table below. There is only one record.

Table 15.4.1.7.8-1 - Precise Basis of the Spectral Calibration Parameters GADS

#	Description	Units	Byte Length	Data Type	Dim.
1	Wavelength of detector pixel	nm	32768	fl	8192
Size (in bytes)			**32768**		

15.4.1.7.9 Spectral Calibration Parameters GADS

SCIAMACHY was equipped with a passive thermal control loop keeping the optical bench temperature stable within 600 mK. Depending on the temperature of the optical bench, the dispersion of the pre-disperse prism produced different spectral properties on the detector arrays. From measurements of the spectral calibration lamp (SLS), a set of spectral calibration parameters was calculated for different positions along the orbit relative to the sun. To fulfill the ultimate scientific requirement for a spectral accuracy of 1/100th of a detector pixel, it was sufficient to define certain orbit phase regions in which the spectral calibration parameters were expected to be fairly constant. These ranges were used as the key into the spectral calibration parameters.

The spectral calibration parameters are a precise basis array of wavelength value for each detector pixel, and a sequence of five coefficients of a 4th order polynomial from a4 to a0 for each detector array and the eight detector arrays are given from 1 to 8 for a total of 40 coefficients.

There are 12 records in this GADS of the type shown below.

Table 15.4.1.7.9-1 - Spectral Calibration Parameters GADSR

#	Description	Units	Byte Length	Data Type	Dim.
1	Orbit phase after eclipse (range: 0 - 1)	-	4	fl	1
2	Coefficients in the 4th order polynomial for each detector array (channel)	-	320	do	40
3	Number of used lines per channel	-	16	us	8
4	Wavelength calibration error per channel	-	32	fl	8
Size (in bytes)			**372**		

One set of spectral calibration parameters is valid for the sun reference measurement. The radiance and the polarisation sensitivity values in the ADSs below are interpolated to this wavelength grid.

15.4.1.7.10 Sun Reference Spectrum GADS

This GADS contains several records (i.e. 12) with solar reference spectra obtained from different measurement modes. Solar radiances obtained from both ESM and ASM calibration measurements are provided in a calibrated and un-calibrated way (see table below).

Solar spectrum Identifier	Content
D0	ESM diffuser, calibrated, ND filter in
D1	ESM diffuser, calibrated, ND filter out
D2	ASM diffuser, calibrated
E0	ESM diffuser, un-calibrated, ND filter in
E1	ESM diffuser, un-calibrated, ND filter out
A0	ASM diffuser, un-calibrated
A1	ASM diffuser, un-calibrated
N1	Placeholder – not used
N2	Placeholder – not used
N3	Placeholder – not used
N4	Placeholder – not used
N5	Placeholder – not used

Each reference spectrum is given in the form of a mean value of different sun diffuser measurements using the bi-directional scattering distribution function (BSDF) of the diffuser to convert the measured radiance into irradiance and the mean values of the corresponding PMD measurements. The individual sun diffuser calibration measurements are not given in the Level 1b product. The reason to provide mean sun reference spectra for the different modes is that during instrument calibration several anomalies were found for different modes. The optimum Sun reference spectrum to use in the Level 2 processing may depend on the kind of retrieval used there. The following identifiers specify the possible types of spectra:

Table 15.4.1.7.10-1 - Solar spectrum Identifier

	Fully Calibrated	Uncalibrated
Diffuser (ESM)	D	E
Diffuser (ASM)	D	A
Occultation	O	U

Sun Solar	S	V

The format of the GADS is defined in the table below.

Table 15.4.1.7.10-2 - Sun Reference Spectrum GADS

#	Description	Units	Byte Length	Data Type	Dim
1	Sun spectrum identifier ("Xn" where "X" indicates the solar measurement mode, according to the table above, and "n" indicates various diffuser angles)	-	2	uc	2
2	Wavelength of the sun measurement	nm	32768	fl	8192
3	Mean sun reference spectrum	Calibrated = photons/ (cm2*nm*s) Uncalibrated = BU/s	32768	fl	8192
4	Radiometric precision of the mean sun reference spectrum		32768	fl	8192
5	Radiometric accuracy of the mean sun reference spectrum		32768	fl	8192
6	Diffuser/Small Aperture Etalon	-	32768	fl	8192
7	Average azimuth mirror position	degrees	4	fl	1
8	Average elevation mirror position (diffuser)	degrees	4	fl	1
9	Average solar elevation angle	degrees	4	fl	1
10	Mean value of the corresponding PMD measurements	BU	28	fl	7
11	PMD out-of-band signal with ND out	BU	28	fl	7
12	PMD out-of-band signal with ND in	BU	28	fl	7
13	Doppler shift at 500 nm	nm	4	fl	1
Size (in bytes)			**163942**		

15.4.1.7.11 Polarisation Sensitivity Parameters Nadir GADS

The polarisation sensitivity is expressed as a large number of different parameters that are dependent on the two positions (azimuth and elevation) of the scanner, so an array of various polarisation sensitivity values for a list of scanner positions is required.
For nadir, a one-dimensional array of two parameters (μ2, μ3) is sufficient, because only the position of the elevation mirror is relevant.

The number of records in the GADS results from pre-flight calibration activities: ESM and ASM position values were selected so that linear interpolation between these values yields an error well below the systematic error of the corresponding parameter. These values are extracted from the initialisation file and used to calculate the present

product component. During application of the polarisation sensitivity parameters the scan mirror positions in the geolocation record of the MDS are used to select the correct interval and calculate an appropriate set of polarisation sensitivity parameters using linear interpolation. The format of each GADS record is shown below.

Table 15.4.1.7.11-1 - Polarisation Sensitivity Parameters Nadir GADSR

#	Description	Units	Byte Length	Data Type	Dim.
1	Elevation mirror position	degrees	4	fl	1
2	μ2 for the elevation mirror position of field 1	-	32768	fl	8192
3	μ3 for the elevation mirror position of field 1	-	32768	fl	8192
Size (in bytes)			**65540**		

15.4.1.7.12 Polarisation Sensitivity Parameters Limb GADS

The polarisation sensitivity is expressed as a large number of different parameters that are dependent on the two positions (azimuth and elevation) of the scanner, so an array of various polarisation sensitivity values for a list of scanner positions is required.
For limb, a two-dimensional array of two parameters (μ2 and μ3) is required, because the positions of both scanner mirrors are arguments to the two parameters, which are necessary for the calculation of the polarisation correction factor.

The number of records in the GADS results from pre-flight calibration activities: ESM and ASM position values were selected so that linear interpolation between these values yields an error well below the systematic error of the corresponding parameter. These values are extracted from the initialisation file and used to calculate the present product component. During application of the polarisation sensitivity parameters the scan mirror positions in the geolocation record of the MDS are used to select the correct interval and calculate an appropriate set of polarisation sensitivity parameters using linear interpolation. The format of each GADS record is shown below.

Table 15.4.1.7.12-1 - Polarisation Sensitivity Parameters Limb GADSR

#	Description	Units	Byte Length	Data Type	Dim.
1	Elevation mirror position	degrees	4	fl	1
2	Azimuth mirror position	degrees	4	fl	1
3	μ2 for the elevation and azimuth mirror position of fields 1 and 2	-	32768	fl	8192
4	μ3 for the elevation and azimuth mirror position of fields 1 and 2	-	32768	fl	8192

Table 15.4.1.7.12-1 - Polarisation Sensitivity Parameters Limb GADSR		
Size (in bytes)	**65544**	

15.4.1.7.13 Polarisation Sensitivity Parameters Occultation GADS

The format of each GADS record is similar to that of Polarisation Sensitivity Parameters Limbs described in the Table 15.4.1.7.12-1.

15.4.1.7.14 Radiance Sensitivity Parameters Nadir GADS

The format of each GADS record is shown below.

Table 15.4.1.7.14-1 - Radiance Sensitivity Parameters Nadir GADSR

#	Description	Units	Byte Length	Data Type	Dim.
1	Elevation mirror position	degrees	4	fl	1
2	Radiance sensitivity for the mirror position of field 1	(BU/s)/(photons/ cm2*nm*sr*s)	32768	fl	8192
Size (in bytes)			**32772**		

15.4.1.7.15 Radiance Sensitivity Parameters Limb GADS

The radiance sensitivity parameters are an interpolated set of the pre-characterised radiance sensitivity function for the eight detector arrays. The radiance sensitivity is dependent on the scanner position, so it is therefore necessary to include an array of radiance sensitivity values for each two-dimensional (10*10 = 100) scanner positions.
The number of records in the GADS results from pre-flight calibration activities: ESM and ASM position values were selected so that linear interpolation between these values yields an error well below the systematic error of the corresponding parameter. These values are extracted from the initialisation file and used to calculate the present product component. During application of the polarisation sensitivity parameters the scan mirror positions in the geolocation record of the MDS are used to select the correct interval and calculate an appropriate set of polarisation sensitivity parameters using linear interpolation. The format of each GADS record is shown below.

The radiance sensitivity parameters for the nadir measurements are identified by a fixed value of 360° for the ASM position. ESM and ASM position values in the geolocation records of the MDSs are used to select the correct set of radiance sensitivity parameters from this GADS.

Table 15.4.1.7.15-1 - Radiance Sensitivity Parameters Limb/Occultation with ND GADSR

Table 15.4.1.7.15-1 - Radiance Sensitivity Parameters Limb/Occultation with ND GADSR					
#	Description	Units	Byte Length	Data Type	Dim.
1	Elevation mirror position	degrees	4	fl	1
2	Azimuth mirror position	degrees	4	fl	1
3	Radiance sensitivity for the elevation and azimuth mirror position of field 1 and 2	(BU/s)/(photons/ cm2*nm*sr*s)	32768	fl	8192
Size (in bytes)			**32776**		

15.4.1.7.16 Radiance Sensitivity Parameters Occultation GADS

The format of each GADS record is similar to that of Radiance Sensitivity Parameters Limb GADS described in the Table 15.4.1.7.15-1.

15.4.1.7.17 Errors on Key Data GADS

This GADS consists of one GADSR. The format of the GADSR is shown in the table below:

Table 15.4.1.7.17-1 - Errors on Key Data GADSR					
#	Description	Units	Byte Length	Data Type	Dim.
1	Error on µ2 nadir	-	32768	fl	8192
2	Error on µ3 nadir	-	32768	fl	8192
3	Error on µ2 limb	-	32768	fl	8192
4	Error on µ3 limb	-	32768	fl	8192
5	Error on the radiance sensitivity for the optical bench only	(BU/s)/(photons/ cm2*nm*sr*s)	32768	fl	8192
6	Error on radiance sensitivity for elevation mirror only (nadir viewing)	-	32768	fl	8192
7	Error on radiance sensitivity for elevation and azimuth mirror (limb viewing)	-	32768	fl	8192
8	Error on radiance sensitivity for diffuser and azimuth mirror (sun diffuser measurements).	-	32768	fl	8192
9	Error on BSDF	-	32768	fl	8192
Size (in bytes)			**294912**		

To calculate the errors on the final Level 1b data, the errors on those parts of the Key Data, which are required during the processing of the application program, have to be included in the Level 1b product besides the Key Data itself, as described in the GADSs above.

The parameters for which errors are attached are the following:

- polarisation sensitivity parameters for nadir and limb (μ2 and μ3),
- radiance sensitivity parameters, and
- BSDF function.

The error on the radiance sensitivity parameters is given for individual components of the instrument or viewing geometry. For example, the first error is for the optical bench module (OBM) only (field 5). To get the error on the radiance sensitivity for a specific measurement type, the errors have to be combined using the Gaussian error propagation rule for multiplication. The following combinations are required:

- for nadir measurements, fields 5 and 6 (if only the elevation mirror is used)
- for limb or occultation measurements, fields 5 and 7 (if the light is entering the instrument via the azimuth and elevation mirror)
- for sun diffuser measurements, fields 5 and 8 (the light is going via the azimuth mirror onto the sun diffuser on the back side of the elevation mirror, from where it is scattered into the instrument).

The combination of these fields is done as follow:

$$\varepsilon_{Rad} = \text{Square Root } (\varepsilon_{OBM}^{2} + \varepsilon_{\chi}^{2})$$

where ε_{OBM} is field 5 and ε_{χ} is one of the errors given in fields 6 to 8.

15.4.1.7.18 Slit Function Parameters GADS

The slit function parameter GADS is a copy of the Key Data '_SLIT_F' within the SCI_KD1_AX auxiliary file. It is included as GADS because it is needed in the Level 1 to 2 processing step. The actual number of records is equal to the second dimension of the corresponding array in the Key Data file. The format of each GADS is shown below.

Table 15.4.1.7.18-1 - Slit Function Parameters GADS

#	Description	Units	Byte Length	Data Type	Dim.
1	Pixel position for which the slit function is given (0-8191)	-	2	us	1
2	Type of slit function (1=gauss, 2=single hyperbolic, 3=Voigt)	-	1	uc	1
3	FWHM of slit function (pixel)	-	4	fl	1
4	For Voigt : FWHM of Lorenzian part (pixel)	-	4	fl	1
Size (in bytes)			**11**		

15.4.1.7.19 Small Aperture Slit Function Parameters GADS

The small aperture slit function parameters GADS is a copy of the Key Data '_SMALL_AP_SLIT_F' within the SCI_KD1_AX file. It is included as GADS because it is needed in the Level 1 to 2 processing. The actual number of records is equal to the second dimension of the corresponding array in the Key Data file. The format of each GADS is shown below.

Table 15.4.1.7.19-1 - Small Aperture Slit Function Parameters GADS

#	Description	Units	Byte Length	Data Type	Dim.
1	Pixel position for which the slit function is given (0-8191)	-	2	us	1
2	Type of slit function (1=gauss, 2=single hyperbolic, 3=Voigt)	-	1	uc	1
3	FWHM of slit function (pixel), for Voigt: Lorenzian part	-	4	fl	1
4	For Voigt only: FWHM of Gaussian part (pixel)	-	4	fl	1
Size (in bytes)			**11**		

15.4.1.7.20 States of the Product ADS

This ADS provides information concerning the structure of the states in this product. There is one ADSR per state regardless of whether the state has associated MDSRs. The ADSRs are sorted in chronological order. For each state, the state identifier, the measurement category, and the cluster configuration parameters are written. The format of each ADSR is shown below.

Table 15.4.1.7.20-1 - States of the Product ADSR

#	Description	Units	Byte Length	Data Type	Dim.
1	Start time of the scan phase of the state	-	12	mjd	1
2	Flag indicating if MDSRs are attached to the current ADSR (1:no, 0: yes)	-	1	uc	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	-	1	uc	1
4	Orbit phase after eclipse of the state (range: 0-1)	-	4	fl	1
5	Measurement Category	-	2	us	1
6	State ID	-	2	us	1
7	Duration of scan phase of the state	1/16 s	2	us	1

Table 15.4.1.7.20-1 - States of the Product ADSR					
8	Longest integration time	1/16 s	2	us	1
9	Number of clusters	-	2	us	1
10	Cluster Configuration	-	1088	Clcon	64
11	MDS type for this state (1 = nadir, 2 = limb, 3 = occultation, 4 = monitoring)	-	1	uc	1
12	Number of repeated geolocation and Level-0 headers	-	2	us	1
13	Number of Integrated PMD Values	-	2	us	1
14	Number of Different Integration times in all clusters	-	2	us	1
15	Various integration times in this state	1/16 s	128	us	64
16	Number of Fractional Polarisation Values per Integration Time	-	128	us	64
17	Number of Fractional Polarisation Values	-	2	us	1
18	Number of DSRs	-	2	us	1
19	Length of DSR	bytes	4	ul	1
Size (in bytes)			**1387**		

Note: The number of 64 elements for the cluster configuration field is due to the maximum number of clusters of the instrument measurement configuration.

15.4.1.7.21 PMD Data Packets ADS

This ADS contains all PMD data packets extracted from the Level 0 for all states where MDSRs are completed in the product (i.e., no dark states and no unprocessed states).

Table 15.4.1.7.21-1 - PMD Data Packets ADSR					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Start time of the PMD data packet	-	12	mjd	1
2	Flag indicating if MDS DSRs are attached to the current ADS DSR (always set to zero for this ADS)	-	1	uc	1
3	PMD data packet of the level 0 data	-	6820	uc	6820
Size (in bytes)			**6833**		

15.4.1.7.22 Auxiliary Data Packets of Observation States ADS

This ADS contains all auxiliary data packets extracted from the Level 0 for all states where MDSRs are completed in the product (i.e., no dark states and no unprocessed states).

Table 15.4.1.7.22-1 - Auxiliary Data Packets ADSR

Table 15.4.1.7.22-1 - Auxiliary Data Packets ADSR					
#	Description	Units	Byte Length	Data Type	Dim.
1	Start time of the auxiliary data packet	-	12	mjd	1
2	Attachment Flag indicating if MDS DSRs are attached to the current ADS DSR (always set to zero for this ADS)	-	1	uc	1
3	Auxiliary data packet of the level 0 data	-	1666	uc	1666
Size (in bytes)			**1679**		

15.4.1.7.23 Leakage Current Parameters (newly calculated partial set) ADS

A new set of leakage current parameters, as described for the constant and variable fraction GADSs, is constructed out of three newly calculated partial leakage current sets given here. These were extracted by an external facility to generate the leakage current auxiliary data file. The newly calculated partial sets are in most cases not present in the Level 1b product, they are only calculated during the envisaged monthly in-flight calibration activity. This ADS consists of several records of the type shown below.

Table 15.4.1.7.23-1 - Leakage Current Parameters (newly calculated partial set)					
#	Description	Units	Byte Length	Data Type	Dim.
1	Start time of the first dark measurement state which was used to calculate this ADSR	-	12	mjd	1
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)	-	1	uc	1
3	Start time of the last dark measurement state which was used to calculate this ADSR	-	12	mjd	1
4	Orbit phase after eclipse (range: 0-1)	-	4	fl	1
5	OBM (near radiator), detector (8x), and PMD temperatures	-	40	fl	10
6	Fixed pattern noise for channels 1 to 8	BU	32768	fl	8192
7	Error on the FPN	BU	32768	fl	8192
8	Leakage current for channels 1 to 8	BU/s	32768	fl	8192
9	Error on the leakage current	BU/s	32768	fl	8192
10	Mean noise (mean value of standard deviations per detector element)	BU	32768	fl	8192

Table 15.4.1.7.23-1 - Leakage Current Parameters (newly calculated partial set)					
11	PMD dark offset for all PMDs for amplifier A and B	BU	56	fl	14
12	Error on the PMD offset	BU	56	fl	14
Size (in bytes)			**164021**		

15.4.1.7.24 Average of the Dark Measurements per State ADS

This ADS consists of several records of the type shown below.

Table 15.4.1.7.24-1 - Average of the Dark Measurements per State ADSR					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Start time of the dark measurement state which was used to calculate this ADSR	-	12	mjd	1
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)	-	1	uc	1
3	Average dark measurement spectrum	BU	32768	fl	8192
4	Standard deviation of the dark measurement spectrum	BU	32768	fl	8192
5	PMD dark offset for all PMDs for the amplifier A and B (1A, 1B, 2A, etc ...)	BU	56	fl	14
6	Error on the PMD offset	BU	56	fl	14
7	Solar straylight scattered from azimuth mirror	BU/s	32768	fl	8192
8	Error on the solar straylight	BU/s	32768	fl	8192
9	Straylight offset for PMDs	BU	28	fl	7
10	Error on the PMD straylight offset	BU	28	fl	7
Size (in bytes)			**131253**		

15.4.1.7.25 PPG/Etalon Parameters (newly calculated) ADS

This ADS consists of one ADSR of the type shown below.

Table 15.4.1.7.25-1 - PPG/Etalon Parameters (newly calculated) ADSR					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Start time of the WLS measurement state which was used to calculate this ADSR	-	12	mjd	1
2	Flag indicating if MDSRs are attached to the current ADSR (yes, in the monitoring MDS)	-	1	uc	1
3	Pixel-to-pixel gain factor	-	32768	fl	8192
4	Etalon Correction Factor	-	32768	fl	8192
5	Etalon residual	-	32768	fl	8192

Table 15.4.1.7.25-1 - PPG/Etalon Parameters (newly calculated) ADSR					
6	Average WLS spectrum which has been used for the determination of PPG and Etalon	BU	32768	fl	8192
7	Standard deviation of the WLS spectrum	BU	32768	fl	8192
8	Bad Pixel Mask	-	8192	uc	8192
Size (in bytes)			**172045**		

15.4.1.7.26 Spectral Calibration Parameters (newly calculated) ADS

This ADS consists of one ADSR of the type shown below.

Table 15.4.1.7.26-1 - Spectral Calibration Parameters (newly calculated) ADSR					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Start time of the SLS or sun measurement state which was used to calculate this ADSR	-	12	mjd	1
2	Flag indicating if MDSRs are attached to the current ADSR (always set to zero in this ADS)	-	1	uc	1
3	Orbit phase after eclipse (range: the absolute value is between 0 and 1)	-	4	fl	1
4	Coefficients in the 4th order polynomial for each detector array	-	320	do	40
5	Source of spectral calibration parameters (0=SLS, 1=sun)	-	8	uc	8
6	Number of used lines per channel	-	16	us	8
7	Wavelength calibration error per channel	-	32	fl	8
8	Average SLS or solar spectrum which has been used for the determination of spectral calibration parameters	BU	32768	fl	8192
9	Selected line positions for 3 lines per channel	nm	96	fl	24
Size (in bytes)			**33257**		

If the spectral calibration algorithm is not able to determine a set of coefficients for a certain detector array, the corresponding wavelength calibration error shall be set to -1 (field 7 above).

15.4.1.7.27 Sun Reference Spectrum (newly calculated) ADS

The format of each ADSR in this ADS is shown in the table below.

Table 15.4.1.7.27-1 - Sun Reference Spectrum (newly calculated) ADSR					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Start time of the sun diffuser measurement state which was used to calculate this ADSR	-	12	mjd	1

Table 15.4.1.7.27-1 - Sun Reference Spectrum (newly calculated) ADSR					
2	Flag indicating if MDSRs are attached to the current ADSR (always set to 0 for this ADS)	-	1	uc	1
3	Sun spectrum identifier "XØ" where "X" indicates the solar measurement mode; see Table 15.4.1.7.27-1	-	2	uc	2
4	Neutral density filter flag	-	1	uc	1
5	Wavelength of the sun spectrum	nm	32768	fl	8192
6	Mean sun reference spectrum	Calibrated= photons/ (cm2*nm*s) Uncalibrated= BU/s	32768	fl	8192
7	Relative radiometric precision of the mean sun reference spectrum	-	32768	fl	8192
8	Relative radiometric accuracy of the mean sun reference spectrum	-	32768	fl	8192
9	Diffuser/Small Aperture Etalon	-	32768	fl	8192
10	Average azimuth mirror position	degrees	4	fl	1
11	Average elevation mirror position (diffuser)	degrees	4	fl	1
12	Average solar elevation angle	degrees	4	fl	1
13	Mean value of the corresponding PMD measurements	BU	28	fl	7
14	PMD out-of-band signal	BU	28	fl	7
15	Doppler shift at 500 nm	nm	4	fl	1
Size (in bytes)			**163928**		

15.4.1.7.28 Nadir MDS

This MDS contains measurement data acquired while the instrument was in Nadir viewing mode. The MDS contains multiple MDSRs, each of the format shown below. Note that MDSRs within the MDS may be of different lengths.

Table 15.4.1.7.28-1 - Nadir MDSR Format					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Start time of DSR	-	12	mjd	1
2	DSR length	bytes	4	ul	1
3	Quality indicator (-1 if empty DSR)	-	1	sc	1
4	Scale factor for the straylight values in the signal compound type per channel	-	8	uc	8

Table 15.4.1.7.28-1 - Nadir MDSR Format					
5	Saturation Flags	-	8	uc	8
6	Red grass flag	-	*	uc	
7	Sun Glint / Rainbow quality flag per readout	-	*	uc	*
8	Geolocation	-	*	GeoN	*
9	Level 0 detector module data packet headers	-	*		*
10	Integrated PMD values	BUs	*	fl	*
11	Fractional polarisation values	-	*	PolV	*
12	Cluster data	-	**	Clcon	**
Size (in bytes)			**variable**		

* Number of elements provided in the corresponding States ADSR

** Number of elements and data type for each cluster is provided via the Clcon structure in the corresponding States ADSR.

The sun glint / rainbow quality flags are given for observational MDSs only. The sun glint / rainbow flag is set to 0, or to 1 for medium sun glint danger; to 2 for high sun glint danger, and to 4 for rainbow. If the pixel is so large that rainbow and sun glint occur in the same pixel, the flag is the sum of sun glint and rainbow flags (i.e. 5 or 6).

15.4.1.7.29 Limb MDS

This MDS contains measurement data acquired while the instrument was in Limb viewing mode. The MDS contains multiple MDSRs, each of the format shown below. Note that MDSRs within the MDS may be of different lengths.

Table 15.4.1.7.29-1 - Limb MDSR Format					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Start time of DSR	-	12	mjd	1
2	DSR length	bytes	4	ul	1
3	Quality indicator (-1 if empty DSR)	-	1	sc	1
4	Scale factor for the straight values in the signal compound type per channel	-	8	uc	8
5	Saturation flag	-	*	uc	*
6	Red grass flag	-	*	uc	*

Table 15.4.1.7.29-1 - Limb MDSR Format					
7	Sun Glint / Rainbow quality flag per readout (all flags are set to zero as not used)	-	*	uc	*
8	Geolocation	-	*	GeoL	*
9	Level 0 detector module data packet headers	-	*	L0Hdr	*
10	Integrated PMD values	BUs	*	fl	*
11	Fractional polarisation values	-	*	PolV	*
12	Cluster data	-	**	Clcon	**
Size (in bytes)			**variable**		

* Number of elements provided in the corresponding States ADSR

** Number of elements and data type for each cluster is provided via the Clcon structure in the corresponding States ADSR.

Starting from IPF version 7, a new type of Limb state was made available: a mesospheric mode, scanning altitudes between 60 and 150 km. These measurements were run instead of the routine Limb states for 30 orbits every month on two separate days (see OCR 36). The mesospheric observations are identified by state ID 55, and measurement category 27. The planning details for the limb mesosphere-thermosphere blocks are available on the SOST web page.

15.4.1.7.30 Occultation MDS

This MDS contains measurement data acquired while the instrument was in Occultation viewing mode. The MDS contains multiple MDSRs. The format of each MDSR is identical to that of the Limb MDSR described in Table 15.4.1.7.29-1.

15.4.1.7.31 Monitoring MDS

This MDS contains measurement data acquired while the instrument was in Monitoring mode. The MDS contains multiple MDSRs, each with the format shown below. Note that MDSRs within this MDS may be of different lengths.

Table 15.4.1.7.31-1 - Monitoring MDSR Format					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Start time of DSR	-	12	mjd	1
2	DSR length	bytes	4	ul	1
3	Quality indicator (-1 if empty DSR)	-	1	sc	1

Table 15.4.1.7.31-1 - Monitoring MDSR Format					
4	Scale factor for the straight values in the signal compound type per channel	-	8	uc	8
5	Saturation flag	-	1	uc	1
6	Red Grass flag	-	*	uc	*
7	Geolocation	-	*	GeoCal	*
8	Level 0 detector module data packet headers	-	*	L0Hdr	1
9	Cluster data	-	**	Clcon	**
Size (in bytes)			**variable**		

* Number of elements provided in the corresponding States ADSR

** Number of elements and data type for each cluster is provided via the Clcon structure in the corresponding States ADSR.

15.4.1.8 Size Estimate

The Level 1b product size varies depending on the executed instrument timeline. A maximum estimate is of 400 MB/product.

15.5 LEVEL 2 PRODUCTS

Information on the Level 2 product discontinued can be found in ANNEX 15.7.2.

15.5.1 SCIAMACHY Off-Line Level 2 Product (SCI_OL__2P)

The Level 2 off-line product (SCI_OL__2P) contains retrieved trace gas total columns, profiles, and other geophysical parameters including the corresponding errors, plus a number of additional diagnostics, quality flags and intermediate results.

SCIAMACHY Level 2 off-line products include data as indicated in the following table.

O_3	Total vertical columns retrieved from optical absorption spectroscopy fitting UV and visible wavelength range, using AMF calculation by LIDORT. Profiles from limb observations for UV/visible wavelength range
NO_2	Same as O_3 (vertical columns and limb profiles) but only in the visible wavelength range. Additional Troposheric NO2 from limb/nadir matching
BrO	Same as O_3 (vertical columns and limb profiles)
OClO	Slant column retrieval. Significant amounts expected only in the activated polar vortex
SO_2	Two different SO2 vertical total columns are retrieved. The first column is calculated for anthropogenic pollution scenario (SO2 profile with SO2 peak in the boundary layer); the second column is for volcanic eruption scenario (SO2 profile with SO2 peak between 10 and 11 km)
HCHO	Same as SO2. Retrieval restricted to solar zenith angle below 60°. Noticeable amounts expected above tropical forests and biomass burning regions.
Cloud	Cloud retrieval algorithms using PMDs (OCRA) to determine the fractional cloud cover and a cloud fitting algorithm (SACURA) for cloud top height and other cloud parameters Cloud retrieval from limb measurements (SCODA).
Aerosol	Absorbing Aerosol Index (AAI) from Nadir measurements in UV spectral range
H_2O	Vertical columns. Contrary to the other Nadir trace gas products in the UV/VIS it uses a direct retrieval by AMC DOAS
CHOCHO	Vertical column retrieval
CO	Vertical columns retrieved from IR absorption spectroscopy
CH_4	Vertical column retrieval

15.5.1.1 Input Data

Level 1b consolidated product plus auxiliary data.

15.5.1.2 Auxiliary Data Used

The auxiliary data files required for Level 2 processing are listed in the table below.

Table 15.5.1.2-1 - Auxiliary Data Files for SCIAMACHY Level 2 Processing

Description	Auxiliary File ID
Initialization file	SCI_IN__AX
M-factor file	NOT USED[6]

15.5.1.3 Processing Performed

This is not the applicable document for algorithm details.

The following is a high-level overview of the processing performed for Level 2 product generation.

- Extraction / preprocessing of Level 1b data and evaluation of PCD information.
- Retrieval of geophysical target quantities (total column amounts, cloud cover and top height, aerosol absorption indicator).
- Processing of covariance data of the retrieved quantities (noise assessment).
- Generation of Level 2 product files and related output.

[6] Starting from Level 2 processing baseline 6 the m-factor correction is applied to the Level 0-1b processing step.

Table 15.5.1-1 - SCIAMACHY Level 2 PRODUCT SUMMARY SHEETS

SCIAMACHY Level-2 Off-line product	
PRODUCT ID	SCI_OL__2P
PRODUCT NAME	SCIAMACHY Level-2 Off-line product
DESCRIPTION	This product contains geophysical trace gas columns and profiles, and other geophysical parameters including corresponding errors, plus a number of additional diagnostics, quality flags and intermediate results resulting from the off-line processing of the SCI_NL__1P product measurements.
APPLICATIONS	Measurement of ozone and other atmospheric constituents for meteorology and climatology
DELIVERY TIME	Fully consolidated products available from the PAC starting 1-2 weeks after data take.
COVERAGE	Full orbit, all measurement types
THROUGHPUT	One product per orbit
PRODUCT SIZE	Max. size of approx. 30 MBytes per orbit
AUXILIARY DATA	Summary Quality ADS (SQADS) State Geolocation ADS (LADS) States of the product ADS Geolocation of the Nadir ground pixels ADS Geolocation of the Limb / Occultation measurements ADS
NOTES	Produced off-line from Level 1b data

15.5.1.4 Product Structure

The high-level product structure is shown below:

Table 15.5.1.4-1 – SCIAMACHY consolidated Level 2 Product Structure
Main Product Header
Specific Product Header
Summary of Quality ADS (SQADS)
Geolocation of the States ADS (LADS)
Static Parameter GADS
States of the Product ADS
Geolocation of the Nadir Ground Pixels ADS
Geolocation of the Limb/Occultation measurements ADS
Cloud and Aerosol MDS
Nadir Fitting Window Application MDSs (16 MDSs: 14 planned and 2 spare)
Limb Fitting Window Application MDSs (14 MDSs: 12 planned and 2 spare)
Occultation Fitting Window Application MDSs (14 MDSs: 12 planned and 2 spare)
Ozone Profiles from Nadir measurements MDS
Limb Clouds Data sets

15.5.1.5 Main Product Header

The Main Product Header (MPH) is described in R-3.

15.5.1.6 Specific Product Header

The SPH is a header that conforms to the ASCII conventions defined in R-3. The Ø symbol indicates the position of an ASCII blank space character.

Table 15.5.1.6-1 – Specific Product Header of consolidated Level 2 Product

#	Description	Units	Byte Length	Data Type	Dim.
1	**SPH_DESCRIPTOR=**	keyword	15	uc	15
	quotation mark (“)	-	1	uc	1
	SPH descriptor (Set to “SCI_OL__2PØØØØØØØØØØØØØØØØØØØØ”)	-	28	uc	28
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
2	**STRIPLINE_CONTINUITY_INDICATOR=**	keyword	31	uc	31

Table 15.5.1.6-1 – Specific Product Header of consolidated Level 2 Product					
	Value: +000 = No stripline continuity, the product is a complete segment Other: Stripline Counter	-	4	ac	1
	newline character	terminator	1	uc	1
3	**SLICE_POSITION=**	keyword	15	uc	15
	Value: +001 to NUM_SLICES Default value if no stripline continuity = +001	-	4	ac	1
	newline character	terminator	1	uc	1
4	**NUM_SLICES=**	keyword	11	uc	11
	Number of slices in this stripline Default value if no continuity = +001	-	4	ac	1
	newline character	terminator	1	uc	1
Product Location Information					
5	**START_TIME=**	keyword	11	uc	11
	quotation mark (“)	-	1	uc	1
	Start time of the measurement data in this product UTC time of the first MDSR	utc	27	uc	27
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
6	**STOP_TIME=**	keyword	10	uc	10
	quotation mark (“)	-	1	uc	1
	Time of the end of the measurement data in this product UTC time of the last MDSR	utc	27	uc	27
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
7	**START_LAT=**	keyword	10	uc	10
	Latitude of the satellite nadir at the START_TIME WGS84 latitude, positive = North	1e-6 deg	11	al	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
8	**START_LONG=**	keyword	11	uc	11
	Longitude of the satellite nadir at the START_TIME WGS84 longitude, positive = East, 0 = Greenwich	1e-6 deg	11	al	1
	<10-6degE>	units	10	uc	10
	newline character	terminator	1	uc	1
9	**STOP_LAT=**	keyword	9	uc	9
	Latitude of the satellite nadir at the STOP_TIME WGS84 latitude, positive = North	1e-6 deg	11	al	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
10	**STOP_LONG=**	keyword	10	uc	10

Table 15.5.1.6-1 – Specific Product Header of consolidated Level 2 Product

	Longitude of the satellite nadir at the STOP_TIME WGS84 longitude, positive = East, 0 = Greenwich	1e-6 deg	11	al	1
	<10-6degE>	units	10	uc	10
	newline character	terminator	1	uc	1
11	**DECONT =**	keyword	7	uc	7
	quotation mark (")	-	1	uc	1
	Decontamination flag for each detector channel (Default set to "NNNNNNNNØØØØØØØØØØØØØØØØØØØØØØØØØØØØØØØØØ") 8*char plus 33*blank	-	41	uc	1
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
Other Product Information					
12	DB_SERVER_VER=	keyword	14	uc	14
	quotation mark (")	-	1	uc	1
	Version number of database server Format: NN.MM, currently 05.01	-	5	uc	5
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
13	FITTING_ERROR_SUM=	keyword	18	uc	18
	quotation mark (")	-	1	uc	1
	Quality summary of the fitting errors: GOOD or FAIR or BADØ	keyword	4	uc	4
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
14	NO_OF_NADIR_FITTING_WINDOWS=	keyword	28	uc	28
	Number of Nadir fitting windows	-	4	Ac	1
	newline character	terminator	1	uc	1
15	NAD_FIT_WINDOW_UV0=	keyword	19	uc	19
	quotation mark (")	-	1	uc	1
	Wavelength range of fitting window given as a pattern of two wavelengths like: xxxx-yyyy (e.g., Ø325-Ø335; missing digits shall be written as blank spaces)	variable	9	uc	9
	Blank Space character (Ø)	-	1	uc	1
	Acronyms for the fitting parameter	variable	20	uc	20
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1

Table 15.5.1.6-1 – Specific Product Header of consolidated Level 2 Product					
16-30	**The field above is repeated for NAD_FIT_WINDOW_UV1 to NAD_FIT_WINDOW_UV9, and next for NAD_FIT_WINDOW_IR0 to NAD_FIT_WINDOW_IR5 8 of the 9 fitting windows in the UV and visible wavelength range are planned, and 1 is spare. 5 of the 6 fitting windows in the IR wavelength range are planned, and 1is spare. If a fitting window is not used, the string between quotation marks is filled by "EMPTYØØØØØØØØØ" 52 uc each (18/14/20)**	-	780	uc	780
31	**NO_OF_LIMB_FITTING_WINDOWS=**	keyword	27	uc	27
	Number of Limb fitting windows	-	4	ac	1
	newline character	terminator	1	uc	1
32	**LIM_FIT_WINDOW_PTH= Limb fitting specifications for pTH**	keyword	19	uc	19
	quotation mark (")	-	1	uc	1
	Wavelength range of fitting window given as a pattern of two wavelengths like: xxxx-yyyy (e.g., Ø325-Ø335; missing digits shall be written as blank spaces) If a fitting window is not used, the string between quotation marks is filled by "EMPTYØØØØØØØØØ"	variable	9	uc	9
	Blank Space character (Ø)	-	1	uc	1
	Acronym for the driving parameter of this fitting window (e.g., O3ØØ)	variable	20	uc	4
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
33	**LIM_FIT_WINDOW_UV0=**	keyword	19	uc	19
	quotation mark (")	-	1	uc	1
	Wavelength range of fitting window given as a pattern of two wavelengths like: xxxx-yyyy (e.g., Ø325-Ø335; missing digits shall be written as blank spaces)	variable	9	uc	9
	Blank Space character (Ø)	-	1	uc	1
	Acronym for the driving parameter of this fitting window (e.g., O3ØØ)	variable	20	uc	4
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1

Table 15.5.1.6-1 – Specific Product Header of consolidated Level 2 Product					
34-45	**The field above is repeated for LIM_FIT_WINDOW_UV1 to LIM_FIT_WINDOW_UV7, and next for LIM_FIT_WINDOW_IR0 to LIM_FIT_WINDOW_IR4 6 of the 7 fitting windows in the UV and visible wavelength range are planned, and 1 is spare. 4 of the 5 fitting windows in the IR wavelength range are planned, and 1 is spare. If a fitting window is not used, the string between quotation marks is filled by "EMPTYØØØØØØØØØ"**	-	624	uc	624
46	**NO_OF_OCCL_FITTING_WINDOWS=**	keyword	27	uc	27
	Number of occultation fitting windows default value +000 if no occultation fitting windows.	-	4	ac	4
	newline character	terminator	1	uc	1
47	**OCC_FIT_WINDOW_PTH=**	keyword	19	uc	19
	quotation mark (")	-	1	uc	1
	Occultation fitting window specifications -pTH with rough wavelength range . (e.g., Ø325-Ø335; missing digits shall be written as blank spaces) If a fitting window is not used, the string between quotation marks is filled by "EMPTYØØØØØØØØØ"	variable	9	uc	9
	Blank Space character (Ø)	-	1	uc	1
	Acronym for the driving parameter of this fitting window	variable	20	uc	4
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
48	**OCC_FIT_WINDOW_UV0=**	keyword	19	uc	19
	quotation mark (")	-	1	uc	1
	Occultation fitting window specifications with rough wavelength range . (e.g., Ø325-Ø335; missing digits shall be written as blank spaces)	variable	9	uc	9
	Blank Space character (Ø)	-	1	uc	1
	Acronym for the driving parameter of this fitting window (e.g., O3ØØ)	variable	20	uc	4
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
49-60	**The field above is repeated for OCC_FIT_WINDOW_UV1 to OCC_FIT_WINDOW_UV7, and next for OCC_FIT_WINDOW_IR0 to OCC_FIT_WINDOW_IR4**	-	624	uc	624

Table 15.5.1.6-1 – Specific Product Header of consolidated Level 2 Product					
	6 of the 7 fitting windows in the UV and visible wavelength range are planned, and 1 is spare. **4 of the 5 fitting windows in the IR wavelength range are planned, and 1 is spare.** **If a fitting window is not used, the string between quotation marks is filled by "EMPTYØØØØØØØØØ" 60** **52 uc each (18/14/20)**				
61	Spare (blank characters (Ø))	-	64	uc	64
	newline character	terminator	1	uc	1
DSDs for Attached Data Sets					
62	DSD (A) for the SQ ADS	-	280	dsd	1
63	DSD (A) State Geolocation ADS (L ADS)	-	280	dsd	1
64	DSD (A) for the Static parameters	-	280	dsd	1
65	DSD (A) for the States of the Product ADS	-	280	dsd	1
66	DSD(A) for the Geolocation of the Nadir Ground Pixels ADS	-	280	dsd	1
67	DSD(A) for the Geolocation of the Limb/Occultation Measurements ADS 67	-	280	dsd	1
68	DSD (M) for the Clouds and Aerosol MDS	-	280	dsd	1
69-84	DSDs for the Nadir Fitting Window Application 16 MDSs: 14 planned and 2 spare; unused entries set to NOT USED as described in R-3	-	4480	dsd	14
85-98	DSDs for the Limb Fitting Window Application 14 MDSs: 12 planned and 1 spare unused entries set to NOT USED as described in R-3	-	3920	dsd	14
99-112	DSDs (M) for the Occultation Fitting Window Application MDSs. (14 MDSs: 12planned and 1 spare; unused entries set to NOT USED as described in R-3)	-	3920	dsd	14
113	DSDs (M) for the Ozone Profiles from Nadir measurements MDS	-	280	dsd	1
114	DSDs (M) for the Limb Cloud measurements MDS	-	280	dsd	1
DSDs for reference files					
115	DSD (R) -Level 1b product from which this product is generated	-	280	dsd	1
116	DSD (R) -Level 2 Initialization file	-	280	dsd	1
117	DSD (R) -Atmospheric Climatologies Data file NOT USED	-	280	dsd	1
118	DSD (R) –M-factor file NOT USED	-	280	dsd	1

Table 15.5.1.6-1 – Specific Product Header of consolidated Level 2 Product					
119	*DSD -Spare (279 blank space characters followed by one newline character)*	-	280	dsd	1
Size (in bytes)			**19115**		

The following ASCII strings are used to fill the DS_NAME fields of the DSDs (refer to R-3).

Table 15.5.1.6-2 – DS_NAME Field Strings	
DSD	**DS_NAME**
DSD (A) -SQ ADS	SUMMARY_QUALITY
DSD (A) -State Geolocation ADS (L ADS)	STATE_GEOLOCATION
DSD (A) -Static Parameters	STATIC_PARAM
DSD (A) -States of the Product ADS	STATES
DSD (A) -Geolocation of the Nadir Ground Pixels ADS	GEOLOCATION_NADIR
DSD (A) -Geolocation of the Limb/Occultation Measurements ADS	GEOLOCATION_LIMB

Table 15.5.1.6-2 – DS_NAME Field Strings	
MSD -Clouds and Aerosol	CLOUDS_AEROSOL
MSD -Nadir Fitting Window Application MDS #1	NAD_UV0_O3
MSD - Nadir Fitting Window Application MDS #2	NAD_UV1_NO2
MSD - Nadir Fitting Window Application MDS #3	NAD_UV2_O3
MSD - Nadir Fitting Window Application MDS #4	NAD_UV3_BRO
MSD - Nadir Fitting Window Application MDS #5	NAD_UV4_H2CO
MSD - Nadir Fitting Window Application MDS #6	NAD_UV5_SO2
MSD - Nadir Fitting Window Application MDS #7	NAD_UV6_OCLO
MSD - Nadir Fitting Window Application MDS #8	NAD_UV7_SO2
MSD - Nadir Fitting Window Application MDS #9	NAD_UV8_H2O
MSD - Nadir Fitting Window Application MDS #10	NAD_UV9_CHOCHO
MSD - Nadir Fitting Window Application MDS #11	NAD_IR0_H2O
MSD - Nadir Fitting Window Application MDS #12	NAD_IR1_CH4
MSD - Nadir Fitting Window Application MDS #13	NAD_IR2_N2O
MSD - Nadir Fitting Window Application MDS #14	NAD_IR3_CO
MSD - Nadir Fitting Window Application MDS #15	NAD_IR4_CO2
MSD - Nadir Fitting Window Application MDS #16	LNM_UV0_NO2
MSD - Limb Fitting Window Application MDS #1	LIM_PTH
MSD - Limb Fitting Window Application MDS #2	LIM_UV0_O3
MSD - Limb Fitting Window Application MDS #3	LIM_UV1_NO2
MSD - Limb Fitting Window Application MDS #4	LIM_UV2_O3
MSD - Limb Fitting Window Application MDS #5	LIM_UV3_BRO
MSD - Limb Fitting Window Application MDS #6	LIM_UV4_H2CO
MSD - Limb Fitting Window Application MDS #7	LIM_UV5_SO2
MSD - Limb Fitting Window Application MDS #8	LIM_UV6_OCLO
MSD - Limb Fitting Window Application MDS #9	LIM_UV7_SPARE
MSD - Limb Fitting Window Application MDS #10	LIM_IR0_H2O

Table 15.5.1.6-2 – DS_NAME Field Strings	
MSD - -Limb Fitting Window Application MDS #11	LIM_IR1_CH4
MSD - Limb Fitting Window Application MDS #12	LIM_IR2_N2O
MSD - Limb Fitting Window Application MDS #13	LIM_IR3_CO
MSD - Limb Fitting Window Application MDS #14	LIM_IR4_SPARE
MSD - Occultation Fitting Window Application MDS #1	OCC_PTH
MSD - Occultation Fitting Window Application MDS #2	OCC_UV0_O3
MSD - Occultation Fitting Window Application MDS #3	OCC_UV1_NO2
MSD - Occultation Fitting Window Application MDS #4	OCC_UV2_O3
MSD - Occultation Fitting Window Application MDS #5	OCC_UV3_BRO
MSD - Occultation Fitting Window Application MDS #6	OCC_UV4_H2CO
MSD - Occultation Fitting Window Application MDS #7	OCC_UV5_SO2
MSD - Occultation Fitting Window Application MDS #8	OCC_UV6_OCLO
MSD - Occultation Fitting Window Application MDS #9	OCC_UV7_SPARE
MSD - Occultation Fitting Window Application MDS #10	OCC_IR0_H2O
MSD - Occultation Fitting Window Application MDS #11	OCC_IR1_CH4
MSD - Occultation Fitting Window Application MDS #12	OCC_IR2_N2O
MSD - Occultation Fitting Window Application MDS #13	OCC_IR3_CO
MSD - Occultation Fitting Window Application MDS #14	OCC_IR4_SPARE
MSD - Ozone Profiles from Nadir measurements MDS	NAD_PROFILE_O3
MSD - Limb Cloud measurements MDS	LIM_CLOUDS
DSD (R) -Level 1b product from which this product is produced	LEVEL_1B_PRODUCT
DSD (R) -Level 2 Initialization file	INITIALISATION_FILE
DSD (R) -Atmospheric Climatologies Data file	ECMWF_FILE
DSD (R) –M-factor Data file	M_FACTOR_FILE
DSD spare	SPARE

The number of 58 DSD records is derived from the fact that there are five ADSs (Summary of Quality, Geolocation of the states, States of the product and two detailed geolocation data sets), one GADS (static parameter), one general MDS about cloud and aerosol data from Nadir, a maximum of 45 fitting window application MDSs (16 Nadir, 14 Limb, 14 Occulation and Ozone profiles from Nadir), one general MDS about clouds from Limb, 4 reference DSD for the input files and one spare record.

15.5.1.7 Data Sets

The following sub-sections describe the individual data sets that together form the consolidated Level 2 product. Data sets are in mixed-binary format. ASCII strings may be included within the data sets, but the string is not surrounded by quotation marks as for the MPH/SPH structures.

15.5.1.7.1 Summary Quality ADS

The Summary Quality ADS provides a summary of the quality flags set for each state. There is one ADSR per state, each with a time stamp to indicate which portion of the product the ADSR pertains to. The format of the ADSR is as follows:

Table 15.5.1.7.1-1 - Summary Quality ADSR Format

#	Description	Units	Byte Size	Data Type	Dim.
1	Start time of the scan phase of the state	-	12	mjd	1
2	Attachment Flag (1 = no MDSRs attached to the current ADSR, 0 otherwise)	-	1	uc	1
3	Error on cloud parameters [a]	-	2	uc	2
4	Aerosol parameter diagnostic [a]	-	2	uc	2
5	Quality of the driving geophysical parameter in each fitting window [a b]	-	44	uc	44
6	RMS of the retrieval algorithm [a b]	-	44	uc	44
7	χ2 of the retrieval algorithm [a b]	-	44	uc	44
8	Goodness of fit of the retrieval algorithm [a b]	-	44	uc	44
Size (in bytes)			**193**		

a. The quality flags are specified as unsigned character having a range from value 0 to 10. 1 represents the best and 10 the worst quality, assigned to the mean value of all quality parameters of a certain kind which are encountered during one state.
b. The 44 flags correspond respectively to the 42 fitting windows applications plus the Ozone profile retrieval from nadir and one spare. Quality flags for not existing datasets due to a smaller number of trace gases are set to zero.

If there are less than the defined number of applications (44 = 16 Nadir + 14 Limb + 14 Occultation applications), or if the quality parameter is not applicable for the specific retrieval algorithm, then the unused quality flags are set to 0.

15.5.1.7.2 State Geolocation ADS

To support the extraction of SCIAMACHY data according to a given geolocation, this LADS gives the geolocation (4 corner co-ordinates) of the scene on-ground which is covered by each state.

Table 15.5.1.7.2-1 - Geolocation LADS

N	Description	Units	Byte Size	Data Type	Dim.
1	Start time of the scan phase of the state	-	12	mjd	1
2	Attachment Flag (1 = no MDSRs attached to the current ADSR, 0 otherwise)	-	1	uc	1
3	4 corner coordinates 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)	-	32	Coord	4
Size (in bytes)			**45**		

The “Coord” data type is defined in Table 15.4.1.7.1-1.

15.5.1.7.3 Static Parameter of the Level 2 off-line Processor (GADS)

Table 15.5.1.7.3-1 - Static parameter GADS

N	Description	Units	Byte Size	Data Type	Dim.
1	XML text of the initialisation file which covers the complete range of static parameters	-	105263	uc	1
Size (in bytes)			**105263**		

The static parameter GADS size does not change from one orbit to the other, but changes with different processor versions. It has a size given in the SPH.

15.5.1.7.4 States of the Product ADS

Each DSR of this ADS corresponds to a certain segment in one of the following MDSs. It describes the parameters of the corresponding state, as far as they are of interest for the data product, which is covered by the MDSs. The ADSRs of this ADS are sorted in chronological order as well as the DSRs of all the other time dependent ADSs (SQADS, LADS, and Geolocation ADS).

Table 15.5.1.7.4-1 - States of the Product ADSR

#	Description	Units	Byte Size	Data Type	Dim.
1	Start Time of DSR	-	12	mjd	1

Table 15.5.1.7.4-1 - States of the Product ADSR					
2	Attachment Flag (1 = no MDSRs attached to the current ADSR, 0 otherwise)	-	1	uc	1
3	State ID	-	2	us	1
4	Duration of scan phase of the state	1/16 s	2	us	1
5	Longest integration time	1/16 s	2	us	1
6	Shortest integration time	1/16 s	2	us	1
7	Number of geolocation records for this state	-	2	us	1
Size (in bytes)			**23**		

15.5.1.7.5 Geolocation of the Nadir Ground Pixels ADS

This ADS provides the detailed geolocation (several ADSRs for each state) for the shortest integration time of the corresponding measurements. In case a fitting window application is using a detector cluster with a larger integration time, the geolocation for this observation must be derived from the geolocation records of its sub-pixels with this shortest integration time. The shortest integration time is not constant over the whole product, but depends on the different states and may vary accordingly. Each ADSR is time stamped to allow cross-reference to the MDSRs. The format of each ADSR is defined below.

Table 15.5.1.7.5-1 - Geolocation of the Nadir Ground Pixels ADSR					
#	**Description**	**Units**	**Byte Size**	**Data Type**	**Dim.**
1	Start Time of DSR	-	12	mjd	1
2	Attachment Flag (1 = no MDSRs attached to the current ADSR, 0 otherwise)	-	1	uc	1
3	Integration time for this geolocation entity	1/16 s	2	us	1
4	Solar zenith angles of the start, middle and end of the integration time at TOA	degrees	12	fl	3
5	Line-of-sight nadir angles of start, middle and end of the integration time at TOA	degrees	12	fl	3
6	Relative azimuth angles of start, middle and end of the integration time at TOA	degrees	12	fl	3
7	Satellite geodetic height at the middle of the integration time	km	4	fl	1
8	Earth radius at the middle of the integration time	km	4	fl	1
9	Sub-Satellite point at the middle of the integration time		8	Coord	1
10	4 corner coordinates of the nadir ground pixel (the first coordinate 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	-	32	Coord	4

Table 15.5.1.7.5-1 - Geolocation of the Nadir Ground Pixels ADSR					
	first in flight direction and the fourth the last in time and flight direction)				
11	Centre coordinate of the nadir ground pixel	-	8	Coord	1
Size (in bytes)			**107**		

15.5.1.7.6 Geolocation of the Limb/Occultation measurements ADS

As the geophysical results of limb or occultation retrievals are always given for a complete state, the geolocation of limb/occultation ADSR is also given for complete states. The format of each ADSR is defined below.

Table 15.5.1.7.6-1 - Geolocation of the Limb/Occultation measurements ADSR

#	Description	Units	Byte Size	Data Type	Dim.
1	Start Time of DSR	-	12	mjd	1
2	Attachment Flag (1 = no MDSRs attached to the current ADSR, 0 otherwise)	-	1	uc	1
3	Integration time for this geolocation entity	1/16 s	2	us	1
4	Solar zenith angles of the start, middle and end of the integration time at TOA	degrees	12	fl	3
5	Line-of-sight nadir angles of start, middle and end of the integration time at TOA	degrees	12	fl	3
6	Relative azimuth angles of start, middle and end of the integration time at TOA	degrees	12	fl	3
7	Satellite geodetic height at the middle of the integration time	km	4	fl	1
8	Earth radius at the middle of the integration time	km	4	fl	1
9	Sub-satellite point at the middle of the integration time	-	8	Coord	1
10	Co-ordinates of tangent ground point of the start, middle and end of the integration time	-	24	Coord	3
11	Tangent height of the start, middle and end of the integration time	km	12	ul	1
Size (in bytes)			**103**		

15.5.1.7.7 Clouds and Aerosol MDS

The Clouds and Aerosols MDS is of variable record length. The actual length is given in the DSRLEN field (the second field). This MDS contains several MDSRs. The format of each MDSR is described below.

Table 15.5.1.7.7-1 - Clouds and Aerosol MDSR Format

#	Description	Units	Byte Size	Data Type	Dim.
1	Start Time of DSR	-	12	mjd	1
2	Data set record length (required because this record has a variable record length)	-	4	ul	1
3	Quality indicator (-1 if empty DSR)	-	1	sc	1
4	Integration time for this DSR	1/16 s	2	us	1
5	Surface Pressure	hPa	4	fl	1
6	Cloud fraction	-	4	fl	1
7	Error on cloud fraction	rel. fraction	4	fl	1
8	Number of PMD sub-pixels for this DSR	-	2	us	1
9	Number of PMD sub-pixels determined to be totally cloudy or totally cloud-free	-	4	us	2
10	Cloud-top height (given relative to sea level)	km	4	fl	1
11	Error on cloud-top height (currently set to -99.99, see product README file)	rel. fraction	4	fl	1
12	Cloud optical depth	km	4	fl	1
13	Error on cloud optical depth (currently set to -99.99, see product README file)	rel. fraction	4	fl	1
14	Cloud type [a]	flags	2	us	1
15	Cloud-top bi-directional reflectance	-	4	fl	1
16	Error on cloud-top bi-directional reflectance	rel. fraction	4	fl	1
17	Effective Lambertian surface reflectance	-	4	fl	1
18	Error on effective Lambertian surface reflectance	rel. fraction	4	fl	1
19	Flags describing the cloud parameter output [b]	flags	2	us	1
20	Absorbing aerosol indicator	-	4	fl	1
21	Aerosol indicator diagnostic	-	4	fl	1
22	Flag describing the aerosol indicator output [c]	flags	2	us	1
23	Number of additional aerosol parameters (na)	-	2	us	1
24	Additional aerosol parameters	-	4*na	fl	2
Size (in bytes)			**variable**		

a. The flags describing the cloud type have to be interpreted bit-wise (the bit numbering convention is defined in R5). They contain the classification of clouds according to the WMO scheme:

bit 0: value 0 = high cloud, 1= low cloud
bit 1: value 0 = water cloud, 1 = ice cloud
bit 2: value 0 = thin cloud, 1 = thick cloud
bits 3-15: not used.

b. The flags describing the cloud processing output have to be interpreted bit-wise. The bit numbering convention is defined in R5. They contain information reflecting some important settings in the initialisation file:
bit 0: source of cloud fraction value 0 = fitting, 1 = PMD
bit 1: source of cloud-top pressure value 0 = ISCCP, 1 = SACURA
bit 2: if bit set, 1 = SACURA fully convergent
bit 3: if bit set, 1 = number of iterations exceeded, average of neighboured pixels taken
bit 4: if bit set, 1 = SACURA: cloud layer size set to constraint
bit 5: if bit set, 1 = SACURA: cloud bottom height set to constraint
bit 6: if bit set, 1 = SACURA: cloud top height set to constraint
bits 7-15: not used.

c. The definition of aerosol components (field 22) is as follows. When the bit is set, the underlined condition is true. According to big-endian, in a two bytes field, bits are counted from 15 to 0):
bit 15: Rayleigh scattering correction successful (no/yes);
bit 14: AAIA computation successfully ended (no/yes);
bit 13-0: not used.

For the current version, the number of additional aerosol parameters (na, field 23) is 3. Additional aerosol parameters (given in field 24) are the residual calculated in the AAIA, the retrieved surface albedo at 380 nm, the ground height used in the AAIA.

15.5.1.7.8 Nadir Fitting Window Application MDSs

There are up to 16 Nadir Fitting Window Application MDSs used in a product (one MDS per fitting window). The content of each MDS is identified in the SPH. Each MDS contains several MDSRs. All MSDRs for all MDSs share a common format that is defined below. MDSR have variable record length. The actual length is given in the DSRLEN field (the second field).

Table 15.5.1.7.8-1 - Nadir Fitting Window Application MDSR Format

#	Description	Units	Byte Size	Data Type	Dim.
1	Start Time of DSR	-	12	mjd	1
2	DSR length (required because this record has a variable length)	-	4	ul	1
3	Quality indicator (-1 if empty DSR)	-	1	sc	1
4	Integration time for this DSR	1/16 s	2	us	1
5	Number of vertical column densities (nvcd) d	-	2	us	1
6	Vertical column density (VCD) of main parameter value	mol/cm2	nvcd*4	fl	1
7	Error on the VCD above	rel. fraction	nvcd*4	fl	1

Table 15.5.1.7.8-1 - Nadir Fitting Window Application MDSR Format					
8	Flag describing the VCD data above a	flags	2	us	1
9	Effective slant column (ESC) density of the main parameter	mol/cm2	4	fl	1
10	Error on the effective slant column density above	rel. fraction	4	fl	1
11	Number of linear fit parameters [n1] [e]	-	2	us	1
12	Total number of fit parameters [n2] [e]	-	2	us	1
13	Linear fitted parameters [e]	-	4 * n1	fl	n1
14	Error on linear fitted parameters e	rel. fraction	4 * n1	fl	n1
15	Cross-correlation matrix entries of the linear fit [e]	-	2 * n1 * (n1-1)	fl	n1 * (n1-1) / 2
16	Non-linear fitted parameters [e]	-	4 * n2	fl	n2
17	Error on non-linear fitted parameters [e]	rel. fraction	4 * n2	fl	n2
18	Cross-correlation entries of the non-linear fit	-	2 * n2 * (n2-1)	fl	n2 * (n2-1) / 2
19	RMS of fit for the fitting window	-	4	fl	1
20	χ2 of the fit	-	4	fl	1
21	Goodness of the fit	-	4	fl	1
22	Iteration number for the fitting window	-	2	us	1
23	Flag describing the above data for linear and non-linear fit b	flags	2	us	1
24	AMF to ground for species	-	4	fl	1
25	Error on AMF to ground	rel. fraction	4	fl	1
26	AMF to cloud-top for species	-	4	fl	1
27	Error on AMF to cloud-top	rel. fraction	4	fl	1
28	Flag describing the AMF data above [c]	flags	2	us	1
29	Temperature of reference spectrum	K	4	fl	1
Size (in bytes)			**variable**		

a. The flags describing the VCD calculation have to be interpreted bit-wise. The bit numbering convention is defined in R5 (when the bit is set the underlined condition is true, bits are counted from 0 to 15).

For field 6, each bit is defined as follows. Only bits from 0 to 7 are used for DOAS.

0: no -yes extended field-of-view calculation

1: no -yes maximum SZA reached, VCD computation impossible

2: no -yes no weighting of AMFs over footprint

3: no -yes linear weighting of AMFs over footprint

4: no -yes parabolic weighting of AMFs over footprint

5-7: not used at present

For AMC-DOAS (retrieval of H2O only) flag 2 is set 'true', all others 'false'.

For IAS in principle all 16 bits are used:

0: convergence reached (no/yes)

1: sza lower than limit, currently 80° (no/yes)

2: residual norm lower than limit, currently 4 (no/yes)

3: maximum absolute value of residual lower than limit, currently 2 (no/yes)

4: error weighting used (no/yes)

5: ratioed measurements used (no/yes)

6-15: α between bounds and |αerr| < limit, a pair of flags for each gas (αerr limit currently 0.5).

b. Field 23 specifies the slant column density fitting. The flags have to be interpreted by bits. The bit numbering convention is defined in R5 (when the bit is set the underlined condition is true, bits are counted from 0 to 15). For AMC-DOAS and IAS this field is not used.

0: no -yes smoothing of measurements

1: no -yes error weighting of fitting

2: no -yes use of ratioed measurements

3: no -yes use of pre-convoluted cross-sections

4: no -yes convolution of cross-sections

5: no -yes convolution of measurement grid

6: literature -SCIAMACHY cross-sections used

7: linear -non-linear fitting

8: no - yes use of SO2 correction

9-11: quality, to be interpreted as 3 bit integer, 0 lowest quality (product is NOT CORRECTED for

an offset. Don't use it), 7 highest quality

12-15: not used at present

c. The flags describing the AMF look-up scheme (field 28) have to be interpreted by bits. The bit numbering convention is defined in R5 (when the bit is set the underlined condition is true, bits are counted from 0 to 15). For AMC-DOAS all flags are set to 'false'):

0: clear -clear & cloud look-up

1: one AMF value -extended field-of-view

2: continental -maritime aerosol present

3: no -yes maximum SZA exceeded

4-15: not used

d. Field 5 allows the output of more than one VCD result per record. This feature is used for NAD_UV8_H2O, NAD_IR1_CH4, NAD_IR3_CO, LMN_UV0_NO2 with the following effect on fields 6 and 7:

For H2O, fields 6 and 7 consist of two entries each: the first entry of field 6 gives the VCD in molecules/cm2, the second in g/cm2. The latter unit is more convenient in the meteorological community. All errors for AMC-DOAS (fields 7, 17, 25) are absolute values. Both entries of field 7 contain the H2O VCD error in g/cm2

The CH4 total columns are dry-air vertical column densities with CO2 as proxy. For CH4 fields 6 and 7 consist of two entries: the first entry contains XCH4 (= VCDCH4,ref * α CH4/ α CO2), the second VCDCH4 (= VCD CH4,ref * α CH4).

For CO fields 6 and 7 consist of two entries: the first entry contains VCD CO corrected with CH_4 scaling (xCO = VCDCO,ref * α CO/ α CH4), the second entry for CO value without CH_4 scaling (VCDCO = VCD CO,ref * α CO).

For tropospheric NO2 from limb-nadir-matching, fields 6 and 7 consist of five entries:

1: Tropospheric vertical column.
2: Uncorrected tropospheric slant column.
To correct for a systematic offset between nadir and limb measurements the reference sector method is used. In this method, however, it is assumed that there is no tropospheric NO2 above the remote Pacific, which is not true. To correct for that, a modelled tropospheric NO2 slant column is added. The uncorrected tropospheric slant column is an intermediate result prior to the above described addition.
3: Corrected stratospheric slant column.
Experience shows that a small but significant offset exists between the slant columns obtained from limb and nadir measurements. This offset is determined by means of the reference sector method. Stratospheric slant columns given in this entry are corrected for this offset.
4: Stratospheric slant column.
Stratospheric columns calculated from the limb profiles and converted into the

slant columns by means of the stratospheric AMF. These columns are not yet corrected for the offset (see above).
5: Stratospheric vertical column.
This entry represents limb profiles integrated from TOA to tropopause and interpolated to the nadir grid.
Entries 2-5 are intermediate results obtained during the retrival.
All corresponding entries of field 7 have value 0, because there are no error calculations available for limb-nadir-matching.

Flags describing the output will be interpreted bit-wise. Please note: not all bits of the following fields are used and some of them are only relevant for the indicated application (DOAS or IAS).

e. Fields 11/12, 13/14 and 16/17 require some special treatment for IAS. Field 11 contains the number of linear fit parameters, which is currently 1, and Field 12 is filled with the total number of fit parameters. This number is currently 5, composed of the number of linear (1) and non-linear fit parameters (1) plus the number of gases (3). In principle, the number of linear fit parameters is composed of reflectance and baseline, which can contribute up to three values each, depending on the polynomial degrees defined by the initialization file. Note that attribute degree in the initialization file specifies the number of coefficient, not the polynomial degree. Baseline is not used at present.
Fields 13 and 14 show value and error of the reflectance in the IAS case. Fields 16 and 17 have currently five entries each, containing the values and errors of the scaling factors of gases (i.e. αCO, αCH4, αH2O) and HWHM. The last entry of Field 16 and 17 is empty (i.e. filled with 0), because value and error of the linear fit parameter are already given in Field 13 and 14, respectively

Because of different reasons some MDS fields are left empty (i.e. have values 0) if AMC-DOAS was used. The AMC-DOAS algorithm allows obtaining a VCD of water vapour directly, omitting an intermediate step of SCD calculation. That is why fields 9 and 10 (SCD and its error) are empty for NAD_UV8_H2O. Since the fitting procedure in the AMC-DOAS algorithm is non-linear, the parameters of linear fitting (fields 13 to 15) are absent. In the field 24 instead of “AMF to ground” the AMF correction factor computed by the AMC-DOAS algorithm is listed, and in the field 25 its error. Fields 26 and 27 are left empty as well, because no AMF to cloud-top is calculated in the AMC-DOAS algorithm. All errors for AMC-DOAS are absolute values and not relative fractions.

15.5.1.7.9 Limb Fitting Window Application MDSs

Each limb MDS consists of several MDSRs containing the retrieval result of one vertically sorted sequence of Limb measurements. A complete Limb scan, given by one limb state, may consist of more than one limb profile depending on the integration time during one azimuth sweep of the corresponding channels from which the fitting window parts were taken. Therefore, the number of records of each Limb MDS is given by the number of Limb states and their integration times.

According to the planning of SCIAMACHY operations there will be approximately 30 Limb states per orbit and several integration times for the various channels depending on the expected signal to noise level. This implies a variable number of records for the Limb MDSs.

There are up to 14 Limb Fitting Window Application MDSs used in a product (one MDS per fitting window). The content of each MDS is identified in the SPH. All MSDRs for all MDSs share a common format that is defined below.

Table 15.5.1.7.9-1 - Limb Fitting Window Application MDSR Format					
#	**Description**	**Units**	**Byte Size**	**Data Type**	**Dim.**
1	Start Time of DSR	-	12	mjd	1
1b	DSR length (required because this record may have a variable length)	-	4	ul	1
2	Quality indicator (-1 if empty DSR)	-	1	sc	1
2b	Integration time for this DSRs	1/16s	2	us	1
3	Retrieval Method: 'O' for optimal estimation, 'N' for non linear least square fitting, etc...	-	1	uc	1
4	Height of reference pressure	km	4	fl	1
5	Reference pressure for Hydrostatic Equilibrium	hPa	4	fl	1
6	Reference pressure source 'E' = ECMWF, 'C' = Climatology, etc	-	1	uc	1
7	Number of retrieval levels: [nmain]	-	1	uc	1
8	Number of used measurement levels [nmeas]	-	1	uc	1
9	Number of fitted main gas species [n1]	-	1	uc	1
10	Number of fitted closure parameters: [n2]	-	1	uc	1
10 b	Number of fitted other parameters [n3]	-	1	uc	1
11	Number of fitted scaling parameters for auxiliary gases [n4]	-	1	uc	1
11 b	Tangent height at the lower layer boundary	km	(120)	fl	nmain (30)
11 c	Tangent layer pressure at the lower layer boundary	hPa	(120)	fl	nmain (30)
11 d	Tangent layer temperature (mean)	K	(120)	fl	nmain (300)
11 e	Main species which have been fitted on the coarse forward model grid	-	(960)	Layer Rec.	nmain *n1 (60)
11 f	Scaled profiles which have been used for the fit on the coarse forward model grid	-	(960)	Layer Rec.	nmain *n4 (60)
11 g	Measurement Grid	-	(429)	Meas-Grid	nmeas (13)
12	Size of the State Vector (nStVec = n1*nmain+n2 +n3)	-	2	us	1
13	State Vector (nStVec times)	-	nStVec	State vector structure	nStVec
14	Correlation matrix size (mf = 1/2 * nStVec + (nStVec -1))	-	2	us	1
15	Correlation Matrix of the fit (mf values)	-	mf	fl	mf
16	RMS of the fit		4	fl	1
17	$\chi 2$ of the fit	-	4	fl	1

Table 15.5.1.7.9-1 - Limb Fitting Window Application MDSR Format					
18	Goodness of the fit	-	4	fl	1
19	Number of iterations for the fit (ni)	-	2	us	1
20	Measurement summary, number of used and rejected wavelengths	-	4	us	2
21	Convergence Criteria	-	1	b	1
22	Residuals size (nres = nStVec * ni)	-	2	us	1
23	Iteration Step state vector residuals (nres values)	-	nres	fl	nres
24	Number of additional diagnostics (nad)	-	2	us	1
25	Additional diagnostics	-	4*nad(0)	fl	nad
Size (in bytes)			**variable**		

Convergence criteria (field 21) are currently not defined.

Compound data types from previous table are described below:

Table 15.5.1.7.9-2 - Limb Profile Layer (LayerRec) Record structure					
#	**Description**	**Units**	**Byte Size**	**Data Type**	**Dim.**
1	Tangent layer volume mixing ratio	ppV	4	fl	4
2	Error on the tangent layer volume mixing ratio	%	4	fl	4
3	Vertical column density above lower layer boundary	molecule/cm2	4	fl	4
4	Error on the vertical column density above lower layer boundary	%	4	fl	4
Size (in bytes)			**16**		

Table 15.5.1.7.9-3 - Measurement Grid (MeasGrid) Record structure					
#	**Description**	**Units**	**Byte Size**	**Data Type**	**Dim.**
1	Start time of the measurement at that specific layer	-	12	mjd	12
2	Mean tangent height of measurement	km	4	fl	4
3	Pressure at tangent height	hPa	4	fl	4
4	Temperature at tangent height	K	4	fl	4
5	Number of fitting windows	-	1	uc	1
6	Minimum wavelength over all fitting windows	nm	4	fl	4
7	Maximum wavelength over all fitting windows	nm	4	fl	4
Size (in bytes)			**33**		

Table 15.5.1.7.9-4 - State Vector (StateVec) structure					
#	Description	Units	Byte Size	Data Type	Dim.
1	Value of the State vector entry	-	4	fl	4
2	Error of the value of the state vector entry	%	4	fl	4
3	Type of the value of the state vector entry (Annotation)	-	4	b	4
Size (in bytes)			**12**		

15.5.1.7.10 Limb Clouds MDSs

This component is of variable record length. The actual length is given in the DSRLEN field (the second field). The number of records is depending on the number of limb states and the number of columns per limb state.

Table 15.5.1.7.10-1 - Limb Clouds Data Set MDSR Format					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start time of the limb clouds record	-	12	mjd	1
2	Data set record length	-	4	ul	1
3	Quality indicator (-1 if empty DSR)	-	1	sc	1
4	Integration time for this DSRs	-	2	us	1
5	Diagnostics of the cloud detection algorithm, details see below	-	1	b	1
6	Flag for normal water clouds	-	1	uc	1
7	Maximum value of CIR for normal water clouds	-	4	fl	1
8	Height of maximum value of CIR for normal water clouds	Km	4	fl	1
9	Height index of maximum value of CIR for normal water clouds	-	1	uc	1
10	Flag for ice clouds	-	1	uc	1
11	Maximum value of CIR for ice clouds	-	4	fl	1
12	Height of maximum value of CIR for normal water clouds	Km	4	fl	1
13	Height index of maximum value of CIR for ice clouds	-	1	uc	1
14	Flag for polar stratospheric clouds	-	1	uc	1
15	Maximum value of CIR for polar stratospheric clouds	-	4	fl	1
16	Height of maximum value of CIR for polar stratospheric clouds	Km	4	fl	1
17	Height index of maximum value of CIR for ice clouds	-	1	uc	1
18	Flag for noctilucent clouds	-	1	uc	1
19	Not used at present	-	4	fl	1

Table 15.5.1.7.10-1 - Limb Clouds Data Set MDSR Format					
20	Maximum height of strictly monotonically increasing	Km	4	fl	1
21	Maximum height index of strictly monotonically increasing radiances for noctilucent clouds	-	1	uc	1
22	Number of tangent heights for CIR (m1)	-	2	us	1
23	Tangent heights for CIR	Km	0	fl	m1(0)
24	Number of CIR (m2)	-	2	us	1
25	CIR (m = m1 * m2)	-	0	fl	m(0)
26	Number of additional limb cloud parameters (n)	-	2	us	1
27	Additional limb cloud parameters	-	0	fl	n(0)
Size (in bytes)			**variable**		

The values of the cloud flags have the following meanings:

Flag for normal water clouds (field 6):

0: no clouds,
1: partially cloudy,
2: fully cloudy,
3: bad data or cloud top height too high.

Flag for ice clouds (field 10):

0: water cloud,
1: ice cloud,
2: bad data (MAXHEIGHT_ICL is greater than the warning tangent height, warn_th),
9: strange case (MAXVAL_ICL is greater than the upper bound for the CIR, upper_bound_cir).

Flag for polar stratospheric clouds (field 14):

0: no PSC,
1: PSC.

Flag for noctilucent clouds (field 18):

0: no NLC,
1: NLC criterion 1 fulfilled (radiance increase with height),
2: NLC criterion 2 fulfilled (radiance ratios above threshold),
3: both NLC criteria fulfilled.

The diagnostics of the cloud detection algorithm (field 5) are defined as follows: Each bit indicates whether the algorithm for a certain cloud type succeeded (bit is set) or failed. The assignment of bits is

0: retrieval of normal water clouds succeeded
1: retrieval of ice clouds succeeded

2: retrieval of polar stratospheric clouds succeeded
3: retrieval of noctilucent clouds succeeded
4-7: not used

Fields 22-26 are reserved for colour index ratios as functions of tangent height. At the moment two CIR are considered (1090/750 nm and 1630/750 nm), but the concrete number of CIR is not fixed and is written to field 24. Entries of field 25 run first over tangent heights and then over CIR, i.e. entries 1 to NUMTANH are values of CIR1, entries NUMTANH+1 to 2*NUMTANH are values of CIR2 and so on.
For the current version the number of additional limb cloud parameters (field 30) is 0. Further parameters might be added in future versions.

15.5.1.7.11 Occultation Fitting Window Application MDSs

There are up to 14 Occultation Fitting Window Application MDSs available in a product (one MDS per fitting window) as indicated by the DSDs, but none is currently used.

15.5.1.7.12 Ozone profiles from Nadir measurements MDS

This MDSs is currently not used.

15.5.1.8 Size Estimate

The size of Level 2 consolidated products (version 6.01) is approximately 30.8 MB for a scenario corresponding to 60 states with 30 limb states, zero occultation states, and to 1250 single observations for nadir and limb states respectively.

		bytes
MPH		1247
SPH		19115
SQADS	60 states * 193 bytes / state	11580
State Geolocation	60 states * 45 bytes / state	2700
Static Parameter GADS		60000
States ADS	60 states * 23 bytes / state	1380
Nadir Geolocation ADS	3600 observations * 107 bytes / obs.	385200
Limb Geolocation ADS	2625 limb states * 103 bytes / state	270375
Clouds & Aerosols MDS	3600 observations * 96 bytes / obs.	345600
Nadir Fit. Win. Appl. MDSs (1)	3600 observations * 157 bytes / obs. * 10 MDS used	5652000
Limb Fit. Win. Appl. MDSs (1)	750 observations * 33323 bytes / obs.	24872250
Occultation Fit. Win. Appl. MDSs (1)	Not used	0
Limb Clouds MDSs (1)	100 observations * 66 bytes / obs.	6600

Total product size estimation: 31628047 bytes (1)

1. DSR size corresponding to typical size derived from example case

15.6 AUXILIARY DATA FILES

The following sub-sections describe the Auxiliary Data Files used in the SCIAMACHY operational processing[7]. Information is extracted from R-1. For the Level 1b processing, a new calibration scheme based on a calibration database has been implemented starting from baseline version 8. In-flight calibration parameters, which were previously extracted from LK1, SU1, SP1, and PE1 auxiliary data files, are now derived from the database

15.6.1 Leakage Current Parameter File

This file contains the leakage current correction parameters for SCIAMACHY level 0 to 1b processing. The leakage current parameters are expected to be dependent on the position along the orbit. Therefore, the calculation of these parameters requires dark calibration measurement states as well as the last measurements of the limb states and the orbit phase of the corresponding measurements.

The parameters are divided into a constant fraction of the leakage current and a fraction being variable with orbit phase.

FILE ID: SCI_LK1_AX

TYPE: Auxiliary

USE: Level 1b processing

UPDATED: one leakage current parameter set per orbit.

For baseline version 8, leakage current parameters are stored in a calibration database. Auxiliary files are not maintained except for a single reference file used whenever suitable calibration is not found in the database.

SIZE: approximately 1.2 MB

15.6.1.1 Format

The leakage current correction parameter file includes headers and two global annotation data sets (GADS) as depicted below.

Table 15.6.1.1-1 - Schematic Structure of the Leakage Current Auxiliary file

[7] From SGP version 5.01, the initialisation file, does not use the database files SCI_CS2_AX, SCI_FM2_AX, SCI_UC2_AX and SCI_KEY_AX. However, the processor is still able to read them, and future changes in the setup might require using them again. Their description is available in R-2.

MPH
Auxiliary Data SPH as described in R-4 with 2 DSDs
Leakage Current Parameters Constant Fraction GADS
Leakage Current Parameters Variable Fraction GADS

15.6.1.1.1 Constant Fraction GADS

The format of the Leakage Current Parameters Constant Fraction GADS within the auxiliary data file is identical to the format of the corresponding GADS in the Level 1b product specified in Table 15.4.1.7.5-1. Level 1b GADS are in fact copied from the auxiliary file.

15.6.1.1.2 Variable Fraction GADS

The format of the Leakage Current Parameters Variable Fraction GADS within the auxiliary data file is identical to the format of the corresponding GADS in the Level 1b product specified in Table 15.4.1.7.6-1. Level 1b GADS are in fact copied from the auxiliary file.

15.6.2 PPG/Etalon Parameter File

This file contains the PPG/Etalon correction parameters for SCIAMACHY level 0 to 1b processing. The PPG/Etalon parameters are not expected to be dependent on the position along orbit. Therefore, the data set consists of just one set of parameters. The calculation of the PPG/Etalon parameters requires one WLS measurement states.

FILE ID: SCI_PE1_AX

TYPE: Auxiliary

USE: Level 1b processing

UPDATED: Once per orbit.

For baseline version 8, PPG/Etalon parameters are stored in a calibration database. Auxiliary files are not maintained except for a single reference file used whenever suitable calibration is not found in the database.

SIZE: approx. 140 KBytes

15.6.2.1 Format

The PPG/Etalon Parameter file includes headers and one global annotation

data set (GADS) as depicted below.

Table 15.6.2.1-1 - Schematic Structure of the PPG/Etalon Auxiliary File

MPH
Auxiliary Data SPH as described in R-4 with 1 DSD
PPG/ Etalon Parameters GADS

15.6.2.1.1 PPG/Etalon Parameters GADS

The format of the PPG/ Etalon Parameters GADS within the auxiliary data file is identical to the format of the corresponding GADS in the Level 1b product specified in Table 15.4.1.7.7-1. Level 1b GADS are in fact copied from the auxiliary file.

15.6.3 Spectral Calibration Parameter File

This file contains the spectral calibration parameters for SCIAMACHY Level 0 to 1b processing.

The spectral calibration parameters are expected to be dependent on the position in orbit. Therefore, the calculation of these parameters requires an orbit phase field for annotation and the application needs them for selection of appropriate parameters. The calculation of the spectral calibration parameters requires one SLS measurement state.

FILE ID: SCI_SP1_AX

TYPE: Auxiliary

USE: Level 1b processing

UPDATED: Once per week

For baseline version 8, spectral calibration parameters are stored in a calibration database. Auxiliary files are not maintained except for a single reference file used whenever suitable calibration is not found in the database.

15.6.3.1 Format

The spectral calibration parameter file includes headers and two global annotation data sets (GADS) as depicted below.

Table 15.6.3.1-1 - Schematic Structure of the Spectral Calibration Auxiliary File

MPH
Auxiliary Data SPH as described in R-4 with 2 DSD
Precise Basis of the Spectral Parameters GADS
Spectral Parameters GADS

15.6.3.1.1 Precise Basis of Spectral Calibration Parameters GADS

The format of the Precise Basis of the Spectral Parameters GADS within the auxiliary data file is identical to the format of the corresponding GADS in the Level 1b product specified in Table 15.4.1.7.8-1. Level 1b GADS are in fact copied from the auxiliary file.

15.6.3.1.2 Spectral Calibration Parameters GADS

The format of the Spectral Calibration Parameters GADS within the auxiliary data file is identical to the format of the corresponding GADS in the Level 1b product specified in Table 15.4.1.7.9-1. Level 1b GADS are in fact copied from the auxiliary file.

15.6.4 Sun Reference Spectrum File

This file contains the sun reference spectrum for the SCIAMACHY level 0 to 1b processing. SCIAMACHY executed one sun diffuser measurement state per day, which yield one sun reference spectrum file per day. The corresponding spectral calibration parameters and the radiance sensitivity included in this file allow the calculation of a complete solar irradiance spectrum for the day. .

FILE ID: SCI_SU1_AX

TYPE: Auxiliary

USE: Level 1b processing

UPDATED: one sun reference spectrum file per day

SIZE: approximately 165 KB

15.6.4.1 Format

The sun reference spectrum file includes headers and one global annotation data set (GADS) as depicted below.

Table 15.6.4.1-1 - Schematic Structure of the Sun Reference Spectrum Auxiliary File

MPH

Auxiliary Data SPH as described in R-4 with 1 DSD
Sun Reference GADS

15.6.4.1.1 Sun Reference Spectrum GADS

The format of the **Sun Reference** GADS within the auxiliary data file is identical to the format of the corresponding GADS in the Level 1b product specified in Table 15.4.1.7.10-1. Level 1b GADS are in fact copied from the auxiliary file.

15.6.5 Key Data (Instrument Characterization) File

Key Data file for the SCIAMACHY Level 0 to 1b processing.

The so-called Key Data file contains one part of the characterisation database of SCIAMACHY used for the operational processing. The Key Data file is provided by the calibration and characterisation team and since 2007 is under the responsibility of the SCIAMACHY QWG.

A new version of the file was provided with Level 1b baseline version 8.

FILE ID: SCI_KD1_AX

TYPE: Auxiliary

USE: Static ADF for Level 1b processing

UPDATED: Infrequently (associated to a specific processing baseline)

SIZE: approximately 75 MB

15.6.5.1 Format

The format of the file consists of an MPH, and Auxiliary Data SPH (as described in R-4) with several DSDs pointing to several GADSs. The GADSs contain ASCII format information as defined in the SCIAMACHY Level 1b IODD (R-1). At present, 39 key data parameters are assembled into the Key data file. The DS_NAME field of the DSDs is set according to the content of the corresponding MDS. The following keywords are present (not necessarily in this order):

#	DS_NAME	Description	Units	Dim.
1	BRDF_s	Bi-directional reflection distribution function measured with s-polarisation detector (ac_ucs / FOV)	sr^{-1}	3
2	BRDF_p	Bi-directional reflection distribution function measured with p-polarisation detector (ac_ucp / FOV)	sr-1	3
3	ELEV_s	Reflection of ESM measured with s-polarisation detector (anauns)	-	2
4	ELEV_p	Reflection of ESM measured with p-polarisation detector (anaunp)	-	2
5	ETA_NAD	Polarisation properties in NADIR mode (OBMs_p*(anauns/anaunp))	-	2
6	XI_NAD	Ratio PMD signal / detector pixel signal (on0pnq / on0pnd)	-	1
7	OBM_s_p	s- over p sensitivity of the instrument without scanner	-	1
8	ETA_LIMB	Polarisation properties in LIMB mode	-	3
9	ZETA_LIMB	Polarisation properties –45/45 in LIMB mode	-	3
10	EL_AZ_p	Elevation and Azimuth scanner calibration with p-polarisation detector (alaulp)	-	3
11	EL_AZ_s	Elevation and Azimuth scanner calibration with s-polarisation detector (alauls)	-	3
12	OMEGA_LIMB		-	3
13	KAPPA_LIMB		-	3
14	XI_LIMB		-	3
15	SIGMA_LIMB		-	3
16	PSI_LIMB		-	3
17	TAU_LIMB		-	3
18	SIGMA_NAD		-	2
19	PSI_NAD		-	1
20	TAU_NAD		-	1
21	OMEGA_NAD		-	2
22	KAPPA_NAD		-	1

#	DS_NAME	Description	Units	Dim.
23	ZETA_NAD		-	2
24	STRAY_UNIFORM		-	1
25	STRAY_GHOST		-	2
26	STRAY_CH1		-	2
27	SPEC_LINE		nm	2
28	SLIT_F		-	2
29	SMALL_AP_SLIT_F		-	2
30	ABS_RAD		(BU/s) / (W/sr.cm3)	1
31	ABS_IRR		(BU/s) / (W/cm3)	1
32	NDF		-	1
33	NDF_s_p		-	1
34	MEM_EFFECT_COEF	Correction factor for the memory effect of the RETICON detector arrays	-	2
35	PMD_CROSS_COEF		-	1
36	BAD_PIXEL_MASK		-	1
37	REF_WLS		BU/s	1
38	FRAUNH_LINE	Spectral calibration: list of used Fraunhofer lines	nm	2
39	NON_LIN		-	2

The general format description of the key data files is defined in document Definition of Instrument Characterisation Data Base, PO-ID-DOR-SY-0037, Issue 1, 1994.

Parameters in fields 28 and 29 are not be used in the Level 0 to 1b processing, but they are copied to GADS on the Level 1b product for use in Level 1b to 2 processing.

15.6.6 M-factor File

M-factor files are an extension to the characterisation database of SCIAMACHY to describe the radiometric degradation of the instrument affecting the light paths for in-flight conditions. Starting from SCIAMACHY Level 1 processing baseline version 8, m-factors are applied to the Level 0-1b processing step (as originally planned) and enclosed into the Level 1b products. Current data version number is 08.31. M-factor files are provided by the University of Bremen.

FILE ID: SCI_MF1_AX

TYPE: Auxiliary

USE: Level 1b processing

M-factors were used in Level 1b processing until IPF version 6.05; for IPF 7.02 m-factor usage in Level 1b processing was deactivated, and it was applied to the Level 2 off-line processing with processor version 5 instead.

UPDATED: daily and delivered by IFE-Bremen (3537 files).

SIZE: approximately 329 KB

15.6.6.1 Format

New m-factor files adopted by baseline version 8 have a single GADS in binary data format with ASCII headers.

Table 15.6.6.1-1 - Schematic Structure of M-factor File

MPH
Auxiliary Data SPH with 1 DSD
M-factor scanner model

The following parameters are envisaged:

#		Unit	Type	Dim	Size
1	Number of (complex) refractive indexes	-	sl	1	4
2	Number of	-	sl	1	4

	contamination layers [nl]				
3	Number of surfaces with contamination [ns]	-	sl	1	4
4	Number of retarder parameters [np]	-	sl	1	4
5	Number of OBM M1 mfactor for science detector [n5]	-	sl	1	4
6	Number of OBM M1 mfactor for PMD [n6]	-	sl	1	4
7	Number of add parameters [n7]	-	sl	1	4
8	Wavelength grid of the science channel detector	nm	fl	8192	32768
9	Refractive index	-	fl	16384	65536
10	Contamination layer thickness	-	fl	nl*ns	24
11	Retarder parameter	-	fl	np	4
12	M1 science channel	-	fl	n5 * 8192	32768
13	M1 PMD channel	-	fl	n6*7	28
14	add_parameter	-	fl	N7	4

15.6.7 Level 1b Initialization File

This initialisation file contains parameters used as initialization information for the Level 0 to 1b processing. Besides the static parameters, the file includes also a set of three spectrum templates, a list of external instrument state parameters which are not available through the ISPs of the instrument, and the polarisation and radiance sensitivity grids GADS.

Unchanged with respect to previous processing baseline (version 7).

FILE ID: SCI_LI1_AX

TYPE: Auxiliary

USE: Static ADF for Level 1b processing

UPDATED: Infrequently (associated to a specific processing baseline)

SIZE: approximately 155 KB

15.6.7.1 Format

The high-level format of the file is shown below.

Table 15.6.7.1-1 - Schematic Structure of the Level 1 Initialization File

MPH
Auxiliary Data SPH as described in R-4 with 5 DSDs
Static Parameters GADS
Spectrum Templates GADS
External State Parameters GADS
Processing Categories GADS
Polarisation and Radiance Sensitivity Grids GADS

15.6.7.1.1 Static Parameters GADS

This GADS is a simple ASCII list consisting of a number of keywords representing the static parameters of the Level 0 to 1b processing followed by the values of these parameters. The position of the parameters in this list is arbitrary, but the structure of the parameter values following a certain parameter's name has to be known by the code reading the static parameters.

15.6.7.1.2 Spectrum Templates GADS

The spectrum data will be used for the retrieval of relative Etalon information. The spectra are given as unitless quantities. The format of this GADS is shown in the table below:

Table 15.6.7.1.2-1 - Spectrum Templates GADS

#	Description	Units	Byte Length	Data Type	Dim.
1	Wavelength	nm	32768	fl	8192
2	External sun reference spectrum	-	32768	fl	8192

3	Template earth-shine spectrum	-	32768	fl	8192
4	External PPG reference spectrum (for Key-data)	-	32768	fl	8192
Size (in bytes)			**131072**		

15.6.7.1.3 External State Parameters GADS

This GADS contains 70 GADSRs. The format of each GADSR is shown in the table below:

Table 15.6.7.1.3-1 - External State Parameters GADSR

N	Description	Units	Byte Length	Data Type	Dim.
1	State Number	-	2	us	1
2	Delay time of measurement after BCPS start	ms	4	fl	1
3	State set-up integration time	ms	4	fl	1
4	Spare	-	3	uc	3
Size (in bytes)			**13**		

15.6.7.1.4 Processing Categories GADS

This GADS contains 20 GADSRs. The format of each GADSR is shown in the table below:

Table 15.6.7.1.4-1 - Processing Category GADS

#	Description	Units	Byte Length	Data Type	Dim.
1	Measurement category	-	2	us	1
2	Processing category (0=other, 1=nadir, 2=limb, 3=occultation, 4=sub-solar, 5=sun diffuser, 6=SLS, 7=WLS, 8=dark, 9=ignore)	-	1	uc	1
Size (in bytes)			**3**		

15.6.7.1.5 Polarisation and Radiance Sensitivity Grids GADS

This GADS contains one GADSR with format as shown in the table below:

Table 15.6.7.1.5-1 - Polarisation and Radiance Sensitivity Grids GADS

Table 15.6.7.1.5-1 - Polarisation and Radiance Sensitivity Grids GADS					
#	**Description**	**Units**	**Byte Length**	**Data Type**	**Dim.**
1	Number of ESM positions for the polarisation sensitivity parameters Nadir (e.g. 10) [NESM,nadir]	-	2	us	1
2	ESM positions for the polarisation sensitivity parameters Nadir	-	4* NESM,nadir	fl	NESM,nadir
3	Number of ESM positions for the polarisation sensitivity parameters Limb (e.g. 10) [NESM,limb]	-	2	us	1
4	ESM positions for the polarisation sensitivity parameters Limb	-	4* NESM,limb	fl	NESM,limb
5	Number of ASM positions for the polarisation sensitivity parameters Limb (e.g. 10) [NASM,limb]	-	2	us	1
6	ASM positions for the polarisation sensitivity parameters Limb	-	4* NASM,limb	fl	NASM,limb
7	Number of ESM positions for the radiance sensitivity parameters (e.g. 10) [NESM,rad]	-	2	us	1
8	ESM positions for the radiance sensitivity parameters	-	4*NESM,rad	fl	NESM,rad
9	Number of ASM positions for the radiance sensitivity parameters (e.g. 10) [NASM,rad]	-	2	us	1
10	ASM positions for the radiance sensitivity parameters	-	4*NASM,rad	fl	NASM,rad
Size (in bytes)			**variable**		

The number of scans mirror positions used for the polarisation and radiance sensitivity component of the Level 1b product is defined in the initialisation file and results from pre-flight calibration activities (the number of 10 in the table above is only an example). ESM and ASM position values are selected so that linear interpolation between these values yields an error well below the systematic error of the corresponding parameter. The scan mirror positions in the geolocation record of the MDS are used to select the correct interval and to calculate an appropriate set of parameters using linear interpolation.

15.6.8 Calibration initialisation File

Initialisation file defining settings for the in-flight calibrations of the SCIAMACHY Level 0 to 1b processor. Newly introduced in the processing baseline version 8 for the changes in the storage/access of calibration parameters. The file is a simple ASCII list consisting of a number of keywords representing the static parameters of the level 0 to 1b processing followed by the values of these parameters. The position of the parameters in this list is arbitrary, but the structure of the parameter values following a certain parameter's name has to be known by the code reading the static parameters.

FILE ID: SCI_LIC_AX

TYPE: Auxiliary

USE: Level 1b processing

UPDATED: Infrequently (associated to a specific processing baseline)

15.6.8.1 Format

The initialisation file includes headers and one GADS with a single DSR described below.

Table 15.6.8.1-1 - Schematic Structure of the Calibration Initialization File

MPH
Auxiliary Data SPH as described in R-4 with 1 DSD
Static Parameters GADS

15.6.9 Level 2 Initialization File

This Initialization file is used to for the generation of Level 2 off-line products, providing processing static parameters. The file size does not change from one orbit to the other, but changes with different processor versions. The current file version is revision 1.19.

FILE ID: SCI_IN__AX

TYPE: Auxiliary

USE: Level 2 processing

UPDATED: infrequently.

There is just one initialisation file associated to a processor version.

SIZE: approximately 95KB

The initialisation file is used to specify the following parameters:

- Overall algorithm control of the Level 1b to 2 processing chain;
- Fitting control for the individual retrievals (choice of parameters to be fitted, fitting convergence criteria, fitting window limits, etc.);
- Parameters controlling cloud fitting and aerosol indicator algorithms.

15.6.9.1 Format

This initialisation file includes headers and one GADS, which contains static parameters divided in several blocks of ASCII data formatted with XML language, reflecting the major components in Level 1b to 2 processing chain and representing the configurational settings needed. The high-level format of the file is shown below. The position of the parameters is arbitrary.

Table 15.6.9.1-1 - Schematic Structure of the Level 2 Initialization File

MPH
Auxiliary Data SPH as described in R-4 with 1 DSD
Static Parameters GADS

15.6.9.1.1 Static Parameters GADS

This GADS contains a single record of XML code. The format of the GADS is shown in table 15.5.1.7.3-1.

15.6.10 Database Server

In addition to the measurement data input provided by the Level 1b product, a broad set of reference data is needed for the Level 1b-2 processing. These data sets are collected in the so-called Database Server, which provides a uniform

programming interface to this data for all retrieval algorithms

The SCIAMACHY Database Server is divided into several files, each combining logically related information and parameters used for the Level 2 processing. Each of these files includes headers and a small number of GADS records. There is just one database server covering the entire mission.

Table 15.6.9.1-1 - Database Server

Database type	File	Content	Number of GADS
Atmospheric climatologies	SCI_PR2_AX	Pressure, temperature, trace gas concentration profiles	13
Cloud database	SCI_CL2_AX	Clouds related parameters	2
Surface database	SCI_SF2_AX	Global surface albedo, global vegetation index, global topography and other surface reflectance data	7
Literature cross-sections database	SCI_CS2_AX	Absorption cross-sections from literature appropriate for SCIAMACHY	13
Line-by-line absorption cross-sections	SCI_BL2_AX		5
Flight-model cross-sections	SCI_FM2_AX	Absorption cross-sections for trace gases measured with the SCIAMACHY flight-model	12
Auxiliary cross-sections	SCI_UX2_AX	Absorption cross-sections from GOME and literature sources, especially used for SO2, BrO and OClO retrievals	25
Undersampling correction	SCI_UC2_AX	Calculated undersampling spectra for DOAS and IAS applications	4
Key database	SCI_KEY_AX	ETA & ZETA key data	2
ESFT spectral data	SCI_ES2_AX	Hitran spectral inputs for SACURA	1
Cloud clearing data	SCI_CC2_AX	PMD minimum reflectance database	1
Background database	SCI_BG2_AX	Corrections to slant columns for SO2, NO2, NCHO, CHOCHO from the Pacific reference sector	4
Air Mass Factor Look-Up-Table	SCI_MF2_AX		1
BIAS slant path factor Look-Up-Table	SCI_PF2_AX	obsolete	
AAIA Rayleigh scattering correction Look-Up-Table	SCI_RC2_AX		1

The current Level 2 initialisation file version 5.00 does not use the database files SCI_CS2_AX, SCI_FM2_AX, SCI_UC2_AX, and SCI_KEY_AX.

15.6.10.1 Format

All database files consist of the following components:

Table 15.6.10.1-1 - Schematic Structure of a Database File

MPH
Auxiliary Data SPH as described in R-4 with DSDs
Data content GADS (several records in each file)

15.6.11 Atmospheric Climatologies Data File

An atmospheric climatology gives reference information about pressure, temperature and trace gas concentration profiles as a function of time during the year and location on Earth. There are various standard climatologies and one reference atmosphere in the SCIAMACHY database. In total 13 GADSR are enclosed:

- MPI climatology from the 2-D chemical-dynamical model developed by the Max-Planck Institute for Chemistry in Mainz, Germany.
- US reference atmospheres provided by Air Force Geophysical Laboratory (AFGL), Hanscom, Mass., USA
- TOMS V8 temperature and O3 conc. profile;
- KNMI O3 conc. profile;
- HALOE NO2 conc. profile;
- BIRA temperature, pressure and BrO conc. profile;
- Boundary layer SO2 profiles from IFE Bremen;
- Volcanic SO2 profiles from IFE Bremen;
- CIRA temperature profiles (for new IR retrieval algorithms)
- GLATM temperature, pressure and concentration profiles for several molecules (two files)
- Single BIAS reference atmosphere (derived from the AFGL US Standard atmosphere) with trace species for BIAS applications (obsolete);
- WMO Aerosol coefficients

Details on the format of the specific GADS can be found in R-2.

15.6.12 Cloud Parameters Data File

The cloud reference parameters given in the database are the following:

- ISCCP Data Base

- Cloud Albedo Climatology

Details on the format of the specific GADS can be found in R-2.

15.6.13 Surface Data Bases File

The surface parameters given in the database are the following:

- Global topography
- Global albedo climatology
- Spectral reflectance climatology
- Glitter albedo climatology
- Global reflection climatology (GLER)
- TOMS albedo climatology
- Refined global topography

Details on the format of the specific GADS can be found in R-2.

15.6.14 Literature Reference Cross-Sections Data Base File

The database contains absorption cross-section and cross-section coefficients (O3 Hartley-Huggins bands) as function of molecular species, wavelength and temperature. Databases are available from different measurement campaigns, documented in the literature. The database consists of the following components:

- O3 Reference Spectra (literature)
- NO2 Reference Spectra (literature)
- Vandaele NO2 Reference Spectra
- H2O Reference Spectra (literature)]
- BrO Reference Spectra (literature)
- Wilmouth BrO Reference Spectra
- SO2 Reference Spectra (literature)
- HCHO Reference Spectra (literature)]
- Cantrell HCHO Reference Spectra
- OClO Reference Spectra (literature)
- Kromminga OClO Reference Spectra
- O4 Reference Spectra (literature)
- Theoretical Ring spectrum

Details on the format of the specific GADS can be found in R-2.

15.6.15 Line by Line Absorption Cross-Sections File

This file contains absorption cross-sections for trace gases in selected parts of channels 7 and 8, for the BIAS reference atmosphere.

15.6.16 Flight-Model Reference Cross-Sections Data File

This database contains absorption cross-section of several molecules, plus a Ring Reference spectrum measured by GOME and the SCIAMACHY flight-model. The cross-sections are given as a function of wavelength and temperature.

- O3 Reference Spectra (GOME-measured)
- NO2 Reference Spectra (GOME-measured)
- Ring Reference Spectra (GOME-measured)
- O3 Reference Spectra (SCIA-measured)
- NO2 Reference Spectra (SCIA-measured)
- BrO Reference Spectra (SCIA-measured)
- SO2 Reference Spectra (SCIA-measured)
- HCHO Reference Spectra (SCIA-measured)
- OClO Reference Spectra (SCIA-measured)
- NO Reference Spectra (SCIA-measured)
- O2 Reference Spectra (SCIA-measured)
- O3D Reference Spectra (derived from GADS 7)

Details on the format of the specific GADS can be found in R-2.

15.6.17 Undersampling correction spectra File

It has been recognised that there is a need to correct the DOAS and IAS fitting for instrumental effects. One such effect is the Doppler shift (in wavelength) between the re-corded sun spectra and the earthshine spectra. So called undersampling correction spectra have been pre-calculated for channels #2, #3, #7 and #8 using the Doppler shift and the slit function information. Correction spectra cover the spectral regions of interest for DOAS and IAS applications.

15.6.18 PMD minimum reflectance library File

The PMD reflectance database is derived from GOME PMD measurements. It contains minimum reflectance values as function of the geolocation. The GOME instrument has only three PMD's in the UV-VIS spectral range. Thus, the database entries for the first three PMD's are based on real GOME measurements and the currently implemented algorithm makes use only of that data.

15.6.19 Air Mass Factor Look-Up Table

This file contains the Air Mass Factor (AMF) look-up tables used for Level 2 processing.

FILE ID: SCI_MF2_AX

TYPE: Auxiliary

USE: Level 2 processing

UPDATED: infrequently

In total three GADSR are enclosed:

- AMF LUT for O3
- AMF LUT for NO2
- AMC DOAS LUT for H2O

15.6.20 AAIA Rayleigh Reflectance Look-Up Table File

This file contains the Rayleigh reflectance look-up table used for the AAIA preprocessing step of the Level 2 processing.

FILE ID: SCI_RC2_AX

TYPE: Auxiliary

USE: Level 2 processing

UPDATED: infrequently.

15.6.21 Background Database

With the introduction of nadir trace gas columns retrieved with DOAS for NO2, SO2, CHOCHO, and HCHO, it became necessary to include a background database correction. Slant column values are known to have an offset to the true values that is dependent from latitude and time. This error is corrected by substracting an offset value from the retrieved slant column. For the determination of the offset it is assumed that no trace gas of interest is present over the Pacific Ocean, in the so-called reference sector (longitudes between 180° and 220°). Slant columns from this sector are averaged over latitude bins and stored in a database that is prefilled and continuously updated during regular processing. Values from the reference sector are the assumed offsets that compensate most of the effect and also some of the ozone interference.

FILE ID: SCI_BG2_AX

TYPE: Auxiliary

USE: Level 2 processing

UPDATED: infrequently.

In total four GADSR are enclosed:

- SO2 background correction
- NO2 background correction
- CHOCHO background correction
- HCHO background correction

15.6.22 ECMWF Data Files

Originally, the SCIAMACHY Level 2 processor was built in a way to use the ECMWF data files as input. These files are common to many instruments and are hence defined in R-4. However the SCIAMACHY processors do not use ECMWF files.

15.6.23 Orbit State Vectors

The Orbit State Vector files available from the FOS or from DORIS data are defined in R-4.

15.7 ANNEX – PRODUCTS DISCONTINUED

Along the mission lifetime several Level 2 product types were discontinued. They are listed in the subsections below. Details on content and data format are available in the previous version of this document.

15.7.1 Fast Delivery Level 2 Product

This product has been discontinued at the end of the operational phase of the mission (May 2012).

Starting from Level 2 baseline version 5 (December 2009), a Fast Delivery processing chain was activated and a new Level 2 product was introduced (SCI_OL__2PN). This product was generated with the Level 2 off-line processor SGP version 5 using Level 1b NRT products as input retrieving geophysical parameters from nadir as well as from limb measurements. The Restituted Attitude files (AUX_FRA) were not used in this processing chain. Format was the same as consolidated Level 2 product (SCI_OL__2P).

15.7.2 Vertical Column Amounts Level 2 Product

This product has been discontinued in the operational processing chain since May 2006.

SCIAMACHY Vertical Column Amounts	
PRODUCT ID	SCI_NL__2P
PRODUCT NAME	SCIAMACHY Vertical Column Amounts
DESCRIPTION	This product contains geophysical Trace Gas Column Densities, Cloud Top Height and Cover, as well as Aerosol Absorption Indicator values resulting from the processing of the Level 1b product measurements.
APPLICATIONS	Measurement of ozone and other atmospheric constituents for meteorology and climatology
DELIVERY TIME	The NRT version of this product was available from PDHS within 3 hours from acquisition. A fully consolidated version was processed systematically off-line and was available after 1 to 2 weeks from the PAC.
COVERAGE	Full orbit, nadir and limb measurements
THROUGHPUT	1 product per orbit
PRODUCT SIZE	max. size of approx. 6 MBytes per orbit
GEOMETRICAL SAMPLING	N/A
AUXILIARY DATA	Summary Quality ADS (SQADS) Geolocation ADS (LADS) Geolocation of the Ground Pixels ADS
ALGORITHMS USED	DOAS type retrievals using pre-calculated AMF look-up table in UV and visible wavelength range
INPUT DATA	Level 1b product plus auxiliary data.
NOTES	Produced systematically from Level 1b data

15.7.3 Selected Vertical Column Amounts for Meteo Users Level 2 Product

This product has been discontinued in the operational processing chain since May 2006.

SCIAMACHY Selected Vertical Column Amounts for Meteo Users	
PRODUCT ID	SCI_RV__2P
PRODUCT NAME	SCIAMACHY Selected Vertical Column Amounts for Meteo Users
DESCRIPTION	This Level 2 SCIAMACHY product contains selected vertical column amounts of the NRT Vertical Column Amounts product.
APPLICATIONS	For NRT environmental monitoring
DELIVERY TIME	Available 3 hours after data acquisition from the PDHS.
COVERAGE	Full orbit
THROUGHPUT	One product per orbit (approx. 100 minutes)
PRODUCT SIZE	Maximum size of approx. 200 kB per orbit
GEOMETRICAL SAMPLING	Limb: samples atmosphere between 1 and 100 km.
GEOMETRIC RESOLUTION	Nadir spatial resolution = typically 60 km (across track) x 30 km (along track) --depends on scan speed and integration time Limb spatial resolution = 3 km vertical Occultations = 3 km vertical
GEOMETRIC ACCURACY	Information not available
RADIOMETRIC RESOLUTION	Nadir spatial resolution = typically 60 km (across track) x 30 km (along track) --depends on scan speed and integration time Limb spatial resolution = 3 km vertical Occultations = 3 km vertical
RADIOMETRIC ACCURACY	N/A
AUXILIARY DATA	No auxiliary data required
ALGORITHMS USED	Extraction only.
INPUT DATA	Level 2 Vertical Profiles product.

NOTES	Produced systematically from the NRT Level 2 Vertical Column Amounts product. May be converted to BUFR format outside the PDS for distribution to Meteo users.

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