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

**Abstract** : This document contains the SCIAMACHY Product Specifications.

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## AMENDMENT POLICY

This document shall be amended by releasing a new edition of the document in its entirety. The Amendment Record Sheet below records the history and issue status of this document.

### AMENDMENT RECORD SHEET

ISSUE	REVISION	DATE	CHANGE STATUS	ORIGIN
1	A	12/01/96	Issue 1	
1	B	16/02/96	<p>SCR #16, CR #16            Issue 1, Revision B</p> <p>Reason for Change:</p> <p>Updated to reflect information in PO-TN-ESA-GS-0381 and to address RIDs of Feb. 2/96 pertaining to the Level 0 structure.</p> <p>MPH, SPH, DSD, and DSR structures modified.</p> <p>Table added showing generalized Level 0 product structure.</p> <p>RIDs Addressed:</p> <p>ESA/0001: FEP header defined            ESA/0002: PF-Host time stamp clarified</p> <p>ESA/0004: Processing PCD added            ESA/0006: AF PCD ADS and DSD added</p> <p>ESA/0007: page A-3 updated            ESA/0008: page B-3 updated</p> <p>ESA/0009: Table 8.1.1 modified            ESA/0011: TBD changed to Range/Doppler</p> <p>ESA/0013: FEP header defined            ESA/0014: Table 8.4.7.4-2 corrected</p> <p>CSF/1: filename in MPH corrected</p> <p>CSF/2: page A-3 updated</p> <p>CSF/3: MPH PCD information updated</p> <p>CSF/5: DSD added to Level 0 SPH</p>	



ISSUE	REVISION	DATE	CHANGE STATUS	ORIGIN
			CSF/6: Section on AATSR updated and re-issued CSF/8: AATSR_O Summary Sheet updated	
1	C	04/04/96	SCR #38, CR #38 Issue 1, Revision C  Reason for Change:  Updated Sections 1-6, 17 and Annex A to reflect changes discussed at the Products Review Meeting #1, March 5-8, 1996, as per action item "AI MDA 6 April 96" from PO-MN-ESA-00416, Pg. 35.	Products Review Meeting #1
2	A	20/05/96	SCR #71, CR #71 Issue 2  Reason for Change:  Separate volume created.  Updated with new product information from Document A-3.	
2	B	30/03/97	SCR #145, CR #145 Issue 2, Revision B  Reason for Change:  Level 1 and Level 2:  SPH formats updated, some keywords and data types changed PROCESSING_SOFTWARE_VERSION removed from SPH. Field is in the MPH. Time and positioning info added to SPHs. Reference DSDs added to SPHs. SQADS moved to directly follow SPH. lat/long changed to ENVISAT format. Spares added to accommodate future changes.  1 byte attachment flag added to ADSRs as per Envisat format. Size estimates updated. Data sets from SCIA_MO1 merged into the Level 1B product. Auxiliary data: AX files given standard AX SPH.  Information from IODD defined SPHs moved to a GADS where needed. Spares added to accommodate future changes. Field 5 of Table 15.6.12.1.2-1 and field 5 of Table 15.6.12.1.3-1 changed to units of Kelvin.	
3	A	11/07/98	SCR #169, CR #169 Issue 3	



ISSUE	REVISION	DATE	CHANGE STATUS	ORIGIN
			Reason for Change: Updated for new release of ESA IODD documents: <ul style="list-style-type: none"> <li>• SCIAMACHY Level 0 to Level 1B Processing Input/Output Data Definition, ENV-TN-DLR-SCIA-005, Issue 4/B, March 27, 1998; and</li> <li>• SCIAMACHY Level 1B to Level 2 NRT Processing Input/Output Data Definition, ENV-TN-DLR-SCIA-0010, Issue 3, March 19, 1998.</li> </ul> Also updated for comments from fax DPMO/JMJ/ENV, 1215/98.	
3	B	13/11/98	SCR #218, CR #218 Issue 3, Revision B  Reason for Change: Updated for the following SPRs: SPR-42000-0197-CSF to SPR-42000-0206-CSF, SPR-42000-0213-CSF, SPR-42000-0214-CSF, SPR-42000-0246-CSF to SPR-4200-0252-CSF.	
3	C	30/11/99	Issue 3, Revision C  Reason for Change: Updated for the following faxes: <ul style="list-style-type: none"> <li>• DOT/JMJ/ENV, 1142/99;</li> <li>• PO-FX-ESR-GS-1465.</li> </ul>	
3	D	6/06/2000	Issue 3, Revision D  Reason for Change: Updated according to SCIAMACHY Level-2 / Off-Line IODD ENV-ID-DLR-SCI-2200-0004 issue 1, 29/11/99	PDS V3
3	E	13/11/00	Issue 3, Revision E	

ISSUE	REVISION	DATE	CHANGE STATUS	ORIGIN
			Reason for Change: <ul style="list-style-type: none"> <li>SCIAMACHY Level 0 to Level 1B Processing Input/Output Data Definition, ENV-TN-DLR-SCIA-005, Issue 5, July, 21 2000; and</li> </ul> 7. SCIAMACHY Level 1B to Level 2 NRT Processing Input/ Output Data Definition, ENV-TN-DLR-SCIA-0010, Issue 3/B, May 29, 2000.	
3	F	30/5/2001  26/9/2001	Reason for Change:  wrong dim in table 15.5.1.7.7-1  Addition of GADS in Table 15.4.1.6-2 to be compliant to IODD	
3	G	6/10/2002  16/6/2003	Modifications to level 2 off-line product specifications New Aux file definition added:SCI_INI_AX  Reason for change: <b>L2 OL I/O DD</b> ENV-ID-DLR-SCI-2200-4 of 27/08/2002 issue 4/b  Modifications according to corrections suggested by DLR, plus new baseline. All changes reported in Register of changes.	<b>L2 OL I/O DD: ENV-ID-DLR-SCI-2200-4</b>  Level 1b to 2 NRT processing IODD: <b>ENV-TN- DLR-SCIA-0010 Issue 3/ C of 23.May.2003</b>
3	H	16/04/2004	Modifications according to new IODD issue for corrections on units for Nadir and Limb Geolocation ADS	<b>L2 OL IODD: ENV-ID-DLR-SCI-2200-4 Issue 4/D of 23.March.2004</b>
3	I	25/10/2004	Modifications according to new IODD for Off-line Level2 Product and corrections on NRT level1b to 2 IODD	<b>L2 OL IODD: ENV-ID-DLR-SCI-2200-4 Issue 4/E of 17 Aug. 2004</b>  <b>L1bto2 NRT IODD: ENV-TN-DLR-SCIA-</b>

ISSUE	REVISION	DATE	CHANGE STATUS	ORIGIN
				0010 Issue 3/ D of 16Aug. 2004
3	J	1/12/2004	Modifications according to amendments of L0 to L1b IODD, L1b to L2 NRT See register of changes for details.	<p>L0 to L1b NRT IODD: ENV-TN-DLR-SCIA-0005 Issue 5/ A of 25/10/ 2004</p> <p>L1bto2 NRT IODD: ENV-TN-DLR-SCIA-0010 Issue 3/ D of 02/11/ 2004</p> <p>L2 OL IODD: ENV-ID-DLR-SCI-2200-4 Issue 4/E of 3 Nov. 2004</p>
3	K	31/03/2006 First release	<p>Modifications according to: L0 to L1b IODD, L1b to L2 OFL IODD, L0 to L1b ADF.</p> <p>See register of changes for details.</p> <p><b>WARNING MESSAGE:</b> NRT Processing for SCI NL 2P product is being suspended with start of operations SCIAMACHY IPF L1b 6.01.</p>	<p>L0 to L1b NRT IODD: ENV-TN-DLR-SCIA-0005 Issue 6 of 6/9/ 2005</p> <p>L2 OL IODD: ENV-ID-DLR-SCI-2200-4 Issue 4/G of 9 Mar. 2006</p> <p>L0 to L1b Conf. Mgt ADF: ENV-CMA-DLR-SCIA-0062 Issue 1/B of 20 Mar. 2006</p>
		24/04/2006 Second release	Taking into account updated L0 to L1b IODD	L0 to L1b NRT IODD: ENV-TN-DLR-SCIA-0005 Issue 6/A of 4/4/

ISSUE	REVISION	DATE	CHANGE STATUS	ORIGIN	
				2006	
		06/05/2006 Final release	Taking into account updated L1b to L2 OFL IODD	L2 OL IODD: ENV-ID- DLR-SCI- 2200-4 Issue 4/G of 2 May 2006	
		27/06/2007	Implementing minor corrections raised by Sciamachy DPQC		
		23/06/2008	Fixing old typos		
3	L	06/07/2009	Aligning with SCIAMACHY Level 0 to 1b Processing I/O DD Issue 6/A:	SCIAMACHY Level 0 to 1b Processing I/O DD ENV-TN-DLR-SCIA-0005 Issue 6/A - 04. April 2006	
			<ul style="list-style-type: none"> <li>Reference to DPM:</li> <li>-&gt;N/A</li> </ul>		
			<ul style="list-style-type: none"> <li>Radiance sensitiv. GADS Nadir (corrected cut/paste error)</li> <li>-&gt;Already fixed in 3K</li> </ul>		
			<ul style="list-style-type: none"> <li>Sun reference file: replaced figure:</li> <li>-&gt; Table 15.3.1.1-1 "Schematic Structure of the Sun Reference Spectrum File" already aligned</li> </ul>		
			<ul style="list-style-type: none"> <li>Other editorial changes not reported in Track Change Record (to ensure alignment):</li> <li>-&gt; C1</li> </ul>		
			<ul style="list-style-type: none"> <li>Introduction updated</li> <li>Introduction updated for Nadir IR</li> <li>Mission extension changed form 2014 to 2013</li> <li>-&gt; C2</li> </ul>		SCIAMACHY_L2_OFL_IO DD_v5_ ENV-ID-DLR-SCI-2200-4
			<ul style="list-style-type: none"> <li>Product description updated, new applications inserted</li> <li>-&gt;C3</li> </ul>		
			<ul style="list-style-type: none"> <li>Product component table updated: H2O, volcanic SO2 and limb clouds added</li> <li>-&gt;C4</li> </ul>		
			<ul style="list-style-type: none"> <li>SPH example entries updated, especially new nadir fitting windows for H2O, volcanic SO2 added</li> <li>-&gt; C5</li> </ul>		
			<ul style="list-style-type: none"> <li>Changes in DSD: NAD_UV7_H2O and LIM_CLOUDS added, NAD_UV7_SPARE renamed to NAD_UV8_SPARE, SPARE readded, numbers and size updated</li> </ul>		



ISSUE	REVISION	DATE	CHANGE STATUS	ORIGIN
			<ul style="list-style-type: none"> <li>• -&gt;C6</li> </ul>	
			<ul style="list-style-type: none"> <li>• Explanation for 44 applications fixed</li> <li>• -&gt; C7</li> </ul>	
			<ul style="list-style-type: none"> <li>• Component size of XML initialization file updated</li> <li>• -&gt;C8</li> </ul>	
			<ul style="list-style-type: none"> <li>• Grammar fixed</li> <li>• -&gt;C9</li> </ul>	
			<ul style="list-style-type: none"> <li>• Remarks concerning AMC-DOAS added</li> <li>• Footnote added</li> <li>• -&gt; C10</li> </ul>	
			<ul style="list-style-type: none"> <li>• Comments to fields 9 (NUM_RLEVEL) and 21 (STVEC_SIZE) corrected</li> <li>• -&gt; C11</li> </ul>	
			<ul style="list-style-type: none"> <li>• Section Limb Clouds Data Set added (SCR 25)</li> <li>• Explanation for ice cloud flag = 3 (bad data) and 9 (strange case) added</li> <li>• -&gt;C12</li> </ul>	
			<ul style="list-style-type: none"> <li>• BIAS changed to IAS</li> <li>• -&gt; C13</li> </ul>	
			<ul style="list-style-type: none"> <li>• Typo corrections</li> <li>• -&gt;C13</li> </ul>	
			<ul style="list-style-type: none"> <li>• Key Data db added (ETA.Zeta)</li> <li>• New profile climatologies added</li> <li>• -&gt;C14</li> </ul>	
			<ul style="list-style-type: none"> <li>• BIAS reference atmosphere marked as obsolete</li> <li>• -&gt;C15</li> </ul>	
			<ul style="list-style-type: none"> <li>• Typo correction p94 (96)</li> <li>• -&gt;C16</li> </ul>	
			<ul style="list-style-type: none"> <li>• BIAS Refrence Atmosphere is obsolete for SGP_12OL; section deleted</li> <li>• -&gt;C17</li> </ul>	
			<ul style="list-style-type: none"> <li>• Line-by-Line Absorption Cross-Sections (SCI_BL2_AX) are obsolete for SGP_12OL; section deleted</li> <li>• -&gt;C18</li> </ul>	
			<ul style="list-style-type: none"> <li>• BIAS changed to IAS</li> <li>• -&gt;C19</li> </ul>	
			<ul style="list-style-type: none"> <li>• AMC look-up table for H2O added</li> <li>• -&gt;C20</li> </ul>	
			<ul style="list-style-type: none"> <li>• BIAS Slant Path Factor Look-Up Table (SCI_PF2_AX) is obsolete for SGP_12OL: section has been deleted</li> <li>• -&gt;C21</li> </ul>	
			<ul style="list-style-type: none"> <li>• Typo corrections</li> <li>• -&gt;C22</li> </ul>	This document
			<ul style="list-style-type: none"> <li>• Other Document updates</li> </ul>	



ISSUE	REVISION	DATE	CHANGE STATUS	ORIGIN
			<ul style="list-style-type: none"> <li>-&gt;C23</li> </ul>	
			<ul style="list-style-type: none"> <li>Addition of SCI_OL_2PN product</li> <li>-&gt; C24</li> <li>Changes related to M-factor</li> <li>-&gt;C25</li> </ul>	SCIAMACHY Level 1b to 2 Off-line Processing IODD 5/A, ENV-ID- DLR-SCI- 2200-4
			<ul style="list-style-type: none"> <li>Changes related to Limb Clouds</li> <li>-&gt;C26</li> </ul>	
		21/01/2010	<ul style="list-style-type: none"> <li>Remarks added that errors of AMC-DOAS are absolute values (not fractions) in alignment with IODD 5/A, Date 19. January 2010</li> </ul>	

## REGISTER OF CHANGES

Section	Change	ID
Table 15.4.1.7.1-1	Editorial,: "X" quoted to align with IODD	C1
Section 15.1	(change withdrawn)	C2
Section 15.5.3	Modified table and added paragraph	C3
Table 15.3.1.1-2	Modified table	C4
Table 15.3.1.1-3	Modified field 11, 12, 14, from 28 to 115	C5
Table 15.3.1.1-4	Modified table + added explanation paragraph	C6
Section 15.5.3.6		
Section 15.5.3.7.1	Added paragraph	C7
Table 15.4.1.7.1-2	Modified table	C8
Section 15.5.3.7.7	Text fixed	C9
Table 15.4.1.7.1-3	Added notes to table	C10
Section 15.5.3.7.8	Modified note a. b. and c.	
	Added note d.	
	Added note e.	
Table 15.4.1.7.1-4	Field 12: corrected comment	C11
Section 15.5.3.7.10	New section added	C12
Table 15.4.1.7.1-5	New table added	
Section 15.6.20	BIAS changes to IAS Typo correction	C13
Section 15.6	Footnote added	C14
Table 15.5.1.2 1	Text added	
Table 15.5.1.6 2	Text added KEY_DATA and DBUX	
Section 15.6.9	Text added	C15
Section 15.6.10.1.2	Text modified	C16
Section 15.6.9.1.3	Section description text added to be obsolete	C17
Section 15.6.13	(change withdrawn)	C18
Section 15.6.15.1.1	Added text	C19
Table 15.6.17.1 1	Added SPH and GADS	C20
Section 15.6.17.1	Added text	
Section 15.6.17.1.3	Added new section	
Section 15.6.18	(change withdrawn)	C21
Section 15.5.3	Text changed	C22
Section 15.6.19.1.1		
Section 15.6.5	Text added / changed	C23
Section 15.6.6	Text added / changed	
Section 15.3.1	Text added / changed	
Section 15.4.1	Text added / changed	
Section 15.4.1.8	Text changed	
Section 15.5.1	Text changed	
Table 15.5.3.2 1	Footnote added	
Section 15.5.3.8	Text changed	
Section 15.6.2	Text changed	
Section 15.6.21	Text added / changed	
Section 15.7	Text changed	
Section 15.5.1.7.1	Text changed	

Section	Change	ID
Section 15.5.3.8	Text changed	
Section 15.2	Text added	
Section 15.5.1	Section renamed and Text Added.	
Section 15.5.1 / 15.8.1	Text moved to new Annex section	
Section 15.5.2	Section renamed and Text Added.	
Section 15.5.2 / 15.8.2	Text moved to new Annex section	
Section 15.5.3	Section renamed and Text Added	
Section 15.5.3	Text Removed	
Table 15.6.17.1.2 1	Text changed	
Table 15.2-1	Text added	C24
Figure 15.2-1	Figure changed	
Section 15.5	Text deleted	
Section 15.5	Text added	
Table 15.4.1.2 1	Footnote added	C25
Section 15.5.3.3	Text added	
Table 15.4.1.6 2	Footnote added	
Table 15.5.3.2 1	Text added	
Table 15.5.3.4 1	Text added	C26
Section 15.4.1.7.29	Text added	
Section 15.5.3.7.8	Text added	C27



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## 15. SCIAMACHY PRODUCTS SPECIFICATIONS

### 15.1 INSTRUMENT OVERVIEW

The Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (SCIAMACHY) instrument provides spectra measured from light transmitted, back scattered or reflected by trace gases in the atmosphere. The instrument is designed for the global measurement of trace gases in the troposphere and stratosphere by means of a spectrometer scanning the atmosphere either at nadir or in limb. It records radiation in the range 0.24  $\mu\text{m}$  to 2.4  $\mu\text{m}$  with 8 detector modules. The goal is to allow small optical absorptions (as small as  $2\text{E-}4$  in some regions of the spectrum) to be detected.

SCIAMACHY is designed to measure the global distribution of trace gases, aerosols and clouds in both the troposphere and the stratosphere. The abundances of a number of atmospheric constituents which are targeted species include:

- in the troposphere -  $\text{O}_3$ ,  $\text{O}_4$ ,  $\text{N}_2\text{O}$ ,  $\text{NO}_2$ ,  $\text{CH}_4$ ,  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{HCHO}$  and aerosols and, in polluted conditions,  $\text{SO}_2$
- in the stratosphere -  $\text{O}_3$ ,  $\text{O}_2$ ,  $\text{O}_2^*$ ,  $\text{O}_4$ ,  $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{BrO}$ ,  $\text{N}_2\text{O}$ ,  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{CH}_4$  plus under volcanic eruption  $\text{SO}_2$ , plus under ozone hole conditions  $\text{OCIO}$  and  $\text{ClO}$ .

SCIAMACHY makes spectral measurements in passive limb and nadir looking spectrometer observations to permit ground based computation of the trace constituent concentrations.



<b>Table 15.1-1 - SCIAMACHY Instrument Characteristics</b>	
<b>GEOMETRIC:</b>	<p>Nadir viewing:            IFOV: 0.045 deg (across track) * 1.8 deg (along track)            Max Swath width: 960 km            Typical footprint: 30 k (along track) * 60 km (across track)</p> <p>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 is +/- 44 deg. relative to satellite velocity and is adjusted in order to cover the same atmospheric volume as for nadir measurements within 5 minutes.</p>
<b>SPECTRAL:</b>	<p>8 detector modules are utilized operating in the 0.24–2.4 <math>\mu\text{m}</math> spectral region. Detector modules 1-5 operate in the 0.25 to 1.05 <math>\mu\text{m}</math> region, and modules 6-8 operate in the 1 to 2.4 <math>\mu\text{m}</math> region.            channel 1 &amp; 2 = 240 - 400 nm,            channel 3 to 5 = 400 - 1000 nm,            channel 6 = 1000 -1700 nm            channel 7 = 1940 - 2040 nm, channel 8 = 2265 - 2380 nm</p> <p>Polarization (Polarization Measurement Devices, PMD) is measured in several channels;            PMD channel 1 = 320 -380 nm, PMD channel 2 = 450 - 520 nm            PMD channel 3 = 620 - 700 nm, PMD channel 44 = 800 -900 nm            PMD channel 5 = 1500 -1700 nm, PMD channel 6 = 2265 -2380 nm            PMD channel 7 = 45° detector = 800 - 900 nm</p>



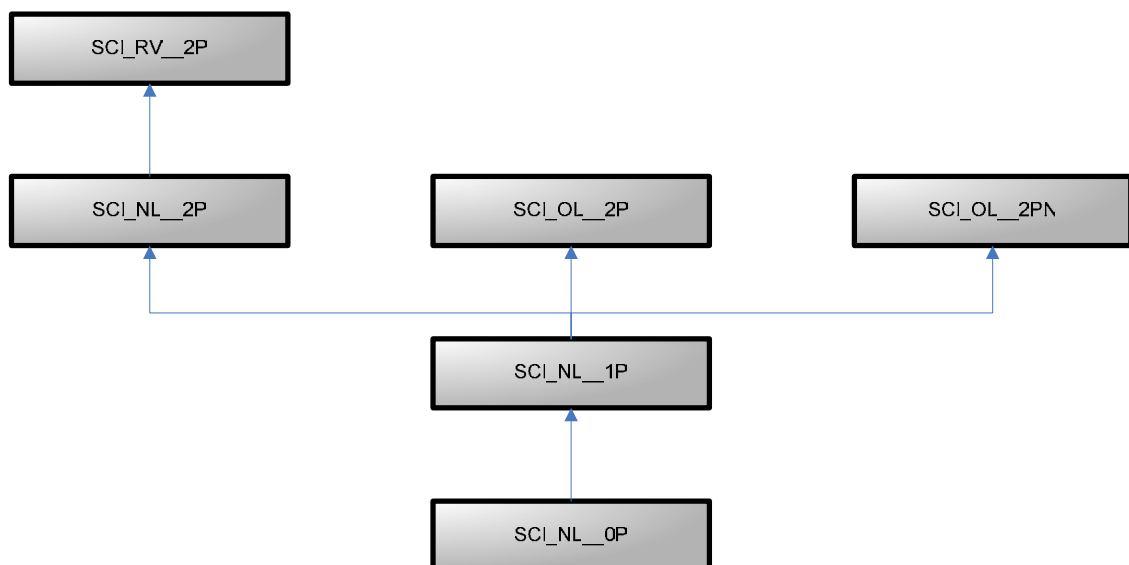
## 15.2 PRODUCTS OVERVIEW

The SCIAMACHY products may be classified as Level 0, 1B or 2. The characteristics of each product are summarized in Table 15.2-1 and Figure 15.2-1.

**Table 15.2-1- SCIAMACHY Products**

Instrument / mode	Product ID	Description
SCIAMACHY	SCI_NL__0P	SCIAMACHY Level 0
	SCI_NL__1P	Geolocated and Calibrated Spectra contains: Geolocated and Radiometrically and Spectrally Calibrated Limb and Nadir radiance spectra
	SCI_NL__2P	Vertical Column Amounts Geolocated vertical column amounts. Note that the NRT processing has been suspended since IPF version 6 (May 2006); from level 2 off-line version 5 a new processing chain the Fast Delivery level 2 processing (SCI_OL__2PN) has been activated
	SCI_OL__2P	Geolocated vertical column amounts from off-line processing, cloud-top pressure, cloud fractional cover and aerosols parameters, geolocated profiles from trace gas species.
	SCI_OL__2PN	Geolocated vertical column amounts from fast delivery processing, cloud-top pressure, cloud fractional cover and aerosols parameters, geolocated profiles from trace gas species. Note these products are processed within 24 hours from acquisition.
	SCI_RV__2P	Selected Vertical Column Amounts for Meteo users

**Figure 15.2-1 - SCIAMACHY Product Tree**







**WARNING MESSAGE:** NRT Processing for SCI\_NL\_2P product was suspended with operations SCIAMACHY IPF L1b 6.0 in May 2006. Starting from level 2 off-line version 5 (December 2009) a new processing chain, the Fast Delivery level 2 processing (SCI\_OL\_2PN) has been activated. This processing chain is based on the level 2 off-line processor using NRT level 1b products as input. The SCI\_OL\_2PN product contains as well nadir as limb products..

### 15.2.1 Product Specific Notation

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

**Table 15.2.1-1 - SCIAMACHY Notation**

Notation	Description
%	Percent
(BU/s)*sr	Binary units per second of a solid angle
(BU/s) / (photons/cm <sup>2</sup> * nm * s)	Binary units per second per radiance
-	No unit
1/16 s	Time of BCPS (62.5 ms)
BU	Binary units of signal read-outs
BU/s	Binary units per second
day	Day
degree	General Angle (360 per circle)
keyword	A keyword in the format definition
km	Kilometre
Lat/Long	Geographical Co-ordinate
10 <sup>-2</sup> m	10 <sup>-2</sup> metre
10 <sup>-5</sup> m/s	10 <sup>-5</sup> metre per second
mbar	Pressure
mol/cm <sup>2</sup>	Column density
mol/cm <sup>3</sup>	Density
ms	Millisecond
nm	Nanometre (Wavelength)
photons / (cm <sup>2</sup> * nm * sr * s)	Radiance
ppV	Volume mixing ratio; parts per Volume
Rel. fraction	Relative fraction
s	Second
terminator	Terminator of fields
µs	Microsecond

The following acronyms are used to describe data structures used in the products:

**Table 15.2.1-2 - SCIAMACHY Data Structures**

Notation	Description
Clcon	Cluster configuration
Coord	Geographical co-ordinate
Flags	Quality Flags
GeoL	Geolocation for limb measurements
GeoN	Geolocation for nadir measurements
GeoCal	Geolocation for calibration measurements
MJD	Modified Julian Date for the year 2000
PolV	Fractional polarisation values
L0Hdr	Level 0 header structure

### 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 is composed of time ordered and annotated Instrument Source Packets (in instrument data units) with a main and specific product header. There are 3 different types of source packets: Detector, PMD, and Auxiliary Data Packets. The SCIAMACHY Level 0 product is the basis of all data processing to create the higher level SCIAMACHY Products. The product is produced systematically. The NRT version of the product is available from the PDHS 3 hours after data acquisition. The OFL (fully consolidated) version is available from the LRAC 1-2 weeks after acquisition.

##### 15.3.1.1 Input Data

Annotated ISPs as received from the Front End Processor (FEP) plus auxiliary data.

##### 15.3.1.2 Auxiliary Data Used

The Level 0 product requires the following auxiliary information (refer to Volume 6):

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

As defined in Volume 6. A detailed description of the Instrument Source Packets is provided in Document A-1.

## 15.4 LEVEL 1B PRODUCTS

There is one SCIAMACHY Level 1B product. Information regarding this product is extracted from the SCIAMACHY Level 0 to Level 1B IODD (Document R-35).

### 15.4.1 SCIAMACHY Level 1B

Level 1 SCIAMACHY products are geolocated spectra, radiometrically and spectrally calibrated radiance for nadir, limb, and sun/moon occultation geometries. The Level 1B product is the foundation for further processing. The product is produced systematically. The NRT version of the product is available from the PDHS 3 hours after data acquisition. The L1b OFL (fully consolidated) version is generated at D-PAC, 1-2 weeks after acquisition.

#### 15.4.1.1 Input Data

Level 0 product plus auxiliary data.

#### 15.4.1.2 Auxiliary Data Used

The auxiliary data files required for Level 1B processing are listed in the table below.

**Table 15.4.1.2-1 - Auxiliary Data Files for SCIAMACHY Level 1B Processing**

Description	Auxiliary File ID
Leakage Current Parameters file	SCI_LK1_AX
PPG/Etalon Parameters file	SCI_PE1_AX
Spectral Calibration Parameters file	SCI_SP1_AX
Sun Reference 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)	SCI_MF1_AX <sup>1</sup>
Envisat-1 Restitude Attitude Data File	AUX_FRA_AX (described in Product Spec. Volume 16)
Orbit state vectors (one of following)	DOR_NAV_0P
	AUX_FPO_AX
	AUX_FRO_AX
	DOR_POR_AX
	DOR_VOR_AX

#### 15.4.1.3 Processing Performed

This is not the applicable document for algorithm details. The following is a high level overview of the processing performed for Level 1B product generation.

<sup>1</sup> Note that version IPF 7 does not use SCI\_MF1\_AX files for processing – but it will be used for level 2 processing



- 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 files and related output data.

**15.4.1.4 Product Structure**

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

**Table 15.4.1.4-1 - SCIAMACHY Level 1B Product Structure**

MPH
SPH (includes 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/ Occultation without ND GADS
Polarization Sensitivity Parameters Limb/ Occultation with ND GADS
Radiance Sensitivity Parameters Nadir GADS
Radiance Sensitivity Parameters Limb/Occultation without ND GADS
Radiance Sensitivity Parameters Limb/Occultation with ND GADS
Errors on Key Data GADS
Slit Function Parameters GADS
Small Aperture Slit Function Parameters GADS States of the Product ADS
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

**15.4.1.5 Main Product Header**

The Main Product Header is described in Volume 5.

### 15.4.1.6 Specific Product Header

The SPH is an ASCII header which conforms to the ASCII conventions defined in Volume 5. The Ø symbol indicates the position of an ASCII blank space character.

**Table 15.4.1.6-1 - Specific Product Header of Level 1B Product**

N	Description	Units	Byte Length	Data Type	Dim.
1	<b>SPH_DESCRIPTOR=</b>	keyword	15	uc	15
	quotation mark (“)	-	1	uc	1
	<b>SPH descriptor</b> (Set to SCI_NL__1P SPECIFIC HEADER)	-	28	uc	28
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
2	<b>STRIPLINE_CONTINUITY_INDICATOR=</b>	keyword	31	uc	31
	Value: +000 = No stripline continuity, the product is a complete segment Other: Stripline Counter	-	4	Ac	1
	newline character	terminator	1	uc	1
3	<b>SLICE_POSITION=</b>	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	<b>NUM_SLICES=</b>	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
	<i>Product Location Information</i>				
5	<b>START_TIME=</b>	keyword	11	uc	11
	quotation mark (“)	-	1	uc	1
	<b>Start time of the measurement data in this product</b> UTC time of first MDSR	utc	27	uc	27
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
6	<b>STOP_TIME=</b>	keyword	10	uc	10
	quotation mark (“)	-	1	uc	1
	<b>Time of the end of the measurement data in this product (last MDSR time)</b> UTC time of last MDSR	utc	27	uc	27
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
7	<b>START_LAT=</b>	keyword	10	uc	10
	<b>Latitude of the satellite nadir at the START_TIME</b> WGS84 latitude, positive = North	10-6 deg	11	Al	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
8	<b>START_LONG=</b>	keyword	11	uc	11
	<b>Longitude of the satellite nadir at the START_TIME</b> WGS84 longitude, positive = East, 0 = Greenwich	10-6 deg	11	Al	1

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

N	Description	Units	Byte Length	Data Type	Dim.
	<10-6degE>	units	10	uc	10
	newline character	terminator	1	uc	1
9	<b>STOP_LAT=</b>	keyword	9	uc	9
	<b>Latitude of the satellite nadir at the STOP_TIME</b> WGS84 latitude, positive = North	10-6 deg	11	AI	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
10	<b>STOP_LONG=</b>	keyword	10	uc	10
	<b>Longitude of the satellite nadir at the STOP_TIME</b> WGS84 longitude, positive = East, 0 = Greenwich	10-6 deg	11	AI	1
	<10-6degE>	units	10	uc	10
	newline character	terminator	1	uc	1
11	<b>Spare (blank characters (Ø))</b> For initialisation file version starting at 4.0 the first 33 characters provide init file version and decontamination flag: INIT_VERSION=xxxx DECONT= ddddddd with for each channel d='n' or 'y', example: INIT_VERSION= 401 DECONT=nnnnnyyy	-	50	uc	50
	newline character	terminator	1	uc	1
	<i>Data version information</i>				
12	<b>KEY_DATA_VERSION=</b>	keyword	17	uc	17
	quotation mark (")	-	1	uc	1
	Key Data version (pattern XX.XX, e.g. 01.25)	-	5	uc	5
	quotation mark (")	-	1	uc	1
	newline character	terminator	1	uc	1
13	<b>M_FACTOR_VERSION=</b>	keyword	17	uc	17
	quotation mark (")	-	1	uc	1
	Key Data version (pattern XX.XX, e.g. 01.25)	-	5	uc	5
	quotation mark (")	-	1	uc	1
	Newline character	terminator	1	uc	1
	<i>Product Quality Information</i>				
14	<b>SPECTRAL_CAL_CHECK_SUM=</b>	keyword	23	uc	23
	quotation mark (")	-	1	uc	1
	Range of spectral calibration error $\epsilon$ (summary): GOOD if $\epsilon \leq 0.02$ FAIR if $0.02 < \epsilon \leq 0.05$ BADØ if $\epsilon > 0.05$	-	4	uc	4
	quotation mark (")	-	1	uc	1
	Newline character	terminator	1	uc	1
15	<b>SATURATED_PIXEL=</b>	keyword	16	uc	16
	quotation mark (")	-	1	uc	1
	Number of saturated detector pixels n (summary): GOOD if n = 0 FAIR if $0 < n \leq 100$ BADØ if n > 100	-	4	uc	4
	quotation mark (")	-	1	uc	1
	Newline character	terminator	1	uc	1
16	<b>DEAD_PIXEL=</b>	keyword	11	uc	11

**Table 15.4.1.6-1 - Specific Product Header of Level 1B Product**

N	Description	Units	Byte Length	Data Type	Dim.
	quotation mark (“	-	1	uc	1
	Number of dead detector pixels n (summary): 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	<b>DARK_CHECK_SUM=</b>	keyword	15	uc	15
	Currently a spare Difference between measurement and calibrated dark signal (summary) : “GOOD” “FAIR” “BADØ” boundaries still tbd	keyword	6	Ac	6
	New-line character	terminator	1	uc	1
18	<b>NO_OF_NADIR_STATES=</b>	keyword	19	uc	19
	Number of Nadir states where MDSRs have been stored, example: +025	-	4	Ac	1
	New-line character	terminator	1	uc	1
19	<b>NO_OF_LIMB_STATES=</b>	keyword	18	uc	18
	Number of Limb states where MDSRs have been stored, example: +025	-	4	Ac	1
	New-line character	terminator	1	uc	1
20	<b>NO_OF_OCCULTATION_STATES=</b>	keyword	25	uc	25
	Number of Occultation states where MDSRs have been stored, example: +025	-	4	Ac	1
	New-line character	terminator	1	uc	1
21	<b>NO_OF_MONI_STATES=</b>	keyword	18	uc	18
	Number of WLS, SLS, and sun diffuser states where MDSRs have been stored and the corresponding processing has been completed (i.e., ‘newly calculated’ ADSRs stored) plus the number of monitoring states where MDSRs have been stored, example: +025	-	4	Ac	1
	New-line character	terminator	1	uc	1
22	<b>NO_OF_NOPROC_STATES=</b>	keyword	20	uc	20
	Number of states present in the processing time window applied to the Level 0 product but not counted in fields 17, 18, 19, 20, 21.3 and 21.6, example: +025	-	4	Ac	4
	New-line character	terminator	1	uc	1
22.3	<b>COMP_DARK_STATES=</b>	keyword	17	uc	17
	Currently a spare Number of processed complete dark states	-	4	Ac	4
	New-line character	terminator	1	uc	1
22.6	<b>INCOMP_DARK_STATES=</b>	keyword	19	uc	19
	Currently a spare Number of incomplete dark states	-	4	Ac	4
	New-line character	terminator	1	uc	1
22.7 <sup>2</sup>	<b>Spare (blank characters (Ø))</b>	-	4	uc	4
	newline character	terminator	1	uc	1
	<i>DSDs for Attached Data Sets</i>				
23	<i>DSD (A) for the SQ ADS</i>	-	280	dsd	1

<sup>2</sup> IODD 6.A here reports “23” instead of “22.7”





**Table 15.4.1.6-1 - Specific Product Header of Level 1B Product**

N	Description	Units	Byte Length	Data Type	Dim.
24	<i>DSD (A) for the Geolocation ADS (L ADS)</i>	-	280	dsd	1
25	<i>DSD (A) for the StaticInstrument Parameters GADS</i>	-	280	dsd	1
26	<i>DSD(G) for the Leakage Current (constant part) GADS</i>	-	280	dsd	1
27	<i>DSD(G) for the Leakage Current (variable part) GADS</i>	-	280	dsd	1
28	<i>DSD (G) PPG/Etalon Parameters GADS</i>	-	280	dsd	1
29	<i>DSD (G) for the Precise Basis Array of Spectral Calibration GADS</i>	-	280	dsd	1
30	<i>DSD (G) for the Spectral Calibration Parameters GADS</i>	-	280	dsd	1
31	<i>DSD (G) for the Sun Reference Spectrum GADS</i>	-	280	dsd	1
32	<i>DSD (G) for the Polarization Sensitivity Nadir GADS</i>	-	280	dsd	1
33	<i>DSD (G) for the Polarization Sensitivity Limb/Occultation without ND GADS</i>	-	280	dsd	1
34	<i>DSD (G) for the Polarization Sensitivity Limb/Occultation with ND GADS</i>	-	280	dsd	1
35	<i>DSD (G) for the Radiance Sensitivity Parameters Nadir GADS</i>	-	280	dsd	1
36	<i>DSD (G) for the Radiance Sensitivity Parameters Limb/ Occultation without NDGADS</i>	-	280	dsd	1
37	<i>DSD (G) for the Radiance Sensitivity Parameters Limb/ Occultation with NDGADS</i>	-	280	dsd	1
38	<i>DSD(G) Errors on Key Data GADS</i>	-	280	dsd	1
39	<i>DSD(G) for the Slit Function Parameters GADS</i>	-	280	dsd	1
40	<i>DSD(G) for the Small Aperture Slit Function Parameters GADS</i>	-	280	dsd	1
41	<i>DSD (A) for the States of the Product ADS</i>	-	280	dsd	1
42	<i>DSD (A) for the PMD Data Packets ADS</i>	-	280	dsd	1
43	<i>DSD (A) for the Auxiliary Data Packets ADS</i>	-	280	dsd	1
44	<i>DSD(A) for the Leakage Current (newly calculated parts) ADS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	-	280	dsd	1
45	<i>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 Volume 5.</i>	-	280	dsd	1
46	<i>DSD (A) PPG/Etalon Parameters (newly calculated) ADS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	-	280	dsd	1
47	<i>DSD (A) for the Spectral Calibration (newly calculated) ADS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	-	280	dsd	1
48	<i>DSD (A) for the Sun Reference Spectrum ADS (newly calculated) ADS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	-	280	dsd	1
49	<i>DSDs (M) for the Nadir MDS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	-	280	dsd	1



**Table 15.4.1.6-1 - Specific Product Header of Level 1B Product**

N	Description	Units	Byte Length	Data Type	Dim.
50	<i>DSDs (M) for the Limb MDS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	-	280	dsd	1
51	<i>DSDs (M) for the Occultation MDS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	-	280	dsd	1
52	<i>DSDs (M) for the Monitoring MDS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	-	280	dsd	1
	<i>DSDs for reference files</i>				
53	<i>DSD (R) for the Level 0 product</i>	-	280	dsd	1
54	<i>DSD (R) for the Leakage Current Parameters file</i>	-	280	dsd	1
55	<i>DSD (R) for the PPG/Etalon Parameters file</i>	-	280	dsd	1
56	<i>DSD (R) for the Spectral Calibration Parameters file</i>	-	280	dsd	1
57	<i>DSD (R) for the Sun Reference Spectrum file</i>	-	280	dsd	1
58	<i>DSD (R) for the Key Data file (Instrument Characterization file)</i>	-	280	dsd	1
59	<i>DSD (R) for the M-factor file</i>	-	280	dsd	1
60	<i>DSD (R) for the Initialisation file</i>	-	280	dsd	1
61	<i>DSD (R) for the Orbit State Vector File used</i>	-	280	dsd	1
62	<i>DSD(R) for the Attitude Data File</i>	-	280	dsd	1
63	<i>DSD -Spare (279 blank space characters followed by 1 newline character)</i>	-	280	Dsd_sp	1
	<b>size (in bytes)</b>		<b>10213</b>		

\*The sum of fields 17 to 21 equals the total number of states in the processing time window.

The field DSD\_NAME in the DSDs are filled as specified in the table below:

**Table 15.4.1.6-2 - DS\_NAME Field**

DSD	DS_NAME
<i>DSD (A) for the SQ ADS</i>	SUMMARY_QUALITY
<i>DSD (A) for the Geolocation ADS (L ADS)</i>	GEOLOCATION
<i>Static instrument parameters (GADS)</i>	INSTRUMENT_PARAMS
<i>DSD(G) for the Leakage Current (constant part) GADS</i>	LEAKAGE_CONSTANT
<i>DSD(G) for the Leakage Current (variable part) GADS</i>	LEAKAGE_VARIABLE
<i>DSD (G) PPG/Etalon Parameters GADS</i>	PPG_ETALON



**Table 15.4.1.6-2 - DS\_NAME Field**

<b>DSD</b>	<b>DS_NAME</b>
<i>DSD (G) for the Presise Basis Array of Spectral Calibration GADS</i>	SPECTRAL_BASE
<i>DSD (G) for the Spectral Calibration GADS</i>	SPECTRAL_CALIBRATION
<i>DSD (G) for the Sun Reference Spectrum GADS</i>	SUN_REFERENCE
<i>DSD (G) Polarization Sensitivity Nadir GADS</i>	POL_SENS_NADIR
<i>DSD (G) Polarization Sensitivity Limb/Occultation without ND GADS</i>	POL_SENS_LIMB
<i>DSD (G) Polarization Sensitivity Limb/Occultation with ND GADS</i>	POL_SENS_OCC
<i>DSD (G) for the Radiance Sensitivity Nadir GADS</i>	RAD_SENS_NADIR
<i>DSD (G) for the Radiance Sensitivity Limb/Occultation without ND GADS</i>	RAD_SENS_LIMB
<i>DSD (G) for the Radiance Sensitivity Limb/Occultation with ND GADS</i>	RAD_SENS_OCC
<i>DSD(G) for the Errors on Key Data</i>	ERRORS_ON_KEY_DATA
<i>DSD(G) for the Slit Function Parameters GADS</i>	SLIT_FUNCTION
<i>DSD(G) for the Small Aperture Slit Function Parameters GADS</i>	SMALL_AP_SLIT_FUNCTION
<i>DSD (A) for the States ADS</i>	STATES
<i>DSD (A) for the PMD Data Packets ADS</i>	PMD_PACKETS
<i>DSD (A) for the Auxiliary Data Packets ADS</i>	AUXILIARY_PACKETS
<i>DSD(A) for the Leakage Current (newly calculated parts) ADS</i>	NEW_LEAKAGE
<i>DSD(A) for the Average of the Dark Measurement per State ADS.</i>	DARK_AVERAGE
<i>DSD (A) PPG/Etalon Parameters (newly calculated) ADS</i>	NEW_PPG_ETALON
<i>DSD (A) for the Spectral Calibration (newly calculated) ADS</i>	NEW_SPECTRAL_CALIBRATION
<i>DSD (A) for the Sun Reference Spectrum (newly calculated) ADS</i>	NEW_SUN_REFERENCE
<i>DSDs (M) for the Nadir MDS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	NADIR
<i>DSDs (M) for the Limb MDS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	LIMB
<i>DSDs (M) for the Occultation MDS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	OCCULTATION
<i>DSDs (M) for the Monitoring MDS. If not used for this product, set to NOT USED as defined in Volume 5.</i>	MONITORING
<i>DSD (R) for the Level 0 product</i>	LEVEL_0_PRODUCT
<i>DSD (R) for the Leakage Current Parameters file</i>	LEAKAGE_FILE
<i>DSD (R) for the PPG/Etalon Parameters file</i>	PPG_ETALON_FILE

**Table 15.4.1.6-2 - DS\_NAME Field**

<b>DSD</b>	<b>DS_NAME</b>
<i>DSD (R) for the Spectral Calibration Parameters file</i>	SPECTRAL_FILE
<i>DSD (R) for the Sun Reference Spectrum file</i>	SUN_REF_FILE
<i>DSD (R) for the Key Data file (Instrument Characterization file)</i>	KEY_DATA_FILE
<i>DSD (R) for the M-factor file</i>	NOT_USED <sup>3</sup>
<i>DSD (R) for the Initialisation file</i>	INIT_FILE
<i>DSD (R) for the Orbit State Vector file used</i>	ORBIT_FILE
<i>DSD(R) for the Attitude Data File</i>	ATTITUDE_FILE

**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/SPH structures.

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<sup>3</sup> In IPF version 7 it is not in use, but in the corresponding OFL L2 processing version 5 is in use ("M\_FACTOR\_FILE").

### 15.4.1.7.1 Common Structures

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

N	Description	Units	Byte Size	Data Type	Dim.
1	Latitude (convention defined in Volume A)	10-6 deg	4	sl	1
2	Longitude (convention defined in Volume A)	10-6 deg	4	sl	1
Size			8		

N	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	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		

N	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 <sup>a</sup>	1/10 BU	1	uc	1
	size (in bytes)		4		

- a. 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.

N	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	BU	4	ul	1

Table 15.4.1.7.1-4 - Rsig Structure					
	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)				
2	<b>Straylight<sup>a</sup></b>	1/10 BU	1	uc	1
	<b>size (in bytes)</b>		5		

a. 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 15.4.1.7.1-5 - Esig Structure					
N	Description	Units	Byte Length	Data Type	Dim.
1	<b>Memory effect correction</b>	BU	1	sc	1
2	<b>Signal value of one detector element</b>	BU	2	us	1
3	<b>Straylight<sup>a</sup></b>	1/10 BU	1	uc	1
	<b>size (in bytes)</b>		4		

a. 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.

**Remark :** Esig is now equal to data type Rsig. The location for memory effect is currently a spare (reserved for non-linearity correction).

Table 15.4.1.7.1-6 - Esigc Structure					
N	Description	Units	Byte Length	Data Type	Dim.
1	<b>Signal value of one detector element and memory effect correction coded into one unsigned long value</b> (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	<b>Straylight<sup>a</sup></b>	1/10 BU	1	uc	1
	<b>size (in bytes)</b>		5		

a. 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.

**Remark :** Esigc is now equal to data type Rsigc. The location for memory effect is currently a spare (reserved for non-linearity correction).

Table 15.4.1.7.1-7 - PoIV Structure					
N	Description	Units	Byte Length	Data Type	Dim.
1	<b>Fractional polarization values Q</b> (6 values derived from	-	48	fl	12

	PMDs, 5 values derived from the overlapping regions, and one model value below 300 nm)				
2	<b>Errors on Q values</b>	-	48	fl	12
3	<b>Fractional polarization values U (6 values derived from the PMDs and one model value below 300 nm)</b>	-	48	fl	12
4	<b>Errors on the U values</b>	-	48	fl	12
5	<b>Representing wavelength for the fractional polarisation values and the 45 degree PMD</b>	nm	52	fl	13
6	<b>GDF parameters</b>	-	12	fl	3
	<b>size (in bytes)</b>		<b>256</b>		

**Table 15.4.1.7.1-8 - GeoL Structure**

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

**Table 15.4.1.7.1-9 - GeoN Structure**

N	Description	Units	Byte Length	Data Type	Dim.
1	<b>Position of ESM compared to zero position</b>	degrees	4	fl	1
2	<b>Solar zenith angles of start, middle, and end of the integration time at TOA</b>	degrees	12	fl	3
3	<b>Solar azimuth angles of start, middle, and end of the integration time at TOA</b>	degrees	12	fl	3
4	<b>Line of sight nadir angles of start, middle, and end of the integration time at TOA</b>	degrees	12	fl	3
5	<b>Line of sight azimuth angles of start, middle, and end of the integration time at TOA</b>	degrees	12	fl	3
6	<b>Satellite height at the middle of the integration time</b>	km	4	fl	1
7	<b>Earth radius at the middle of the integration time</b>	km	4	fl	1
8	<b>Sub-satellite point at the middle of the integration time</b>	-	8	Coord	1
9	<b>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</b>	-	32	Coord	4

**Table 15.4.1.7.1-9 - GeoN Structure**

	first in flight direction and the fourth the last in time and flight direction)				
10	<b>Center co-ordinate of the nadir ground pixel</b>	-	8	Coord	1
	<b>size (in bytes)</b>		<b>108</b>		

**Table 15.4.1.7.1-10 - GeoCal Structure**

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

**Table 15.4.1.7.1-11 - L0Hdr Structure**

N	Description	Units	Byte Length	Data Type	Dim.
1	<b>Level 0 Product Header (consists of the Packet header (6 bytes) and the Data field Header (66 bytes) as defined in A-1.</b>	-	72	uc	72
	<b>size (in bytes)</b>		<b>72</b>		

**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 this ADS.

There are several ADSRs in the ADS. The format of the ADSR is shown below.

**Table 15.4.1.7.2-1 - Summary Quality ADSR**

N	Description	Units	Byte Length	Data Type	Dim.
1	<b>Start time of the scan phase of the state</b>	-	12	mjd	1
2	<b>Flag indicating if MDS DSRs are attached to the current ADS DSR (1= no MDSRs, 0 otherwise)</b>	-	1	uc	1
3	<b>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.</b>	nm	32	fl	8
4	<b>Standard deviation of the wavelength differences from field 3. Set to zero in the case of a corrupted state or an unprocessed state.</b>	nm	32	fl	8
5	<b>Spare (Number of missing readouts in state)</b>	-	2	us	1



6	<b>Mean difference of leakage current or offset per channel and PMD</b> (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
7	<b>Sun glint region flag</b> 0 = no sun glint or corrupted state or unprocessed state 1 = sun glint	-	1	uc	1
8	<b>Rainbow region flag</b> 0 = no rainbow or corrupted state or unprocessed state 1 = rainbow	-	1	uc	1
9	<b>SAA region flag</b>	-	1	uc	1
10	<b>Number of hot pixel per channel and PMD</b> (order : 1 to 8 and A to F and 45°)	-	30 <sup>4</sup>	us	30
11	<b>Spare for additional flags</b>	-	10	uc	10
	<b>size (in bytes)</b>	-	182	-	-

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

#### 15.4.1.7.3 Geolocation of the States ADS

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

There are several ADSRs per ADS. The format of each ADSR is shown below.

N	Description	Units	Byte Length	Data Type	Dim.
1	<b>Start time of the scan phase of the state</b>	-	12	mjd	1
2	<b>Flag indicating if MDS DSRs are attached to the current ADS DSR</b> (1= no MDSRs, 0 otherwise)	-	1	uc	1

<sup>4</sup> Probably wrong in Prod Spec 3/J



**Table 15.4.1.7.3-1 - Geolocation of the States ADSR**

3	<p><b>For Nadir:</b>  <b>4 corner co-ordinates of the ground scene which is covered by the state</b> (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)</p> <p><b>For Limb:</b>                  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.</p> <p><b>For Occultation:</b>                  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.</p> <p><b>For all other states:</b>                  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.</p> <p>If state is corrupted, values are set to zero.</p>	-	32	Coord	4
	<b>size (in bytes)</b>	-	45	-	-

An ADSR will occur for states that are not processed but appear in the processing time window applied to the level 0 product. This will be 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 co-ordinates are representing the tangent ground point of the beginning and the end of the state and for all other measurements (calibration and monitoring) these co-ordinates 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**

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

**Table 15.4.1.7.4-1 - Static Instrument Parameters**

N	Description	Units	Byte Length	Data Type	Dim.
1	n_lc_min	-	1	uc	1
2	ds_n_phases (~12)	-	1	uc	1

N	Description	Units	Byte Length	Data Type	Dim.
3	ds_phase_boundarie (# = 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
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 the GADS is defined in the table below. There is only one record.

N	Description	Units	Byte Length	Data Type	Dim.

N	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 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 leakage current	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 several records of the type shown below.

N	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 (field 1 and 3) for channels 6 to 8	BU/s	12288	fl	3072
4	Error of variable fraction of LC	BU/s	12288	fl	3072
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 PMD 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 8 channels of SCIAMACHY are affected by the existence of leakage current. The detectors used for channel 1 to 5 are random access linear photo-diode arrays and are not expected to be sensitive to the temperature fluctuations foreseen in SCIAMACHY. Therefore, it is expected that a monthly update of

the leakage current parameters is sufficient to do an appropriate leakage current correction for these channels. Channel 6 to 8, however, are measuring in the near infra-red which requires a different type of detector material. These detectors are very sensitive to temperature fluctuations of the surrounding material (mainly the optical bench) and themselves. Therefore, two types of leakage current parameters are required:

- The default leakage current pattern is always (for all orbital positions and all integration or exposure times) valid for the channels 1 to 5 and the PMDs 1 to 4 and 7 (45° sensor) and serves as a basis for the other detectors.
- A set of differences in leakage current corresponding to the orbital position which may be interpolate for a certain orbital position before applying it to the default leakage current pattern of channel 6 to 8 and PMDs 5 and 6.

There is one additional parameter variable over orbit position which is the solar straylight scattered from the azimuth mirror. This parameter is valid for all 8 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 parameters.

The ‘Orbit phase after eclipse’ field of the variable fraction leakage current parameters may have a range between ‘0’ and ‘1’. ‘0’ represents the time 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 which are required for appropriate determination of the leakage current parameters has to be determined during the satellite commissioning phase. It is assumed the number will be fixed after the 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

Coded into the PPG parameters will be the existence of dead pixels by setting the corresponding detector value to zero.

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

<b>Table 15.4.1.7.7-1 - PPG/Etalon Parameters GADS</b>
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Table 15.4.1.7.7-1 - PPG/Etalon Parameters GADS					
N	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 <sup>a</sup>	-	8192	uc	8192
	size (in bytes)		139264	-	-

a. The bad pixel mask will indicate 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.

Table 15.4.1.7.8-1 - Precise Basis of the Spectral Calibration Parameters GADS					
N	Description	Units	Byte Length	Data Type	Dim.
1	Wavelength of detector pixel	-	32768	fl	8192
	size (in bytes)	-	32768	-	-

#### 15.4.1.7.9 Spectral Calibration Parameters GADS

SCIAMACHY is equipped with a passive thermal control loop which keeps the optical bench temperature stable within 600 mK. Depending on the temperature of the optical bench, the dispersion of the pre-disperse prism produces different spectral properties on the detector arrays. From measurements of the spectral calibration lamp, a set of spectral calibration parameters will be calculated for each position in orbit relative to the sun. To fulfil the ultimate scientific requirement for a spectral accuracy of 1/100th of a detector pixel, it is sufficient to define certain orbit phase regions in which the spectral calibration parameters are expected to be fairly constant. These ranges will be used as the key into the spectral calibration parameters.

The spectral calibration parameters area 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 which gives a total of 40 coefficients.

There are several records in this GADS of the type shown below. It is assumed that the number of records will be fixed during the commissioning phase.

N	Description	Units	Byte Length	Data Type	Dim.
1	<b>Orbit phase after eclipse</b> (range: the absolute value is between 0 and 1)	-	4	fl	1
2	<b>Coefficients in the 4th order polynomial for each detector array (channel)</b>	-	320	do	40
3	<b>Number of used lines per channel</b>	-	16	us	8
4	<b>Wavelength calibration error per channel</b>		32	fl	8
	<b>size (in bytes)</b>	-	372	-	-

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

#### 15.4.1.7.10 Sun Reference Spectrum GADS

The sun 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 this level 1b product, but they have been given in an earlier level 1b product which was covering the time period of the sun diffuser measurements. However, there may be sun reference spectra obtained from different measurement modes. The reason for this is that during instrument calibration several anomalies were found for different modes. The optimum Sun reference to use in Level 2 processing may depend on the kind of retrieval used there. The various modes are specified by the following identifier:

	<b>Calibrated</b>	<b>Uncalibrated</b>
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. There is only one record.

N	Description	Units	Byte Length	Data Type	Dim.
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Table 15.4.1.7.10-1 - Sun Reference Spectrum GADS					
1	Sun spectrum identifier (“Xn” where “X” may indicate various types of solar measurement, according to the table above, and “n” may indicate various diffuser angles)	-	2	Uc	2
2	Wavelength of the sun measurement	nm	32768	fl	8192
3	Mean sun reference spectrum (uncalibrated has as unit BU/s)	photons/cm <sup>2</sup> *nm*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 which 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 parameter ( $\mu_2, \mu_3$ ) is sufficient, because only the position of the elevation mirror is relevant.

The number of records in the GADS depends on the result of the final pre-flight calibration activity. Then ESM and ASM position values will be selected so that linear interpolation between these values yields an error which is well below the systematic error of the corresponding parameter. These values will be placed into the initialisation file and used from there 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					
N	Description	Units	Byte Length	Data Type	Dim.
1	Elevation mirror position	degrees	4	fl	1
2	$\mu_2$ nadir for the elevation mirror position of field 1	-	32768	fl	8192
3	$\mu_3$ nadir for the elevation mirror position of field 1	-	32768	fl	8192
	size (in bytes)	-	65540	-	-

**15.4.1.7.12 Polarisation Sensitivity Parameters Limb/Occultation without ND GADS**

The format of each GADS record is similar to that of Polarisation Sensitivity Parameters Limbs/Occultation with ND described in the Table 15.4.1.7.13-1.

**15.4.1.7.13 Polarisation Sensitivity Parameters Limb/Occultation with ND GADS**

The polarisation sensitivity is expressed as a large number of different parameters which 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 ( $\mu_2$ ,  $\mu_3$ ) is sufficient, because only the position of the elevation mirror is relevant.

For limb, a two-dimensional array of two parameters ( $\mu_2$  and  $\mu_3$ ) 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 depends on the result of the final pre-flight calibration activity. Then ESM and ASM position values will be selected so that linear interpolation between these values yields an error which is well below the systematic error of the corresponding parameter. These values will be placed into the initialisation file and used from there 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 15.4.1.7.13-1 - Polarisation Sensitivity Parameters Limb/Occultation with ND GADSR					
N	Description	Units	Byte Length	Data Type	Dim.
1	Elevation mirror position	degrees	4	fl	1

Table 15.4.1.7.13-1 - Polarisation Sensitivity Parameters Limb/Occultation with ND GADSR					
2	Azimuth mirror position	degrees	4	fl	1
3	$\mu_2$ limb for the elevation and azimuth mirror position of field 1 and 2	-	32768	fl	8192
4	$\mu_3$ limb for the elevation and azimuth mirror position of field 1 and 2	-	32768	fl	8192
	size (in bytes)	-	65544	-	-

**15.4.1.7.14 Radiance Sensitivity Parameters Nadir with ND GADS**

The format of each GADS record is shown below.

Table 15.4.1.7.14-1 - Radiance Sensitivity Parameters Nadir GADSR					
N	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/cm <sup>2</sup> *nm*sr*s)	32768	fl	8192
	size (in bytes)		32772		

**15.4.1.7.15 Radiance Sensitivity Parameters Limb/Occultation without ND GADS**

The format of each GADS record is similar to that of Radiance Sensitivity Parameters Limb/Occultation with ND GADS described in the Table 15.4.1.7.16-1.

**15.4.1.7.16 Radiance Sensitivity Parameters Limb/Occultation with ND GADS**

The radiance sensitivity parameters will be 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 depends on result of the final pre-flight calibration activity. Then ESM and ASM position values will be selected so that linear interpolation between these values yields an error which is well below the systematic error of the corresponding parameter. These values will be placed into the initialisation file and used from there to calculate the present product component. During application of the radiance 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 radiance sensitivity parameters using linear interpolation.

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.

The format of each GADS record is shown below.

<b>Table 15.4.1.7.16-1 - Radiance Sensitivity Parameters Limb/Occultation with ND GADSR</b>					
N	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/cm <sup>2</sup> *nm*sr*s)	32768	fl	8192
	size (in bytes)		32776		

#### 15.4.1.7.17 Errors on Key Data GADS

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

<b>Table 15.4.1.7.17-1 - Errors on Key Data GADS</b>					
N	Description	Units	Byte Length	Data Type	Dim.
1	Error on $\mu_2$ nadir	-	32768	fl	8192
2	Error on $\mu_3$ nadir	-	32768	fl	8192
3	Error on $\mu_2$ limb	-	32768	fl	8192
4	Error on $\mu_3$ limb	-	32768	fl	8192
5	Error on the radiance sensitivity for the optical bench only	(BU/s)/(photons/cm <sup>2</sup> *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 part of the Key Data which are required during the processing of the application programme have to be included in the level 1b product besides the Key Data itself, as described in the ADSs before. The parameters for which errors are attached with errors are the following:



- polarisation sensitivity parameters for nadir and limb ( $\mu_2$  and  $\mu_3$ ),
- radiance sensitivity parameters, and
- the BSDF function.

The error on the radiance sensitivity parameters is given for individual components of the instrument or viewing geometry. 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 field 5 and 6 (if only the elevation mirror is used)
- for limb or occultation measurements field 5 and 7 (if the light is entering the instrument via the azimuth and elevation mirror)
- for sun diffuser measurements field 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:

$$\epsilon_{\text{Rad}} = \text{Square\_Root} (\epsilon_{\text{OBM}}^2 + \epsilon_{\chi}^2)$$

Where  $\epsilon_{\chi}$  is one of the error given in fields 6 to 8.

#### 15.4.1.7.18 Slit Function Parameters GADS

The slit function parameters is a copy of the Key Data ‘\_SLIT\_F’. It is included as GADS because it is needed in the level 1 to 2 precessing. The number of 40 records is an example, the actual number will be equal to the first dimension of the corresponding parameters on the Key Data file.

The format of each GADS is shown below.

Table 15.4.1.7.18-1 - Slit Function Parameters GADS					
N	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 Lorentzian 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 is a copy of the Key Data \_SMALL\_AP\_SLIT\_F'. It is included as GADS because it is needed in the level 1 to 2 precessing. The number of 40 records is an example, the actual number will be equal to the first dimension of the corresponding parameters on the Key Data file.

The format of each GADS is shown below.

<b>Table 15.4.1.7.19-1 - Small Aperture Slit Function Parameters GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Length</b>	<b>Data Type</b>	<b>Dim.</b>
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 : Lorentzian part	-	4	fl	1
4	For voigt only : FWHM of Lorentzian 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.

The format of each ADSR is shown below.

<b>Table 15.4.1.7.20-1 - States of the Product ADSR</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Length</b>	<b>Data Type</b>	<b>Dim.</b>
1	Start time of the scan phase of the state	-	12	mjd	1
2	Flag indicating if MDS DSRs are attached to the current ADS DSR (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	$\frac{1}{16}$ s	2	us	1
8	Longest integration time	$\frac{1}{16}$ s	2	us	1
9	Number of clusters	-	2	us	1
10	Cluster Configuration	-	1088	Clcon	64
11	MDS 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 different Integration Time	-	128	us	64
17	Total Number of Fractional Polarisation Values	-	2	us	1
18	Number of DSRs	-	2	us	1
19	Length of DSR	-	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 64 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).

N	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 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).

N	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 in the constant and variable fraction GADSs before, may be constructed out of three newly calculated partial leakage current sets given here. These will be 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) ADSR					
N	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
11	PMD dark offset for all PMDs for the amplifier A and B (1A, 1B, 2A, etc ...)	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

The format of each ADSR is shown below.

Table 15.4.1.7.24-1 - Average of the Dark Measurements per State ADSR					
N	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

Table 15.4.1.7.24-1 - Average of the Dark Measurements per State ADSR					
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**

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

Table 15.4.1.7.25-1 - PPG/Etalon Parameters (newly calculated) ADSR					
N	Description	Units	Byte Length	Data Type	Dim.
1	Start time of the first 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
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**

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

Table 15.4.1.7.26-1 - Spectral Calibration Parameters (newly calculated) ADSR					
N	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 (yes, in the Monitoring MDS)	-	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 was not able to determine a set of coefficients for a certain detector array the corresponding wavelength calibration error shall be set to -1.

#### 15.4.1.7.27 Sun Reference Spectrum (newly calculated) ADS

For each solar measurement, the Sun Reference ADS has two records: the first record is the calibrated spectrum (NB only the ESM Diffuser mode is absolutely calibrated, the other modes carry rough approximations of the intensity), the second record is not calibrated for intensity (units are in BU).

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

N	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
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" may indicate various types of solar measurement; see the corresponding Sun Reference Spectrum GADS field 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	photons/ cm <sup>2</sup> *nm*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 is 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.

N	Description	Units	Byte Length	Data Type	Dim.
1	Start time of DSR	-	12	mjd	1
2	DSR length	-	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 Flags	-	*	uc	*
6	Red grass flag	-	*	uc	*
7	Sun Glint / Rainbow flags	-	*	uc	*
8	Geolocation	-	*	GeoN	*
9	Level 0 detector module data packet headers	-	*	LOHdr	*
10	Integrated PMD values	BUs	*	fl	*
11	Fractional polarisation values	-	*	PolV	*
12	Cluster data	-	**	**	**
	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.

#### 15.4.1.7.29 Limb MDS

This MDS contains measurement data acquired while the instrument is 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.

N	Description	Units	Byte Length	Data Type	Dim.
1	Start time of DSR	-	12	mjd	1
2	DSR length	-	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 Flags	-	*	uc	*
6	Red grass flag	-	*	uc	*
7	Sun Glint / Rainbow flags (all flags are set to zero if not used)	-	*	uc	*
8	Geolocation	-	*	GeoL	*
9	Level 0 detector module data packet headers	-	*	LOHdr	*
10	Integrated PMD values	BUs	*	fl	*
11	Fractional polarisation values	-	*	PolV	*
12	Cluster data	-	**	**	**
	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 7 a new type of Limb states will be available, a mesospheric mode that scans altitudes between 60 and 150 km. The measurements run instead of the "normal" Limb states for 30 orbits every month on two separate days.

The mesosphere observations are identified with:

state ID = 55

and

measurement category = 27.

**15.4.1.7.30 Occultation MDS**

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

Table 15.4.1.7.31-1 - Monitoring MDSR Format					
N	Description	Units	Byte Length	Data Type	Dim.
1	Start time of DSR	-	12	mjd	1
2	DSR length	-	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	*
7	Geolocation	-	*	GeoCal	*
8	Level 0 detector module data packet headers	-	*	L0Hdr	*
9	Cluster data	-	**	**	**
	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 product size varies depending on the instrument timeline. The estimate provided in R-35 is a maximum of 400 MB/product.

## 15.5 LEVEL 2 PRODUCTS

Since off-line processor version 5, also a level Fast Delivery product SCI\_OL\_\_2PN was introduced. This product is processed with the level 2 off-line processor version using level 1b NRT products as input; restituted Attitude files (AUX\_FRA) are not used for this processing chain.

### 15.5.1 SCIAMACHY Vertical Column Amounts Level 2 Product – SCI\_NL\_\_2P

This product has been discontinued in the operational processing chain since May 2006. For reference the information of the SCI\_NL\_\_2P product can be found in ANNEX 15.8.1.

### 15.5.2 SCIAMACHY Selected Vertical Column Amounts for Meteo Users Level 2 Product – SCI\_RV\_\_2P

This product has been discontinued in the operational processing chain since May 2006. For reference the information of the SCI\_RV\_\_2P product can be found in ANNEX 15.8.2.

### 15.5.3 SCIAMACHY Off-Line Level 2 Product – SCI\_OL\_\_2P

The Level 2 off-line product (SCI\_OL\_\_2P) contains retrieved trace gas vertical columns, profiles and other geophysical parameters including their corresponding errors, plus a number of additional diagnostics, quality flags and intermediate results.

Level 2 off-line products of SCIAMACHY measurements include data as indicated in the following list. It is proposed this list shall be exclusive - parameters specified here represent the maximum amount of information to be retrieved by the level 2 off-line processing. The number of trace gas constituents to be retrieved is related to the availability of processing power and the existence of appropriate reference cross sections. Starting from level 2 off-line version 5 (December 2009) a new processing chain, the Fast Delivery level 2 processing (SCI\_OL\_\_2PN) has been activated. This processing chain is based on the level 2 off-line processor using NRT level 1b products as input. The SCI\_OL\_\_2PN product contains as well nadir as limb products and has the same product format as SCI\_OL\_\_2P.



O <sub>3</sub> :	vertical column retrieved from optical absorption spectroscopy fitting in UV and visible wavelength range, using an AMF calculations by LIDORT. (O <sub>3</sub> profiles from limb observations for UV/visible wavelength range)
NO <sub>2</sub> :	same as O <sub>3</sub> , but only in the visible wavelength range
BrO:	same as O <sub>3</sub>
OCIO:	slant column retrieval
SO <sub>2</sub> :	two different SO <sub>2</sub> vertical columns are retrieved. The first column is calculated for anthropogenic pollution scenario (SO <sub>2</sub> profile with SO <sub>2</sub> peak in the boundary layer); the second one - for volcanic eruption scenario (SO <sub>2</sub> profile with SO <sub>2</sub> peak between 10 and 11 km)
HCHO:	same as BrO, but only for bio mass burning
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:	aerosol absorbing indicator algorithm (AAIA)
H <sub>2</sub> O:	vertical column retrieval by AMC-DOAS
N <sub>2</sub> O:	same as H <sub>2</sub> O
CO:	vertical column retrieved from IR absorption spectroscopy fitting
CO <sub>2</sub> :	same as H <sub>2</sub> O
CH <sub>4</sub> :	same as H <sub>2</sub> O

**15.5.3.1 Input Data**

Level 1B Off-line product plus auxiliary data.

**15.5.3.2 Auxiliary Data Used**

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

Table 15.5.3.2-1 - Auxiliary Data Files for SCIAMACHY Level 2 Processing	
Description	Auxiliary File ID
Initialization file	SCI_IN_AX
M-factor file	SCI_MF1_AX



ECMWF meteorological information	AUX_ECA_AX <sup>5</sup>
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### 15.5.3.3 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).
- ❑ Application of m-factor
- ❑ Generation of Off-line level 2 product files and related output.

### 15.5.3.4 Product Structure

The high level product structure is shown below:

<b>Table 15.5.3.4-1 – SCIAMACHY Off-line Level 2 Product Structure</b>
<b>MPH</b>
<b>SPH</b>
<b>Summary Quality ADS (SQADS)</b>
<b>Geolocation of the States ADS (LADS)</b>
<b>Static Parameter of the level2 off-line processor States of the Product ADS</b>
<b>Geolocation of the Nadir Ground Pixels ADS</b>
<b>Geolocation of the Limb/Occultation measurements ADS</b>
<b>Cloud and Aerosol MDS</b>
<b>Nadir Fitting Window Application MDSs (16 MDSs: 14 planned and 2 spare)</b>
<b>Limb Fitting Window Application MDSs (14 MDSs: 12 planned and 2 spare)</b>
<b>Occultation Fitting Window Application MDSs (14 MDSs: 12 planned and 2 spare)</b>
<b>Ozone Profiles from Nadir measurements MDS</b>
<b>Limb Clouds Data sets</b>

<sup>5</sup>Note that up to this Prod Spec 15\_L the AUX\_ECA\_AX file is not used for processing.



**15.5.3.5 Main Product Header**

The Main Product Header is described in Volume 5.

**15.5.3.6 Specific Product Header**

The SPH is an ASCII header which conforms to the ASCII conventions defined in Volume 5. The Ø symbol indicates the position of an ASCII blank space character.

**Table 15.5.3.6-1 – Specific Product Header of Off-line Level 2 Product**

N	Description	Units	Byte Length	Data Type	Dim.
1	<b>SPH_DESCRIPTOR=</b>	keyword	15	uc	15
	quotation mark (“	-	1	uc	1
	<b>SPH descriptor</b> (Set to “SCI_OL_2P00000000000000000000”)	-	28	uc	28
	quotation mark (“	-	1	uc	1
	newline character	terminator	1	uc	1
2	<b>STRIPLINE_CONTINUITY_INDICATOR=</b>	keyword	31	uc	31
	Value: +000 = No stripline continuity, the product is a complete segment Other: Stripline Counter	-	4	Ac	1
	Newline character	terminator	1	uc	1
3	<b>SLICE_POSITION=</b>	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	<b>NUM_SLICES=</b>	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
<i>Product Location Information</i>					
5	<b>START_TIME=</b>	keyword	11	uc	11
	quotation mark (“	-	1	uc	1
	<b>Start time of the measurement data in this product</b> UTC time of the first MDSR	utc	27	uc	27
	quotation mark (“	-	1	uc	1
	newline character	terminator	1	uc	1
6	<b>STOP_TIME=</b>	keyword	10	uc	10
	quotation mark (“	-	1	uc	1



Table 15.5.3.6-1 – Specific Product Header of Off-line Level 2 Product					
	<b>Time of the end of the measurement data in this product (last MDSR time)</b> UTC time of the last MDSR	utc	27	uc	27
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
7	<b>START_LAT=</b>	keyword	10	uc	10
	<b>Latitude of the satellite nadir at the START_TIME</b> WGS84 latitude, positive = North	1e-6 deg	11	AI	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
8	<b>START_LONG=</b>	keyword	11	uc	11
	<b>Longitude of the satellite nadir at the START_TIME</b> WGS84 longitude, positive = East, 0 = Greenwich	1e-6 deg	11	AI	1
	<10-6degE>	units	10	uc	10
	newline character	terminator	1	uc	1
9	<b>STOP_LAT=</b>	keyword	9	uc	9
	<b>Latitude of the satellite nadir at the STOP_TIME</b> WGS84 latitude, positive = North	1e-6 deg	11	AI	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
10	<b>STOP_LONG=</b>	keyword	10	uc	10
	<b>Longitude of the satellite nadir at the STOP_TIME</b> WGS84 longitude, positive = East, 0 = Greenwich	1e-6 deg	11	AI	1
	<10-6degE>	units	10	uc	10
	newline character	terminator	1	uc	1
11	<b>DECONT =</b>	keyword	7	uc	7
	quotation mark (“)	-	1	uc	1



Table 15.5.3.6-1 – Specific Product Header of Off-line Level 2 Product					
16-30	<p>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</p> <p>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 1 is spare.</p> <p>If a fitting window is not used, the string between quotation marks is filled by “EMPTY0000000000”</p> <p>52 uc each (18/14/20)</p>	-	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., 0325-0335; missing digits shall be written as blank spaces) If a fitting window is not used, the string between quotation marks is filled by “EMPTY0000000000”	variable	9	uc	9
	Blank Space character (Ø)	-	1	uc	1
	Acronym for the driving parameter of this fitting window (e.g., O300)	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., 0325-0335; 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., O300)	variable	20	uc	4
	quotation mark (“)	-	1	uc	1
	Newline character	terminator	1	uc	1

**Table 15.5.3.6-1 – Specific Product Header of Off-line Level 2 Product**

34-45	<p><b>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</b>                      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 "EMPTY0000000000"                      52 uc each (18/14/20)</p>	-	624	uc	624
46	<b>NO_OF_OCCL_FITTING_WINDOWS=</b>	keyword	27	uc	27
	<b>Number of occultation fitting windows</b> default value +000 if no occultation fitting windows.	-	4	Ac	4
	Newline character	terminator	1	uc	1
47	<b>OCC_FIT_WINDOW_PTH=</b>	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 "EMPTY0000000000"	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	<b>OCC_FIT_WINDOW_UV0=</b>	keyword	19	uc
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		<p><b>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</b>                      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</p>	-	624	uc



	quotation marks is filled by “EMPTY0000000000” 60 52 uc each (18/14/20)				
61	<b>Spare (blank characters (Ø))</b>	-	64	uc	64
	newline character	terminator	1	uc	1
<i>DSDs for Attached Data Sets</i>					
62	<i>DSD (A) for the SQ ADS</i>	-	280	dsd	1
63	<i>DSD (A) State Geolocation ADS (L ADS)</i>	-	280	dsd	1
64	<i>DSD (A) for the Static parameters</i>	-	280	dsd	1
65	<i>DSD (A) for the States of the Product ADS</i>	-	280	dsd	1
66	<i>DSD(A) for the Geolocation of the Nadir Ground Pixels ADS</i>	-	280	dsd	1
67	<i>DSD(A) for the Geolocation of the Limb/Occultation Measurements ADS 67</i>	-	280	dsd	1
68	<i>DSD (M) for the Clouds and Aerosol MDS</i>	-	280	dsd	1
69-84	<i>DSDs (M) for the Nadir Fitting Window Application MDSs (16 MDSs: 14 planned and 2spares; unused entries set to NOT USED as described in Volume 5)</i>	-	4480	dsd	14
85-98	<i>DSDs (M) for the Limb Fitting Window Application MDSs (14 MDSs: 12 planned and 1 spare; unused entries set to NOT USED as described in Volume 5) 96109</i>	-	3920	dsd	14
99-112	<i>DSDs (M) for the Occultation Fitting Window Application MDSs. (14 MDSs: 12planned and 1 spare; unused entries set to NOT USED as described in Volume 5)</i>	-	3920	dsd	14
113	<i>DSDs (M) for the Ozone Profiles from Nadir measurements MDS</i>	-	280	dsd	1
114	<i>DSDs (M) for the Limb Cloud measurements MDS</i>	-	280	dsd	1
<i>DSDs for reference files</i>					
115	<i>DSD (R) -Level 1B product from which this product is produced</i>	-	280	dsd	1
116	<i>DSD (R) -Level 2 Initialization file</i>	-	280	dsd	1
117	<i>DSD (R) -Atmospheric Climatologies Data file</i>	-	280	dsd	1
118	<i>DSD -Spare (279 blank space characters followed by 1 newline character)</i>	-	280	Dsd_sp	1
119	<i>DSD -Spare (279 blank space characters followed by 1 newline character)</i>	-	<b>280</b>	<b>Dsd sp</b>	<b>1</b>
	<b>size (in bytes)</b>	-	<b>19115</b>	-	-

The following ASCII strings are used to fill the DS\_NAME field in the DSDs (refer to Volume 5).

The number of 58 DSD records is derived from the fact that there are 5 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 Occultation and Ozone profiles from Nadir) one general MDS about clouds from Limb, 4

reference DSD for the input files and one spare record.

<b>Table 15.5.3.6-2 – DS_NAME Field Strings</b>	
<b>DSD</b>	<b>DS_NAME</b>
<i>DSD (A) -SQ ADS</i>	SUMMARY_QUALITY
<i>DSD (A) -State Geolocation ADS (L ADS)</i>	STATE_GEOLOCATION
<i>DSD (A) -Static Parameters</i>	STATIC_PARAM
<i>DSD (A) -States of the Product ADS</i>	STATES
<i>DSD (A) -Geolocation of the Nadir Ground Pixels ADS</i>	GEOLOCATION_NADIR
<i>DSD (A) -Geolocation of the Limb/Occultation Measurements ADS</i>	GEOLOCATION_LIMB
<i>DSD (M) -Clouds and Aerosol MDS</i>	CLOUDS_AEROSOL
<i>DSD (M) -Nadir Fitting Window Application MDS #1</i>	NAD_UV0_O3
<i>DSD (M) -Nadir Fitting Window Application MDS #2</i>	NAD_UV1_NO2
<i>DSD (M) -Nadir Fitting Window Application MDS #3</i>	NAD_UV2_O3
<i>DSD (M) -Nadir Fitting Window Application MDS #4</i>	NAD_UV3_BRO
<i>DSD (M) -Nadir Fitting Window Application MDS #5</i>	NAD_UV4_H2CO
<i>DSD (M) -Nadir Fitting Window Application MDS #6</i>	NAD_UV5_SO2
<i>DSD (M) -Nadir Fitting Window Application MDS #7</i>	NAD_UV6_OCLO
<i>DSD (M) -Nadir Fitting Window Application MDS #8</i>	NAD_UV7_SO2
<i>DSD (M) -Nadir Fitting Window Application MDS #9</i>	NAD_UV8_H2O
<i>DSD (M) -Nadir Fitting Window Application MDS #10</i>	NAD_UV9_SPARE
<i>DSD (M) -Nadir Fitting Window Application MDS #11</i>	NAD_IR0_H2O
<i>DSD (M) -Nadir Fitting Window Application MDS #12</i>	NAD_IR1_CH4
<i>DSD (M) -Nadir Fitting Window Application MDS #13</i>	NAD_IR2_N2O
<i>DSD (M) -Nadir Fitting Window Application MDS #14</i>	NAD_IR3_CO
<i>DSD (M) -Nadir Fitting Window Application MDS #15</i>	NAD_IR4_CO2
<i>DSD (M) -Nadir Fitting Window Application MDS #16</i>	NAD_IR5_SPARE
<i>DSD (M) -Limb Fitting Window Application MDS #1</i>	LIM_PTH
<i>DSD (M) -Limb Fitting Window Application MDS #2</i>	LIM_UV0_O3
<i>DSD (M) -Limb Fitting Window Application MDS #3</i>	LIM_UV1_NO2
<i>DSD (M) -Limb Fitting Window Application MDS #4</i>	LIM_UV2_O3
<i>DSD (M) -Limb Fitting Window Application MDS #5</i>	LIM_UV3_BRO
<i>DSD (M) -Limb Fitting Window Application MDS #6</i>	LIM_UV4_H2CO
<i>DSD (M) -Limb Fitting Window Application MDS #7</i>	LIM_UV5_SO2
<i>DSD (M) -Limb Fitting Window Application MDS #8</i>	LIM_UV6_OCLO
<i>DSD (M) -Limb Fitting Window Application MDS #9</i>	LIM_UV7_SPARE
<i>DSD (M) -Limb Fitting Window Application MDS #10</i>	LIM_IR0_H2O
<i>DSD (M) -Limb Fitting Window Application MDS #11</i>	LIM_IR1_CH4
<i>DSD (M) -Limb Fitting Window Application MDS #12</i>	LIM_IR2_N2O
<i>DSD (M) -Limb Fitting Window Application MDS #13</i>	LIM_IR3_CO
<i>DSD (M) -Limb Fitting Window Application MDS #14</i>	LIM_IR4_SPARE

<b>Table 15.5.3.6-2 – DS_NAME Field Strings</b>	
<i>DSD (M) -Occultation Fitting Window Application MDS #1</i>	OCC_PTH
<i>DSD (M) -Occultation Fitting Window Application MDS #2</i>	OCC_UV0_O3
<i>DSD (M) -Occultation Fitting Window Application MDS #3</i>	OCC_UV1_NO2
<i>DSD (M) -Occultation Fitting Window Application MDS #4</i>	OCC_UV2_O3
<i>DSD (M) -Occultation Fitting Window Application MDS #5</i>	OCC_UV3_BRO
<i>DSD (M) -Occultation Fitting Window Application MDS #6</i>	OCC_UV4_H2CO
<i>DSD (M) -Occultation Fitting Window Application MDS #7</i>	OCC_UV5_SO2
<i>DSD (M) -Occultation Fitting Window Application MDS #8</i>	OCC_UV6_OCLO
<i>DSD (M) -Occultation Fitting Window Application MDS #9</i>	OCC_UV7_SPARE
<i>DSD (M) -Occultation Fitting Window Application MDS #10</i>	OCC_IR0_H2O
<i>DSD (M) -Occultation Fitting Window Application MDS #11</i>	OCC_IR1_CH4
<i>DSD (M) -Occultation Fitting Window Application MDS #12</i>	OCC_IR2_N2O
<i>DSD (M) -Occultation Fitting Window Application MDS #13</i>	OCC_IR3_CO
<i>DSD (M) -Occultation Fitting Window Application MDS #14</i>	OCC_IR4_SPARE
<i>DSD (M) -Ozone Profiles from Nadir measurements MDS</i>	NAD_PROFILE_O3
<i>DSD (M) – Limb Cloud measurements MDS</i>	LIM_CLOUDS
<i>DSD (R) -Level 1B product from which this product is produced</i>	LEVEL_1B_PRODUCT
<i>DSD (R) -Level 2 Initialization file</i>	INITIALISATION_FILE
<i>DSD (R) -Atmospheric Climatologies Data file</i>	ECMWF_FILE
<i>DSD (R) –M-factor Data file</i>	M_FACTOR_FILE
<i>DSD spare</i>	SPARE

### 15.5.3.7 Data Sets

The following sub-sections describe the individual data sets which together form the Off-line 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.

#### 15.5.3.7.1 Summary Quality ADS

The SQ 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 shall be as follows:

<b>Table 15.5.3.7.1-1 - SQ ADSR Format</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	<b>Start time of the scan phase of the state</b>	-	12	mjd	1

Table 15.5.3.7.1-1 - SQ ADSR Format					
2	Attachment Flag (1 = no MDSRs attached to the current ADSR, 0 otherwise)	-	1	uc	1
3	Error on cloud parameters <sup>a</sup>	-	2	uc	2
4	Aerosol parameter diagnostic <sup>a</sup>	-	2	uc	2
5	Quality of the driving geophysical parameter in each fitting window <sup>a b</sup>	-	44	uc	44
6	RMS of the retrieval algorithm <sup>a b</sup>	-	44	uc	44
7	$\chi^2$ of the retrieval algorithm <sup>a b</sup>	-	44	uc	44
8	Goodness of fit of the retrieval algorithm <sup>a b</sup>	-	44	uc	44
Size:			193		

a. The quality flags are specified as unsigned bytes having a range from value 0 to 10. '0' 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 which are not existing in the data due to a smaller number of trace gas data sets shall be 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 will be set to '0'.

#### 15.5.3.7.2 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 15.5.3.7.2-1 - Geolocation ADSR					
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			45		

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

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



Table 15.5.3.7.3-1 - 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 (the present size is an estimation)	-	Variable (60000)	uc	1
<i>Size</i>			<b>Variable</b>		

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

#### 15.5.3.7.4 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 15.5.3.7.4-1 - States of the Product ADSR					
N	Description	Units	Byte Size	Data Type	Dim.
1	<b>Start Time of DSR</b>	-	12	MJD	1
2	<b>Attachment Flag</b> (1 = no MDSRs attached to the current ADSR, 0 otherwise)	-	1	uc	1
3	<b>State ID</b>	-	2	us	1
4	<b>Duration of scan phase of the state</b>	1/16 s	2	us	1
5	<b>Longest integration time</b>	1/16 s	2	us	1
6	<b>Shortest integration time</b>	1/16 s	2	us	1
7	<b>Number of geolocation records for this state</b>	-	2	us	1
<i>Size:</i>			<b>23</b>		

#### 15.5.3.7.5 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 the case where 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 timestamped to allow cross-reference to the MDSRs. The format of each ADSR is defined below.

Table 15.5.3.7.5-1 - Geolocation of the Nadir Ground Pixels ADSR

N	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
8b	Sub-Satellite point at the middle of the integration time		8	Coord	1
9	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 first in flight direction and the fourth the last in time and flight direction)	-	32	Coord	4
10	Centre coordinate of the nadir ground pixel	-	8	Coord	1
Size:			107		

#### 15.5.3.7.6 Geolocation of the Limb/Occultation measurements ADS

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

Table 15.5.3.7.6-1 - Geolocation of the Limb/Occultation measurements ADSR

N	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

Table 15.5.3.7.6-1 - Geolocation of the Limb/Occultation measurements ADSR					
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	cm	12	ul	1
Size:			103		

#### 15.5.3.7.7 Clouds and Aerosol MDS

The Clouds and Aerosols MDS contains several MDSRs. The format of each MDSR is described below.

Table 15.5.3.7.7-1 - Clouds and Aerosol MDSR Format					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start Time of DSR	-	12	mjd	1
1b	Data set record length (required because this record may have a variable record length)	-	4	ul	1
2	Quality indicator (-1 if empty DSR)	-	1	sc	1
3	Integration time for this DSR	1/16 s	2	us	1
3b	Surface Pressure	hPa	4	fl	1
4	Cloud fraction	-	4	fl	1
5	Error on cloud fraction	rel. fraction	4	fl	1
6	Number of PMD sub-pixels for this DSR	-	2	us	1
7	Number of PMD sub-pixels determined to be totally cloudy or totally cloud-free	-	4	us	2
8	Cloud-top height	km	4	fl	1
9	Error on cloud-top height (currently set to -99.99), see product disclaimer	rel. fraction	4	fl	1
10	Cloud optical depth	km	4	fl	1
11	Error on cloud optical depth (currently set to -99.99), see product disclaimer	rel. fraction	4	fl	1
12	Cloud type <sup>a</sup>	flags	2	us	1

Table 15.5.3.7.7-1 - Clouds and Aerosol MDSR Format					
13	Cloud-top bi-directional reflectance	-	4	fl	1
14	Error on cloud-top bi-directional reflectance	rel. fraction	4	fl	1
15	Effective Lambertian surface reflectance	-	4	fl	1
16	Error on effective Lambertian surface reflectance	rel. fraction	4	fl	1
17	Flags describing the cloud parameter output <sup>b</sup>	flags	2	us	1
18	Absorbing aerosol indicator	-	4	fl	1
19	Aerosol indicator diagnostic	-	4	fl	1
20	Flag describing the aerosol indicator output <sup>b</sup>	flags	2	us	1
21	Number of additional aerosol parameters (na)	-	2	us	1
22	Additional aerosol parameters <sup>c</sup>	-	4*Na	fl	2
Size:			Variable		

a. The flags describing the cloud type have to be interpreted bit-wise. The bit numbering convention is defined in Prod Spec Annex Volume A. 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 by bits. The bit numbering convention is defined in Volume A. They contain information reflecting some important settings in the initialisation file:

- bit 0: value 0 = source of cloud fraction fitting, 1= source of cloud fraction PMD
- bit 1: value 0 = source of cloud-top pressure ISCCP, 1 = source of cloud-top pressure fitting :

SACURA

- bit 2: if bit set, 1 = SACURA: full convergent
- bit 3: if bit set, 1 = number of iterations exceeded, average of neighbored 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.

**constraints are provided in disclaimer**

c. The definition of aerosol components is (when the bit is set the underlined condition is true, bits are counted from 0 to 15):

- bit 0: no-yes Rayleigh scattering correction successful
- bit 1: no-yes AAIA computation successfully ended
- bit 2-15: not used

### 15.5.3.7.8 Nadir Fitting Window Application MDSs

There are up to 14 Nadir Fitting Window Application MDSs used in a product (one MDS per fitting window). The contents of each MDS is identified in the SPH. Each MDS contains several MDSRs. All MDSRs for all MDSs share a common format which is defined below:

Table 15.5.3.7.8-1 - Nadir Fitting Window Application MDSR Format					
N	Description	Units	Byte Size	Data Type	Dim.
1	<b>Start Time of DSR</b>	-	12	mjd	1
1b	<b>DSR length</b> (required because this record may have a variable length)	-	4	ul	1
2	<b>Quality indicator</b> (-1 if empty DSR)	-	1	sc	1
3	<b>Integration time for this DSR</b>	1/16 s	2	us	1
3b	<b>Number of vertical column densities (nvcd)</b> <sup>d</sup>	-	2	us	1
4	<b>Vertical column density (VCD) of main parameter value</b>	mol/cm2	nvcd*4	fl	1
5	<b>Error on the VCD above</b>	rel. fraction	nvcd*4	fl	1
6	<b>Flag describing the VCD data above</b> <sup>a</sup>	flags	2	us	1
6b	<b>Effective slant column (ESC) density of the main parameter</b>	mol/cm2	4	fl	1
6c	<b>Error on the effective slant column density above</b>	rel. fraction	4	fl	1
7	<b>Number of linear and non-linear fitted parameters (2 values: [ n1 ], [ n2 ])</b> <sup>e</sup>	-	4	us	2
8	<b>Linear fitted parameters</b> <sup>e</sup>	-	4 * n1	fl	n1
9	<b>Error on linear fitted parameters</b> <sup>e</sup>	rel. fraction	4 * n1	fl	n1
10	<b>Cross-correlation matrix entries of the linear fit</b> <sup>e</sup>	-	2 * n1 * (n1-1)	fl	n1 * (n1-1) / 2
11	<b>Non-linear fitted parameters</b> <sup>e</sup>	-	4 * n2	fl	n2
12	<b>Error on non-linear fitted parameters</b> <sup>e</sup>	rel. fraction	4 * n2	fl	n2
13	<b>Cross-correlation entries of the non-linear fit</b>	-	2 * n2 * (n2-1)	fl	n2 * (n2-1) / 2
14	<b>RMS of fit for the fitting window</b>	-	4	fl	1
14 b	$\chi^2$ of the fit	-	4	fl	1
14 c	<b>Goodness of the fit</b>	-	4	fl	1
15	<b>Iteration number for the fitting window</b>	-	2	us	1
16	<b>Flag describing the above data for linear and non-linear fit</b> <sup>b</sup>	flags	2	us	1
17	<b>AMF to ground for species</b>	-	4	fl	1
18	<b>Error on AMF to ground</b>	rel. fraction	4	fl	1
19	<b>AMF to cloud-top for species</b>	-	4	fl	1
20	<b>Error on AMF to cloud-top</b>	rel. fraction	4	fl	1
21	<b>Flag describing the AMF data above</b> <sup>c</sup>	flags	2	us	1

Table 15.5.3.7.8-1 - Nadir Fitting Window Application MDSR Format					
22	Temperature of reference spectrum	K	4	fl	1
Size:			var.		

a. The flags describing the VCD calculation have to be interpreted by bits. The bit numbering convention is defined in Prod Spec Annex Volume A (when the bit is set the underlined condition is true, bits are counted from 0 to 15) Bits 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) flag 2 is set 'true', all others 'false'.

For IAS in principle all 16 bit are used:

- 0: no - yes convergence reached
- 1: no - yes sza lower than limit (currently 80°)
- 2: no - yes residual norm lower than limit (currently 4)
- 3: no - yes maximum absolute value of residual lower than limit (currently 2)
- 4: no - yes error weighting used
- 5: no - yes ratioed measurements used
- 6-11:  $\alpha$  between bounds and  $|\alpha_{err}| < \text{limit}$ , a pair of flags for each gas ( $\alpha_{err}$  currently 0.5)

b. Specifies the slant column density fitting The flags have to be interpreted by bits. The bit numbering convention is defined in Volume A (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, 7 highest quality
- 12-15: not used at present

c. The flags describing the AMF look-up scheme have to be interpreted by bits. The bit numbering convention is defined in Volume A (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 allows the output of more than one VCD result per record. This feature is used for NAD\_UV7\_H2O and NAD\_IR3\_CO, and has the following effect on Fields 5 and 6:

- For H2O [S12] fields 5 and 6 consist of two entries. The first entry of field 5 gives the VCD in molecules/cm<sup>2</sup>, the second in g/cm<sup>2</sup>. The latter unit is more convenient in the meteorological community. Field 6 contains for both entries the absolute error in g/cm<sup>2</sup>.
- For CO fields 5 and 6 consist of two entries. The first entry contains xCO, the second VCDCO (this is only valid if the first gas in the initialization file is CO and the second gas is CH<sub>4</sub>).

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 7/8, 9/10 and 11/12 require some special treatment for IAS.

- Field 7 will contain the number of linear fit parameters, which is currently 1,
- Field 8 will be 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 9 and 10 show value and error of the reflectance in the IAS case.
- Fields 11 and 12 have currently five entries each, containing the values and errors of the scaling factors of gases (i.e.  $\alpha_{CO}$ ,  $\alpha_{CH_4}$ ,  $\alpha_{H_2O}$ ) and HWHM. The last entry of Field 11 and 12 is empty (i.e. filled with 0), because value and error of the linear fit parameter are already given in Field 9 and 10, 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 to obtain a VCD of water vapor directly, omitting an intermediate step of SCD calculation. That is why fields 6b and 6c (SCD and its error) are empty for NAD\_UV7\_H2O. Since the fitting procedure in the AMC-DOAS algorithm is non-linear, the parameters of linear fitting (fields 8-10) are absent. In the field 17 instead of AMF (to ground) the parameter a (the AMF correction factor) computed by the AMC-DOAS algorithm [S12] is listed, and in the field 18 its error. Fields 19 and 20 are left empty as well, because no AMF to cloud-top is calculated in the AMC-DOAS algorithm. All errors for AMC-DOAS (fields 5, 12, 18) are absolute values.

#### 15.5.3.7.9 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 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 contents of each MDS is identified in the SPH. All MDSRs for all MDSs share a common format which is defined

below:

N	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	n <sub>main</sub> (30)
11 c	Tangent layer pressure at the lower layer boundary	hPa	(120)	fl	n <sub>main</sub> (30)
11 d	Tangent layer temperature (mean)	K	(120)	fl	n <sub>main</sub> (300)
11 e	Main species which have been fitted on the coarse forward model grid	-	(960)	Layer Rec.	n <sub>main</sub> *n1 (60)
11f	Scaled profiles which have been used for the fit on the coarse forward model grid	-	(960)	Layer Rec.	n <sub>main</sub> *n4 (60)
11 g	Mesurement Grid	-	(429)	Meas-Grid	n <sub>meas</sub> (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)	-	m <sub>f</sub>	fl	m <sub>f</sub>



Table 15.5.3.7.9-1 - Limb Fitting Window Application MDSR Format					
16	RMS of the fit		4	fl	1
17	$\chi^2$ of the fit	-	4	fl	1
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	Convergency 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
26	Additional diagnostics	-	4*n <sub>ad</sub> (0)	fl	n <sub>ad</sub>
Size:			var.		

Data types are described here below:

Table 15.5.3.7.9-2 - Limb Profile Layer Record structure					
N	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/cm <sup>2</sup>	4	fl	4
4	Error on the vertical column density above lower layer boundary	%	4	fl	4
Size:			16		

Table 15.5.3.7.9-3 - Measurement Grid Record structure					
N	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:			33		

Table 15.5.3.7.9-4 - State Vector structure

N	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
<i>Size:</i>			12		

**15.5.3.7.10 Limb Clouds MDSs**

This component is of variable record length. The actual length is given in the DSRLLEN field (the second field).

Table 15.5.3.7.10-1 - Limb Clouds Data Set MDSR Format

N	Description	Units	Byte Size	Data Type	Dim.
1	<b>Start time of the limb clouds record</b>	-	12	mjd	1
2	<b>Data set record length</b> (required because this record may have a variable record length)	-	4	ul	1
3	<b>Quality indicator</b> (-1 if empty DSR)	-	1	sc	1
4	<b>Integration time for this DSRs</b>	-	2	us	1
5	<b>Diagnostics of the cloud detection algorithm, details see below</b>	-	1	b	1
6	<b>Flag for normal water clouds</b>	-	1	uc	1
7	<b>Maximum value of CIR for normal water clouds</b>	-	4	fl	1
8	<b>Height of maximum value of CIR for normal water clouds</b>	Km	4	fl	1
9	<b>Flag for normal water clouds</b>	-	1	uc	1
10	<b>Flag for ice clouds</b>	-	1	uc	1
11	<b>Maximum value of CIR for ice clouds</b>	-	4	fl	1
12	<b>Height of maximum value of CIR for normal water clouds</b>	Km	4	fl	1
13	<b>Height index of maximum value of CIR for ice clouds</b>	-	1	uc	1
14	<b>Flag for polar stratospheric clouds</b>	-	1	uc	1
15	<b>Maximum value of CIR for polar stratospheric clouds</b>	-	4	fl	1
16	<b>Height of maximum value of CIR for polar stratospheric clouds</b>	Km	4	fl	1
17	<b>Height index of maximum value of CIR for ice clouds</b>	-	1	uc	1
18	<b>Flag for noctilucent clouds</b>	-	1	uc	1
19	<b>not used at present</b>	-	4	fl	1
20	<b>Maximum height of strictly monotonically increasing</b>	Km	4	fl	1
21	<b>Maximum height index of strictly monotonically</b>	-	1	uc	1

Table 15.5.3.7.10-1 - Limb Clouds Data Set MDSR Format					
	<b>increasing radiances for noctilucent clouds</b>				
22	<b>Number of tangent heights for CIR (m1)</b>	-	2	us	1
23	<b>Tangent heights for CIR</b>	Km	0	fl	m1(0)
24	<b>Number of CIR (m2)</b>	-	2	us	1
25	<b>CIR (m = m1 * m2)</b>	-	0	fl	m(0)
26	<b>Number of additional limb cloud parameters (n)</b>	-	2	us	1
27	<b>Additional limb cloud parameters</b>	-	0	fl	n(0)
<i>Size:</i>		<b>var.</b>	66		

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.

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 color 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 will be 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 15) is 0. Further parameters might be added in future versions.

The number of records is depending on the number of limb states and the number of columns per limb state. The number of 100 records is just a realistic estimation for a standard orbit and 4 columns per limb state.

**15.5.3.7.11 Occultation Fitting Window Application MDSs**

There are up to 14 Occultation Fitting Window Application MDSs used in a product (one MDS per fitting window). The contents of each MDS is identified in the SPH. All MDSRs for all MDSs share a common format which is the same as the Limb Fitting Window Application MDS format.

**15.5.3.7.12 Ozone profiles from Nadir measurements MDS**

Most of fields of the MDSR format are still TBD. Consequently, the DSD (in the SPH) which describes this MDS has to be set to 'NOT USED'. This MDS will be used in the product after complete definition of the MDSR format and of the related algorithms. The following table provides a preliminary definition of MDSR format:

Table 15.5.3.7.12-1 - Ozone Profiles from Nadir measurements MDSR Format					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start Time of DSR	-	12	mjd	1
2	Quality indicator (-1 if empty DSR)	-	1	sc	1
3	Integration time for this DSR	1/16 s	2	us	1
...	Next fields TBD	-	TBD	TBD	TBD
Size:			TBD		

**15.5.3.8 Size Estimate**

The size of level-2 off-line product containing is approximately 30.8 MBytes for a scenario which corresponds to 60 states including 30 limb states, zero occultation states, and to 1250 single observations for nadir and limb states respectively:

MPH: 1247 bytes

SPH: 19115 bytes

SQADS: 60 states \* 193 bytes / state = 11580 bytes

State Geolocation: 60 states \* 45 bytes / state = 2700 bytes

Static Parameter GADS: 60000 bytes

States of the product ADS: 60 states \* 23 bytes / state = 1380 bytes



Nadir Geolocation ADS:  $3600 \text{ observations} * 107 \text{ bytes / obs.} = 385200 \text{ bytes}$   
Limb Geolocation ADS:  $2625 \text{ limb states} * 103 \text{ bytes / state} = 270375 \text{ bytes}$   
Clouds & Aerosols MDS:  $3600 \text{ observations} * 96 \text{ bytes / obs.} = 345600 \text{ bytes}$   
Nadir Fit. Win. Appl. MDSs:  $3600 \text{ observations} * 157 \text{ bytes / obs.} * 10 \text{ MDS used} = 5652000 \text{ bytes (1)}$   
Limb Fit. Win. Appl. MDSs:  $750 \text{ observations} * 33323 \text{ bytes / obs.} = 24872250 \text{ bytes (1)}$   
Limb Clouds MDSs:  $100 \text{ observations} * 66 \text{ bytes / obs.} = 6600 \text{ bytes (1)}$   
Occultation Fit. Win. Appl. MDSs: not yet used = 0 bytes (1)  
Total product size estimation: 31748047 bytes (1)

1. DSR size corresponds to typical size derived from example in note attached to the table describing the MDSR format

1. As the product size estimation is based on assumptions the product size value of 30.8 MBytes will be revised.



## 15.6 AUXILIARY DATA FILES

The following sub-sections describe the Auxiliary Data Files used in SCIAMACHY processing<sup>6</sup>. Information is extracted from R-35 and R-36.

### 15.6.1 Leakage Current Parameters

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 in orbit. Therefore, the calculation of these parameters require an orbit phase field for annotation and the application needs them for selection of appropriate parameters. The parameters are divided into a constant fraction of the leakage current and a fraction being variable with orbit phase. The calculation of leakage current parameters requires a certain set of dark calibration measurement states as well as the last measurements of the limb states and the orbit phase of the corresponding measurements.

FILE ID: SCI\_LK1\_AX

TYPE: Auxiliary

USE: Level 1B processing

UPDATED: Approximately one leakage current parameter set per orbit is envisaged.

SIZE: MPH(1247 bytes) + SPH(658 bytes) + GADS(approx. 254 kBytes) = approx. 256 kBytes

#### 15.6.1.1 Format

The high level breakdown of the file is shown below

**Table 15.6.1.1-1 - Schematic Structure of the Leakage Current Parameters**

<b>MPH</b>
<b>SPH -standard Auxiliary Data SPH as described in Volume 16 with 2 DSDs:</b>
<i>DSD for the Constant Fraction GADS</i>
<i>DSD for the Variable Fraction GADS</i>
<b>Constant Fraction GADS</b>
<b>Variable Fraction GADS</b>

<sup>6</sup> The current initialisation file of SGP\_12OL, version 5.01, does not use the data base 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 to use them again. Their description is available in the IODD (SCIAMACHY\_L2\_OFI\_IODD\_v5\_ENV-ID-DLR-SCI-2200-4).

### 15.6.1.1.1 Constant Fraction GADS

The format of the Constant Fraction GADS is described below:

<b>Table 15.6.1.1.1-1 - Leakage Current Parameters (constant fraction) GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Length</b>	<b>Data Type</b>	<b>Dim.</b>
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 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 the constant fraction of the PMD offset	BU	56	fl	14
7	Mean noise (mean value of standard deviations per detector element) per detector element	BU	32768	fl	8192
	size (in bytes)	-	163952	-	-

### 15.6.1.1.2 Variable Fraction GADS

This GADS contains 12 GADSRs, one for each SZA region. The format of the GADSR is shown below:

<b>Table 15.6.1.1.2-1 - Leakage Current Parameters (variable fraction) GADSR</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Length</b>	<b>Data Type</b>	<b>Dim.</b>
1	Orbit phase after eclipse (range: 0-1)	-	4	fl	1
2	OBM (near radiator), detector (channels 6 to 8) and PMD temperatures	K	40	fl	10
3	Variable fraction of the leakage current on top of the constant fraction (field 1 and 3) for channels 6 to 8	BU/s	12288	fl	3072
4	Error of variable fraction of LC	BU/s	12288	fl	3072
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/s	28	fl	7
8	Error on straylight offset for PMDs	BU/s	28	fl	7



9	Variable fraction of the PMD dark offset on top of the constant fraction for PMD 5 and 6	BU	8	fl	2
10	Error on the variable fraction of PMD offset	BU	8	fl	2
	size (in bytes)	-	90228	-	-

### 15.6.2 PPG/Etalon Parameters

This file contains the PPG/Etalon correction parameters for SCIAMACHY level 0 to 1B processing.

The PPG/Etalon parameters are not expected to be depended on the position in 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 starting from level 1b baseline for IPF 7

SIZE: MPH(1247 bytes) + SPH(378 bytes) + GADS(139 kBytes) = approx. 140.9 kBytes

#### 15.6.2.1 Format

The high level structure of the file is shown below.

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

<b>MPH</b>
<b>SPH -ENVISAT Auxiliary Data format (as described in Volume 16) with 1 DSD:</b> <i>DSD for the PPG/Etalon Parameters GADS</i>
<b>PPG/ Etalon Parameters GADS</b>

#### 15.6.2.1.1 PPG/Etalon Parameters GADS

The format of the GADS is shown below.

<b>Table 15.6.2.1.1-1 - PPG/Etalon Parameters GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Length</b>	<b>Data Type</b>	<b>Dim.</b>
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 Maska	-	8192	uc	8192
	size (in bytes)	-	139264	-	-

a. The bad pixel mask will indicate 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.

### 15.6.3 Spectral Calibration Parameters

The spectral calibration parameters are expected to be dependent on the position in orbit. Therefore, the calculation of these parameters require 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

SIZE: MPH(1247 bytes) + SPH(658 bytes) + GADS(33140 bytes) = 35.045 kbytes

#### 15.6.3.1 Format

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

**Table 15.6.3.1-1 - Schematic Structure of the Spectral Calibration Parameters**

<b>MPH</b>
<b>SPH -Auxiliary Data SPH format (defined in Volume 16) with 2 DSD:</b>
<i>DSD for the Precise Basis of the Spectral Parameters GADS</i>
<i>DSD for the Spectral Parameters GADS</i>
<b>Precise Basis of the Spectral Parameters GADS</b>
<b>Spectral Parameters GADS</b>

##### 15.6.3.1.1 Precise Basis of Spectral Calibration Parameters GADS

This GADS contains several GADSRs of the format shown below.

N	Description	Units	Byte Length	Data Type	Dim.
1	<b>Wavelength of detector pixel</b>	-	32768	fl	8192
	<b>size (in bytes)</b>	-	<b>32768</b>	-	-

##### 15.6.3.1.2 Spectral Calibration Parameters GADS

This GADS contains several GADSRs of the format shown below.



Table 15.6.3.1.2-1 - Spectral Calibration Parameters GADSR					
N	Description	Units	Byte Length	Data Type	Dim.
1	<b>Orbit phase after eclipse</b> (range: the absolute value is between 0 and 1)	-	4	fl	1
2	<b>Coefficients in the 4th order polynomial for each detector array</b>	-	320	do	40
3	<b>Number of used lines per channel</b>	-	16	us	8
4	<b>Wavelength calibration error per channel</b>	-	32	fl	8
	<b>size (in bytes)</b>	-	<b>372</b>	-	-

#### 15.6.4 Sun Reference Spectrum

This file contains the sun reference spectrum of the SCIAMACHY level 0 to 1B processing.

The sun reference spectrum will be measured once per day and is valid for this period. The corresponding spectral calibration parameters and the radiance sensitivity included in this file allow the calculation of a complete solar irradiance spectrum for this day. The sun reference spectrum requires one sun diffuser measurement state.

FILE ID: SCI\_SU1\_AX

TYPE: Auxiliary

USE: Level 1B processing

UPDATED: one sun reference spectrum file per day

SIZE: MPH(1247 bytes) + SPH(378 bytes) + GADSs(approx. 164 kBytes) = approx. 165.6 kBytes

##### 15.6.4.1 Format

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

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

<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 1 DSD:</b>
<i>DSD for the Sun Reference GADS</i>
<b>Sun Reference GADS</b>

##### 15.6.4.1.1 Sun Reference Spectrum GADS

The format of the GADS is shown below.

Table 15.6.4.1.1-1 - Sun Reference Spectrum GADS					
N	Description	Units	Byte Length	Data Type	Dim.
1	Sun spectrum identifier (“Dn” for sun diffuser, “OØ” for occultation, “SØ” for subsolar ; “n” may indicate various diffuser angles)	-	2	uc	2
2	Wavelength of the sun measurement	nm	32768	fl	8192
3	Mean sun reference spectrum	photons/ cm <sup>2</sup> * nm * 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	-	-

Only one set of spectral calibration parameter in the Spectral Calibration Parameters GADS is valid for the Sun Reference Spectrum GADS. The correct choice is indicated by the “Index to spectral calibration parameters” field.

### 15.6.5 Key Data (Instrument Characterization) File

Key Data file for SCIAMACHY level 0 to 1B processing.

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

The Key data file core name is given by SCI\_KD1\_\_AX following the convention of the ENVISAT ground segment. The core name is followed by the generation time, and by the start and stop validity times.

FILE ID: SCI\_KD1\_\_AX  
 TYPE: Auxiliary  
 USE: Level 1B processing  
 UPDATED: Infrequently



SIZE: Estimated at 50 MB in R-35

### 15.6.5.1 Format

The format of the file will consist of an MPH, and Auxiliary Data SPH (as described in Volume 16) with several DSDs pointing to several GADSs. The GADSs will contain ASCII format information as defined in the SCIAMACHY Level 1B IODD (R-35).

For the time being 39 key data parameters are assembled into one Keydata file. The DS\_NAME field of the DSDs will be set according to the content of the corresponding MDS. The following keywords are present (not necessarily in this order):

N	DS_NAME	Description	Units	Di m.
1	BRDF_s	Bi-directional reflection distribution function measured with s-polarisation detector(ac_ucs / FOV)	Sr <sup>-1</sup>	3
2	BRDF_p	Bi-directional reflection distribution function measured with p-polarisation detector (ac_ucp / FOV)	Sr <sup>-1</sup>	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	-	3

N	DS_NAME	Description	Units	Di m.
		scanner calibration with s-polarisation detector (alauls)		
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
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.cm <sup>3</sup> )	1
31	ABS_IRR		(BU/s) / (W/cm <sup>3</sup> )	1
32	NDF		-	1
33	NDF_s_p		-	1
34	MEM_EFFECT_COEF		-	2
35	PMD_CROSS_COEF		-	1
36	BAD_PIXEL_MASK		-	1
37	REF_WLS		(BU/s)	1
38	FRAUNH_LINE		Nm	2
39	NON_LIN		-	2

### 15.6.6 m-Factor File

The m-factor file are an extension to the characterisation database of SCIAMACHY to describe the degradation of the instrument during flight.

FILE ID: SCI\_MF1\_AX

TYPE: Auxiliary

USE: Level 1B processing until version level 1b IPF 6.05, for IPF 7.02 m-

factor usage in Level 1B processing is deactivated, instead it is used for Level 2 Off-line processing for processor version 5.01

UPDATED: none, until IPF 6.05. Since level 2 off-line processor 5.01 m-factors are updated daily and delivered by IFE-Bremen.

SIZE: Estimated at 1 Mbytes in R-35.

#### 15.6.6.1 Format

The format of the file will consist of an MPH, and Auxiliary Data SPH (as described in Volume 16) with several DSDs pointing to several GADSs. The GADS will contain ASCII format information as defined in the SCIAMACHY Level 1B IOOD (R-35).

For the time being 10 m-factor parameters in the same number of m-factor files are expected by the SOS team [R10]. The DS\_NAME field of the DSDs will be set according to the content of the corresponding MDS or m-factor file. The following keywords are envisaged:

- • from sun diffuser measurements
- M\_CAL
  
- • from sun occultation
- M\_DL
- M\_PL
- M\_QL
  
- • from sub-solar calibration
- M\_DN
- M\_PN
- M\_QN
  
- • from WLS measurements
- M\_NDF
  
- • spare m-factor set (e.g. from moon occultation)
- M\_DS
- M\_PS
- M\_QS

#### 15.6.7 Level 1B Initialization File

This file contains initialization information for the Level 1 processor.

The initialisation file core name is given by SCI\_LI1\_\_AX following the convention of the ENVISAT ground segment. The core name is followed by the generation time, and by the start and stop validity times.

FILE ID: SCI\_LI1\_AX  
 TYPE: Auxiliary  
 USE: Level 1B processing  
 UPDATED: infrequently  
 SIZE: MPH(1247 bytes) + SPH(1498 bytes) + GADSs(variable) = estimated at 150 kbytes

**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 2 Initialization File**

<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 5 DSD:</b> <i>DSD pointing to the Static Parameters GADS</i> <i>DSD pointing to the Spectrum Templates GADS</i> <i>DSD pointing to the External State Parameters GADS</i> <i>DSD pointing to the Processing Categories GADS</i> <i>DSD pointing to the Polarisation and Radiance Sensitivity Grids GADS</i>
<b>Static Parameters GADS</b>
<b>Spectrum Templates GADS</b>
<b>External State Parameters GADS</b>
<b>Processing Categories GADS</b>
<b>Polarisation and Radiance Sensitivity Grids GADS</b>

**15.6.7.1.1 Static Parameters GADS**

As described in R-35.

**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**

N	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**

The format of this GADS is shown in the table below:

Table 15.6.7.1.4-1 - Processing Categories GADS					
N	Description	Units	Byte Length	Data Type	Dim.
11	Measurement category	-	2	us	1
3	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**

The format of this GADS is shown in the table below:



Table 15.6.7.1.5-1 - Polarisation and Radiance Sensitivity Grids GADS					
N	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 scan mirror positions used for the polarisation and radiance sensitivity component of the level 1B product are defined by this GADS of the initialisation file. The numbers of 10 in the table above are only examples and consistent with the definition of the level 1B product. The actual number for each individual category of parameter depends on the result of the final pre-flight calibration activity. Then ESM and ASM position values will be selected so that linear interpolation between these values yields an error which is well below the systematic error of the corresponding parameter. During application of these 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 parameters using linear interpolation.

### 15.6.8 Level 2 Initialization File

This file contains the following parameters:

- ❑ overall control of the level 1B to 2 processing chain
- ❑ DOAS/BIAS fitting specifications (windows, reference spectra, fitting control, etc.)
- ❑ parameters controlling the Air Mass Factor look-up

- parameters controlling cloud fitting and aerosol retrieval algorithm

FILE ID: SCI\_LI2\_AX

TYPE: Auxiliary

USE: Level 2 processing

UPDATED: infrequently

SIZE: MPH(1247 bytes) + SPH(378 bytes) + GADS(7000) = approx. 8.5 kbytes

### 15.6.8.1 Format

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

**Table 15.6.8.1-1 - Schematic Structure of the Level 2 Initialization File**

<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 1 DSD:</b>
<i>DSD pointing to the Initialization Parameters GADS</i>
<b>Initialization GADS</b>

#### 15.6.8.1.1 Initialization Parameters GADS

As described in R-36.

### 15.6.9 Atmospheric Climatologies (Profiles) 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 two standard climatologies and one reference atmosphere in this file:

- MPI climatology provided by the Max-Planck Institute for Chemistry in Mainz, Germany, and
- the US standard atmosphere provided by Air Force Geophysical Laboratory (AFGL), Hanscom, Mass., USA.
- Single BIAS reference atmosphere (derived from the US AFGL standard atmosphere) (obsolete)

FILE ID: SCI\_PR2\_AX

TYPE: Auxiliary

USE: Level 2 processing

UPDATED: infrequently

SIZE: MPH(1247 bytes) + SPH(938 bytes) + GADSs(approx. 116 kBytes) = approx. 118 kBytes

### 15.6.9.1 Format

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

**Table 15.6.9.1-1 - Schematic Structure of the Atmospheric Climatologies File**

<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 3 DSD:</b>
<i>DSD pointing to the MPI Climatology GADS</i>
<i>DSD pointing to the USA Climatology GADS</i>
<i>DSD pointing to the BIAS Reference Atmosphere GADS</i>
<b>MPI Climatology GADS</b>
<b>USA Climatology GADS</b>
<b>BIAS Reference Atmosphere GADS</b>

#### 15.6.9.1.1 MPI Climatology GADS

The format of the MPI GADS is shown in the table below.

<b>Table 15.6.9.1.1-1 - MPI Climatology GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	<b>Number of atmospheric layers</b>	-	2	us	1
2	<b>Number of reference latitudes</b>	-	2	us	1
3	<b>Number of molecules</b>	-	2	us	1
4	<b>Number of seasons</b>	-	2	us	1
5	<b>Number of months</b>	-	2	us	1
6	<b>Cumulative days for pT-profiles</b>	-	24	us	12
7	<b>Cumulative days for concentration profiles</b>	-	8	us	4
8	<b>Molecule names</b>	ascii	25	uc	25

Table 15.6.9.1.1-1 - MPI Climatology GADS					
9	Number of concentration profiles per molecule	-	2	us	1
10	Number of temperature and pressure profiles	-	2	us	1
11	Reference latitudes	degrees	72	fl	18
12	Atmospheric layer altitudes	km	136	fl	34
13	Pressure profiles	hPa	29376	fl	7344
14	Temperature profiles	K	29376	fl	7344
15	Molecule profiles	ppmV	48960	fl	12240
<i>Size of Component:</i>			<b>107991</b>		

The height grid of all the profiles is given from 60.6 km down to 0.2 km, a total of 34 entries. Reference latitudes are given from -85.0 degrees in steps of 10.0 degrees up to +85.0 degrees, a total of 18 entries.

The molecule names are given in ASCII as 5 left-adjusted fields (one for each molecule) of 5 characters. Unused characters shall be set to the ASCII blank character.

In the molecule profile field (15) the different molecules are referred to by indices. The molecule indices in the MPI climatologies above have the following meaning:

1 = O<sub>3</sub>

2 = NO<sub>2</sub>

3 = HCHO

4 = BrO

5 = OCIO

Temperature and pressure profiles are stored as function of height (the height grid), latitude zone and month of the year. The ordering of the temperature and pressure profiles is as follows: The first profile value is valid for the first reference latitude (-85.0 degrees), the first month of the year (January) and the first height grid value (60.6 km). Profiles then run over the height grid followed by the month and finally latitude zone, giving a total of 7344 profile entries (18\*12\*34 = 7344). The order of nesting and cycling of the profiles is: height, zone, month, being height the innermost cycle (runs faster) and month the outermost (runs slower).

Trace gas concentration profiles are stored as function of height, latitude zone, season of the year and molecule number. Four seasons are considered (spring=1, summer=2, autumn=3, winter=4). The ordering of the concentration profiles is as follows: The first profile value is valid for the first molecule number (5 molecules are provided in this MPI climatology, see above), the first reference latitude (-85.0 degrees), the first season of the year (spring) and the first height grid value (60.6 km). Profiles run first over height grid then over season, then over latitude zone and finally over the molecule number, giving a total of 12240 profile entries (5\*18\*4\*34 = 12240). The order of nesting and cycling of



the profiles is: season, height, zone, month, being season the innermost cycle (runs faster) and month the outermost (runs slower).

### 15.6.9.1.2 USA Climatology GADS

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

Table 15.6.9.1.2-1 - USA Climatology GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Number of atmospheric layers	-	2	us	1
2	Number of reference latitudes	-	2	us	1
3	Number of seasons	-	2	us	1
4	Number of molecules	-	2	us	1
5	Cumulative days	-	4	us	2
6	Molecule names	ascii	20	uc	20
7	Number of profiles per category	-	2	us	1
8	Reference Latitudes	degrees	24	fl	6
9	Atmospheric layer altitudes	km	184	fl	46
10	Pressure profiles	hPa	1104	fl	276
11	Temperature profiles	K	1104	fl	276
12	Molecule profiles	ppmV	4416	fl	1104
<i>Size of Component:</i>			<b>6866</b>		

The height grid of all the profiles is given from 100 km down to 0 km, a total of 46 entries.

The molecule names are given in ASCII as 7 left-adjusted fields (one for each molecule) of 5 characters. Unused characters shall be set to the ASCII blank character.

In the molecule profile field (12) the different molecules are referred to by indices. The molecule indices in the USA climatologies above have the following meaning:

- 1 = O<sub>3</sub>
- 2 = NO<sub>2</sub>
- 3 = HCHO
- 4 = SO<sub>2</sub>

The number of profiles per category are not given by an individual latitude



zone and time stamp, but using an index for the following scenarios:

- 1 = tropic for all seasons
- 2 = mid-latitude summer
- 3 = mid-latitude winter
- 4 = sub-arctic summer
- 5 = sub-arctic winter
- 6 = US standard atmosphere

The number of latitude zones (3) and the number of seasons (2) is given in the table above. Temperature and pressure profiles are stored as function of height (height grid) and profile category. The ordering of the temperature and pressure profiles is as follows: The first profile value is valid for the first profile category (tropic for all seasons) and the first height grid value (100 km). Profiles run over the height grid and then over profile category, giving a total of 276 profile entries ( $6 \times 46 = 276$ ).

Trace gas concentration profiles are stored as function of height, profile category and molecule number. The ordering of the concentration profiles is as follows: The first profile value is valid for the first molecule number (4 molecules are provided in the USA climatology), the first profile category (tropic for all seasons) and the first height grid value (100 km), running over height grid then profile category and finally the molecule number, giving a total of 1104 profile entries ( $4 \times 6 \times 46 = 1104$ ).

#### 15.6.9.1.3 BIAS Reference Atmosphere GADS

This section is not more used, since it is obsolete for SGP\_12OL.

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

<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	Number of atmospheric levels	-	2	us	1
2	Number of molecules	-	2	us	1
3	Molecule names	ascii	25	uc	25
4	Atmospheric levels altitudes	km	68	fl	17
5	Pressure profiles	hPa	68	fl	17
6	Temperature profiles	K	68	fl	17
7	Molecule profiles	ppmV	340	fl	85
<i>Size of Component:</i>			<b>573</b>		

The height grid of all the profiles is given from 57.8 km down to 0 km, a total of 17

entries.

The molecule names are given in ASCII as 5 left-adjusted fields (one for each molecule) of 5 characters. Unused characters shall be set to the ASCII blank character.

In the molecule profile field (7) the different molecules are referred to by indices with the following meaning:

1 = H<sub>2</sub>O 2 = CO<sub>2</sub> 3 = N<sub>2</sub>O 4 = CO 5 = CH<sub>4</sub>

Temperature and pressure profiles are stored as a function of height (the height grid); total entries = 2\*17 = 34.

Trace gas concentration profiles are stored as a function of height and molecule number. The ordering of the concentration profiles follows the molecule indexing; total entries = 5\*17 = 85.

#### 15.6.10 Cloud Parameters Data File

The cloud reference parameters given in the data base are the following:

- ISCCP Data Base
- Cloud Albedo Climatology

FILE ID: SCI\_CL2\_AX

TYPE: Auxiliary

USE: Level 2 processing

UPDATED: infrequently

SIZE: MPH(1247 bytes) + SPH(678 bytes) + GADSs(approx. 539  
kbytes) =

approx. 541 kbytes

##### 15.6.10.1 Format

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

**Table 15.6.10.1-1 - Schematic Structure of the Cloud Parameters Data File**



<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 2 DSD:</b>
<i>DSD pointing to the ISCCP Data Base GADS</i>
<i>DSD pointing to the Cloud Reflectance Data Base GADS</i>
<b>ISCCP Data Base GADS</b>
<b>Cloud Reflectance Data Base GADS</b>

**15.6.10.1.1 | ISCCP Data Base GADS**

The ISCCP Data Base GADS is described in the table below.

<b>Table 15.6.10.1.1-1 - ISCCP Data Base GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	<b>Number of reference latitudes</b>	-	2	us	1
2	<b>Number of reference longitudes</b>	-	2	us	1
3	<b>Number of months entries in the data base</b>	-	2	us	1
4	<b>Reference latitudes</b>	degrees	288	fl	72
5	<b>Reference longitudes</b>	degrees	576	fl	144
6	<b>Cloud-top pressures</b>	hPa	497664	fl	124416
<i>Size of Component:</i>			<b>498534</b>		

Reference latitudes are given from 88.75 degrees in steps of 2.5 degrees down to -88.50 degrees, a total of 72 entries. Reference longitudes are given from 1.25 degrees in steps of 2.5 seconds up to 358.75 degrees, a total of 144 entries.

Cloud-top pressure is given beginning with the first month (January), the first latitude zone (88.75 degrees) and the first longitude zone (1.25 degrees) running over longitude then latitude and finally month giving a total of  $12 \times 72 \times 144 = 124416$  values. The order of nesting and cycling of the profiles is: month, latitude, longitude being month the innermost cycle (runs faster) and longitude the outermost (runs slower)

**15.6.10.1.2 Cloud Reflectance Data Base GADS**

The GADS format is described in the table below.



Table 15.6.10.1.2-1 - Cloud Reflectance Data Base GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Number of asymmetry parameters	-	2	us	1
2	Number of reference zenith angles	-	2	us	1
3	Number of reference azimuths	-	2	us	1
4	Number of reference wavelengths for escape function correction	-	2	us	1
5	Number of reference zenith angles for escape function correction	-	2	us	1
6	Number of different cloud types	-	2	us	1
7	Reference wavelengths	nm	100	fl	25
8	Reference asymmetry parameters for different cloud types	-	32	fl	8
9	Spectral dependent asymmetry parameters for different cloud types. Looping about cloud type and then wavelength.	-	800	fl	2
10	Reference azimuths	-	48	fl	12
11	Cosines of reference zenith angles	sr.-1	36	fl	9
12	Cosines of reference escape function zenith angles	sr.-1	44	fl	11
13	Raw data cloud-top reflectance	-	31104	fl	7776
14	Raw data escape function	-	8800	fl	2200
<i>Size of Component:</i>			40976		

Cloud-top reflectance data depend on cloud type, wavelength and the viewing geometry, i.e., the zenith angles of incident and reflected radiation. Inside the SGP\_12N the required cloud-top albedo is calculated from the raw data given in the table above. This step is necessary because the AMF look-up tables are only classified according to Lambertian lower boundary reflectance. The Lambertian reflectance has no angular variation, but there is a marked dependence on the cloud optical depth and the albedo of the underlying ground surface. Both these effects enter through the “escape function” term of the bi-directional reflectance; this term describes the transmission loss through a cloud of finite optical depth.

The cloud-top reflectances are given as a function of the cloud type (the reference asymmetry parameter) and the viewing geometry. The first entry is valid for the first cloud type, the first azimuth, the first incident zenith angle and the first zenith angle of reflected radiation. Cloud-top values run over the cloud type, then over azimuth, then over the zenith angle of incident radiation and lastly over the zenith angle of reflection, giving a total of 7776 entries ( $8*12*9*9=7776$ ).

The wavelength dependency of calculated cloud-top albedos come from the escape function which is a correction formalism to take into account the transmission loss through a cloud which originates from photons reflected from the underlying surface. Thus, the computed escape function depends on the cloud optical depth, the ground



albedo and the wavelength.

Raw escape function data are given as function of cloud-type, the viewing geometry (zenith angle) and the wavelength. The first entry is valid for the first cloud type, the first zenith angle and the first wavelength. Escape function data run over the cloud type, then zenith angle and finally wavelength, giving a total of 2200 entries (8\*11\*25-2200).

**15.6.11 Surface Data Bases File**

The surface parameters given in the data base are the following:

- ❑ Global Topography
- ❑ Global Albedo Climatology
- ❑ Spectral Reflectance Climatology
- ❑ Glitter Albedo Climatology

FILE ID: SCI\_SF2\_AX

TYPE: Auxiliary

USE: Level 2 processing

UPDATED: infrequently

SIZE: MPH(1247 bytes) + SPH(1218 bytes) + GADSs(approx. 1.305 MB) = approx. 1.307 MB

**15.6.11.1 Format**

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

<b>Table 15.6.11.1-1 - Schematic Structure of the Surface Data Bases File</b>
<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 4 DSD:</b> <i>DSD pointing to the Global Topography GADS</i> <i>DSD pointing to the Global Albedo Climatology GADS</i> <i>DSD pointing to the Spectral Reference Climatology GADS</i> <i>DSD pointing to the Glitter Albedo Climatology GADS</i>
<b>Global Topography GADS</b>
<b>Global Albedo Climatology GADS</b>
<b>Spectral Reference Climatology GADS</b>
<b>Glitter Albedo Climatology GADS</b>

**15.6.11.1.1 Global Topography GADS**



The GADS format is described in the table below.

<b>Table 15.6.11.1.1-1 - Global Topography GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	<b>Number of reference latitudes</b>	-	2	us	1
2	<b>Number of reference longitudes</b>	-	2	us	1
3	<b>Height</b>	m	129600	us	64800
<i>Size of Component:</i>			<b>129604</b>		

The global topography data base contains the height as function of latitude and longitude with a spatial resolution of 1° \* 1° degrees. The first entry is valid for a latitude from -89 (until 90° ) and a longitude of 0°, running first over latitude and longitude afterwards, a total of 64800 (360\*180 = 64800) entries.

#### 15.6.11.1.2 Global Albedo Climatology GADS

The GADS format is described in the table below.

<b>Table 15.6.11.1.2-1 Global Albedo Climatology GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	<b>Number of reference latitudes</b>	-	2	us	1
2	<b>Number of reference longitudes</b>	-	2	us	1
3	<b>Number of seasons</b>	-	2	us	1
4	<b>Albedo</b>	-	1036800	fl	259200
5	<b>Vegetation Index</b>	-	129600	us	64800
<i>Size of Component:</i>			<b>1166406</b>		

The global albedo data base contains the albedo as function of latitude and longitude with a spatial resolution of 1\*1 degrees and a time resolution of 3 months representing the 4 seasons of a year, a total of 259200 (360\*180\*4 = 259200) entries. The first entry is valid for a latitude from -89 (until 90°) and a longitude of 0°, running first over season then over latitude and finally the longitude. The first season given in the data base represents 'winter'. The order of nesting and cycling of the profiles is: latitude, longitude, season being latitude the innermost cycle (runs faster) and season the outermost (runs slower)

The vegetation index is a function of latitude and longitude with a spatial resolution of 1\*1 degrees, a total of 64800 (360\*180 = 64800) entries. The first entry is valid for a latitude from -89°until 90°and a longitude of 0°, running first over latitude then longitude.

**15.6.11.1.3 Spectral Reflectance Climatology GADS**

The GADS format is described in the table below.

<b>Table 15.6.11.1.3-1 Spectral Reflectance Climatology GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	<b>Number of surface types</b>	-	2	us	1
2	<b>Surface types</b>	ascii	55	uc	55
3	<b>Number of wavelengths</b>	-	2	us	1
4	<b>Wavelengths</b>	nm	528	fl	132
5	<b>Spectral reflectance</b>	-	2640	fl	660
<i>Size of Component:</i>			<b>3227</b>		

The spectral reflectance data base contains the albedo as function of surface type and wavelength, a total of 660 (5\*132) entries. The wavelength is given from 240.0 nm up to 2500.0 nm, with a total of 132 entries.

The surface types are given in ASCII as five left-adjusted fields (one for each molecule) of 11 characters. Unused characters shall be set to the ASCII blank character.

In the spectral reflectance field (5) the different surface types are referred to by indices. The surface type contains 5 entries representing five different surface types. The surface types are:

- 1 = sand
- 2 = soil
- 3 = snow
- 4 = vegetation
- 5 = water

These surface types are also valid for the vegetation indices of the previous GADS.

#### 15.6.11.1.4 Glitter Albedo Climatology GADS

The GADS format is described in the table below.

Table 15.6.11.1.4-1 Glitter Albedo Climatology GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Number of glitter albedo sun zenith angles	-	2	us	1
2	Number of glitter albedo wavelengths	-	2	us	1
3	Glitter albedo reference sun zenith angles	-	128	fl	32
4	Glitter albedo reference wavelengths	nm	164	fl	41
5	Glitter albedo	-	5248	fl	1312
<i>Size of Component:</i>			<b>5544</b>		

Additionally, a glitter albedo data base is included which is given as function of sun zenith angle, wavelength and wind speed, a total of 1312 entries ( $32 \times 41 = 1312$ ). The sun zenith angle is given in steps from 0.0 degrees to 89.99 degrees, a total of 32 entries. The wavelength is given in steps from 200 nm up to 2500 nm, a total of 41 entries. The first entry of the glitter albedo is valid for the first wavelength and the first sun zenith angle. The data is running first over sun zenith angle and then wavelength.

#### 15.6.12 Literature Reference Cross-Sections Data Base File

The data base contains absorption cross-section and cross-section coefficients (O3 Hartley-Huggins bands) as function of molecule species, wavelength and temperature. Data bases are available from different measurement campaigns, documented in the literature.

FILE ID: SCI\_CS2\_AX  
 TYPE: Auxiliary  
 USE: Level 2 processing  
 UPDATED: infrequently  
 SIZE: MPH(1247 bytes) + SPH(2618 bytes) + GADSs(approx. 814 kbytes) = approx. 817.5 kBytes

##### 15.6.12.1 Format

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

Table 15.6.12.1-1 - Structure of the Literature Cross Sections Data Base File
MPH



<b>Table 15.6.12.1-1 - Structure of the Literature Cross Sections Data Base File</b>	
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 9 DSD:</b>	
<i>DSD pointing to the O3 Reference Spectra GADS</i>	
<i>DSD pointing to the NO2 Reference Spectra GADS</i>	
<i>DSD pointing to the H2O Reference Spectra GADS</i>	
<i>DSD pointing to the BrO Reference Spectra GADS</i>	
<i>DSD pointing to the SO2 Reference Spectra GADS</i>	
<i>DSD pointing to the HCHO Reference Spectra GADS</i>	
<i>DSD pointing to the OCIO Reference Spectra GADS</i>	
<i>DSD pointing to the O4 Reference Spectra GADS</i>	
<i>DSD pointing to the Theoretical Ring Spectrum GADS</i>	
<b>O3 Reference Spectra GADS</b>	
<b>NO2 Reference Spectra GADS</b>	
<b>H2O Reference Spectra GADS</b>	
<b>BrO Reference Spectra GADS</b>	
<b>SO2 Reference Spectra GADS</b>	
<b>HCHO Reference Spectra GADS</b>	
<b>OCIO Reference Spectra GADS</b>	
<b>O4 Reference Spectra GADS</b>	
<b>Theoretical Ring Spectrum GADS</b>	

**15.6.12.1.1 O3 Reference Spectra GADS**

The GADS format is described in the table below.

<b>Table 15.6.12.1.1-1 O3 Reference Spectra GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	<b>Molecule name</b>	ascii	5	uc	5
2	<b>Number of atmospheric levels</b>	-	2	us	1
3	<b>Number of spectral segments (O3, BP-spectra and Hartley-Huggins bands)</b>	-	2	us	1
4	<b>Maximum number of temperatures</b>	-	2	us	1
5	<b>Maximum number of coefficients</b>	-	2	us	1
6	<b>Number of temperature per segment</b>	-	6	us	3
7	<b>Number of coefficient per segment</b>	-	6	us	3
8	<b>Number of spectral entries per segment (O3, BP-spectra, Hartley-Huggins bands)</b>	-	6	us	3

Table 15.6.12.1.1-1 O3 Reference Spectra GADS					
9	Type of formula for coefficients	-	1	uc	1
10	Type of wavelength information	-	1	uc	1
12	Temperature grid for first segment	K	4	fl	1
13	Wavelength grid for spectral segment (O <sub>3</sub> , BP-spectra, Hartley-Huggins bands)	nm	47612	fl	11903
14	Cross-section for spectral segment (O <sub>3</sub> , BP-spectra)	cm <sup>2</sup> /mol	47612	fl	11903
15	Cross-section coefficients for spectral segment (O <sub>3</sub> , BP-spectra) within the Hartley-Huggins bands	-	19264	fl	4816
<i>Size of Component:</i>			<b>114525</b>		

The first spectral segment of the O<sub>3</sub> Bass-Paur spectra covers the spectral range from 184.9277 nm up to 253.7749 nm, a total of 5122 entries, and a segment from 253.7749 nm up to 365.3635 nm, a total of 2408 entries. The data from this spectral segment corresponds to a temperature of 195 K. The third segment covers the spectral range from 407.8 nm up to 845.0 nm, a total of 4373 entries (no temperature dependency).

The spectral segment within the Hartley-Huggins bands (the third segment) covers the wavelength range between 253.7749 nm and 365.3635 nm, a total of 2408 entries. This segment contains linear and quadratic cross-section coefficients for the spectral ranges mentioned above.

#### 15.6.12.1.2 NO2 Reference Spectra GADS

The GADS format is described in the table below.

N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (NO <sub>2</sub> , Harwood-Jones spectra)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
6	Number of temperatures (NO <sub>2</sub> , Harwood-Jones spectra)	-	2	us	1
8	Number of spectral entries (NO <sub>2</sub> , Harwood-Jones spectra)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
12	Temperature Grid	K	28	fl	7

Table 15.6.12.1.2-1 NO <sub>2</sub> Reference Spectra GADS					
13	Wavelength grid for spectral segment (NO <sub>2</sub> , Harwood-Jones spectra)	nm	48944	fl	12336
14	Cross-sections per temperature (NO <sub>2</sub> , Harwood-Jones spectra)	cm <sup>2</sup> /mol	48944	fl	12336
<i>Size of Component:</i>			<b>97934</b>		

The spectral segment of the NO<sub>2</sub> Harwood-Jones data covers a wavelength range from 313.1 nm up to 567.73 nm, a total of 1748 entries. The data is available for 7 different temperatures. Each block contains a total of 1748 entries, the complete spectrum contains 12336 entries (1748\*7). The given temperatures are 213 K, 225

#### 15.6.12.1.3 H<sub>2</sub>O Reference Spectra GADS

The GADS format is described in the table below.

Table 15.6.12.1.3-1 H <sub>2</sub> O Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (H <sub>2</sub> O)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of temperatures (H <sub>2</sub> O)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
13	Wavelength grid (H <sub>2</sub> O)	nm	156212	fl	39053
14	Cross-sections (H <sub>2</sub> O)	cm <sup>2</sup> /mol	156212	fl	39053
<i>Size of Component:</i>			<b>312440</b>		

The spectral segment of the H<sub>2</sub>O HITRAN data base spectrum covers a wavelength range from 409.48 nm up to 800 nm, a total of 39053 entries. The cross sections of H<sub>2</sub>O are available for each wavelength entry within the given spectral range, a total of 39053 entries.

#### 15.6.12.1.4 BrO Reference Spectra GADS

The GADS format is described in the table below.



Table 15.6.12.1.4-1 BrO Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of spectral entries (BrO)	-	2	us	1
3	Number of spectral segments (B2O)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of spectral entries (BrO)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
13	Wavelength grid for spectral segment (BrO)	nm	7704	fl	1926
14	Cross-sections for spectral segment (BrO)	cm <sup>2</sup> /mol	7704	fl	1926
<i>Size of Component:</i>			<b>15424</b>		

The spectral segment of the BrO spectrum covers the spectral range from 312.37 nm up to 388.26 nm, a total of 1926 entries. The cross sections of BrO are available for each wavelength entry within the given spectral range, a total of 1926 entries.

#### 15.6.12.1.5 SO<sub>2</sub> Reference Spectra

The GADS format is described in the table below.

Table 15.6.12.1.5-1 SO <sub>2</sub> Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (SO <sub>2</sub> )	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of spectral entries (SO <sub>2</sub> )	-	2	us	1
10	Type of wavelength information	-	1	uc	1
13	Wavelength grid for spectral segment (SO <sub>2</sub> )	nm	22500	fl	5625
14	Cross-sections for spectral segment (SO <sub>2</sub> )	cm <sup>2</sup> /mol	22500	fl	5625
<i>Size of Component:</i>			<b>45016</b>		

The spectral segment of the SO<sub>2</sub> spectrum covers the spectral range from 227.34 nm up to 339.82 nm, a total of 5625 entries. The cross sections of SO<sub>2</sub> are available for each wavelength entry within the given spectral range, a total of 5625 entries.

**15.6.12.1.6 HCHO Reference Spectra GADS**

The GADS format is described in the table below.

Table 15.6.12.1.6-1 HCHO Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (HCHO)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of spectral entries (HCHO)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
13	Wavelength grid for spectral segment (HCHO)	nm	20192	fl	5048
14	Cross-sections for spectral segment (HCHO)	cm <sup>2</sup> /mol	20192	fl	5048
<i>Size of Component:</i>			<b>40400</b>		

The spectral segment of the HCHO spectrum covers the spectral range from 224.58 nm up to 375.99 nm, a total of 5048 entries. The cross sections of HCHO are available for each wavelength entry within the given spectral range, a total of 5048 entries.

**15.6.12.1.7 OCIO Reference Spectra GADS**

The GADS format is described in the table below.

Table 15.6.12.1.7-1 OCIO Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (OCIO)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of spectral entries (OCIO)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
13	Wavelength grid for spectral segment (OCIO)	nm	12840	fl	3210
14	Cross-sections for spectral segment (OCIO)	cm <sup>2</sup> /mol	12840	fl	3210
<i>Size of Component:</i>			<b>25696</b>		

The spectral segment of the OCIO spectrum covers the spectral range from

242.59 nm up to 476.80 nm, a total of 3210 entries. The cross sections of OClO are available for each wavelength entry within the given spectral range, a total of 3210 entries.

#### 15.6.12.1.8 O4 Reference Spectra GADS

The GADS format is described in the table below.

Table 15.6.12.1.8-1 O4 Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (O <sub>4</sub> )	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of spectral entries (O <sub>4</sub> )	-	4	us	2
10	Type of wavelength information	-	1	uc	1
13	Wavelength grid for spectral segment (O <sub>4</sub> )	nm	18688	fl	4672
14	Cross-sections for sec. spectral segment (O <sub>4</sub> )	cm <sup>2</sup> /mol	18688	fl	4672
<i>Size of Component:</i>			<b>37394</b>		

The spectral segments of the O<sub>4</sub> spectrum cover the spectral range from 300.09 nm up to 677.09 nm, a total of 3770 entries and from 1000.00 nm up to 1136.80 nm, a total of 902 nm. The cross sections of O<sub>4</sub> are available for each wavelength entry within the given spectral range, a total of 4672 entries.

#### 15.6.12.1.9 Theoretical Ring Reference Spectra GADS

The GADS format is described in the table below.

Table 15.6.12.1.9-1 Ring Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Spectra type	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (channels)	-	2	us	1

4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of spectral entries (per channel)	-	4	us	2
10	Type of wavelength information	-	1	uc	1
13	Wavelength grid for spectral segment (O <sub>4</sub> )	nm	16	fl	4
14	Ring spectrum values per channel	-	124808	fl	31202
<i>Size of Component:</i>			<b>124842</b>		

There are two segments covering the SCIAMACHY channels 2 and 3. The channel 2 segment contains 9501 points which start at 311.0 nm at a resolution of 0.01 nm. The channel 3 segment contains 21701 points which start at 394.0 nm at 0.01 nm resolution.

### 15.6.13 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.

FILE ID: SCI\_BL2\_AX

TYPE: Auxiliary

USE: Level 2 processing

UPDATED: infrequently

SIZE: MPH(1247 bytes) + SPH(1498 bytes) + GADSs(approx.973 kbytes) = approx. 976 kbytes

#### 15.6.13.1 Format

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

Table 15.6.13.1-1 - Structure of the Line by Line Absorption Cross Sections File



MPH
<b>SPH - Auxiliary Data SPH (defined in Volume 16) with 5 DSD:</b>  <i>DSD pointing to the H2O Reference Spectra GADS</i> <i>DSD pointing to the CO2 Reference Spectra GADS</i> <i>DSD pointing to the N2O Reference Spectra GADS</i> <i>DSD pointing to the CO Reference Spectra GADS</i> <i>DSD pointing to the CH4 Reference Spectra GADS</i>
<b>H2O Reference Spectra GADS</b>
<b>CO2 Reference Spectra GADS</b>
<b>N2O Reference Spectra GADS</b>
<b>CO Reference Spectra GADS</b>
<b>CH4 Reference Spectra GADS</b>

**15.6.13.1.1 H2O Reference Spectra GADS**

The GADS format is described in the table below.

N	Description	Units	Byte Size	Data Type	Dim.
1	<b>Molecule name</b>	ascii	5	uc	5
2	<b>Number of atmospheric levels</b>	-	2	us	1
3	<b>Number of spectral segments (H2O)</b>	-	2	us	1
4	<b>Maximum number of temperatures</b>	-	2	us	1
5	<b>Maximum number of coefficients</b>	-	2	us	1
8	<b>Number of spectral entries per segment</b>	-	6	us	3
10	<b>Type of wavelength information</b>	-	1	uc	1
11	<b>Height grid</b>	km	68	fl	17
13	<b>Wave number information per segment</b>	cm <sup>-1</sup>	48	do	6
14	<b>Cross sections per spectral segment</b>	cm <sup>2</sup> /mol	367404	fl	91851
<i>Size of Component:</i>			<b>367540</b>		

The first spectral segment starts at 4905.0 cm<sup>-1</sup> and contains 1901 spectral points at 17 levels of the BIAS reference atmosphere (17\*1901 = 32317). The second segment starts at 4393.0 cm<sup>-1</sup> and has 1701 spectral points (total entries 17\*1701 = 28917); the third starts at 4223.0 cm<sup>-1</sup> and has 1801

spectral points (total entries  $17 \times 1801 = 30617$ ). The resolution is  $0.01 \text{ cm}^{-1}$  for all segments. The number of atmospheric levels must be the same as the equivalent entry in the BIAS reference atmosphere data set. For the cross-sections the first entry is valid for the first segment, the first atmospheric level and the first wavenumber; the data runs first over wavenumber, then over atmospheric levels and then over segments.

#### 15.6.13.1.2 CO2 Reference Spectra GADS

The GADS format is described in the table below.

Table 15.6.13.1.2-1 CO2 Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (CO <sub>2</sub> )	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of spectral entries per segment	-	2	us	1
10	Type of wavelength information	-	1	uc	1
11	Height grid	km	68	fl	17
13	Wave number information per segment	cm <sup>-1</sup>	16	do	2
14	Cross sections for spectral segment	cm <sup>2</sup> /mol	129268	fl	32317
<i>Size of Component:</i>			<b>129368</b>		

The first spectral segment starts at  $4905.0 \text{ cm}^{-1}$  and contains 1901 spectral points at 17 levels of the BIAS reference atmosphere ( $17 \times 1901 = 32317$ ). The resolution is  $0.01 \text{ cm}^{-1}$  for the segment. The number of atmospheric levels must be the same as the equivalent entry in the BIAS reference atmosphere data set. For the cross-sections, the first entry is valid for the first atmospheric level and the first wavelength; the data runs first over wavenumber then over atmospheric levels.

#### 15.6.13.1.3 N2O Reference Spectra GADS

The GADS format is described in the table below.

Table 15.6.13.1.3-1 N2O Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5

Table 15.6.13.1.3-1 N2O Reference Spectra GADS					
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (N <sub>2</sub> O)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of spectral entries per segment	-	2	us	1
10	Type of wavelength information	-	1	uc	1
11	Height grid	km	68	fl	17
13	Wave number information per segment	cm <sup>-1</sup>	16	do	2
14	Cross sections for spectral segment	cm <sup>2</sup> /mol	115668	fl	28917
<i>Size of Component:</i>			<b>115768</b>		

The first spectral segment starts at 4393.0 cm<sup>-1</sup> and has 1701 spectral points (total entries 17\*1701 = 28917). The resolution is 0.01 cm<sup>-1</sup> for the segment. The number of atmospheric levels must be the same as the equivalent entry in the BIAS reference atmosphere data set. For the cross-sections, the first entry is valid for the first atmospheric level and the first wavelength; the data runs first over wavenumber then over atmospheric levels.

#### 15.6.13.1.4 CO Reference Spectra GADS

The GADS format is described in the table below.

Table 15.6.13.1.4-1 CO Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (CO)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of spectral entries per segment	-	2	us	1
10	Type of wavelength information	-	1	uc	1
11	Height grid	km	68	fl	17
13	Wave number information per segment	cm <sup>-1</sup>	16	do	2
14	Cross sections per spectral segment	cm <sup>2</sup> /mol	122468	fl	30617
<i>Size of Component:</i>			<b>122568</b>		

The first spectral segment starts at  $4223.0 \text{ cm}^{-1}$  and has 1801 spectral points (total entries  $17 * 1801 = 30617$ ). The resolution is  $0.01 \text{ cm}^{-1}$  for the segment. The number of atmospheric levels must be the same as the equivalent entry in the BIAS reference atmosphere data set. For the cross-sections in a given segment, the first entry is valid for the first atmospheric level and the first wavenumber; the data runs first over wavenumber then over atmospheric levels.

#### 15.6.13.1.5 CH4 Reference Spectra GADS

The GADS format is described in the table below.

Table 15.6.13.1.5-1 CH4 Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (CH4)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of spectral entries per segment	-	4	us	2
10	Type of wavelength information	-	1	uc	1
11	Height grid	km	68	fl	17
13	Wave number information per segment	cm-1	32	do	4
14	Cross sections per spectral segment	cm <sup>2</sup> /mol	238136	fl	59534
<i>Size of Component:</i>			<b>238254</b>		

The first spectral segment starts at  $4393.0 \text{ cm}^{-1}$  and has 1701 spectral points (total entries  $17 * 1701 = 28917$ ); the second starts at  $4223.0 \text{ cm}^{-1}$  and has 1801 spectral points (total entries  $17 * 1801 = 30617$ ). The resolution is  $0.01 \text{ cm}^{-1}$  for both segments. The number of atmospheric levels must be the same as the equivalent entry in the BIAS reference atmosphere data set.

For the cross-section, the first entry is valid for the first segment, the first atmospheric level and the first wavelength; the data runs first over wavenumber then over atmospheric levels, and the over segments.

#### 15.6.14 Flight-Model Reference Cross-Sections Data File

The data base contains absorption cross-section of O<sub>3</sub> and NO<sub>2</sub>, plus a Ring Reference spectrum which will all be measured by the SCIAMACHY flight-model. The cross-sections are given as a function of wavelength and temperature. All spectra are separated into a number of spectral segments.





FILE ID: SCI\_FM2\_AX  
 TYPE: Auxiliary  
 USE: Level 2 processing  
 UPDATED: infrequently  
 SIZE: MPH(1247 bytes) + SPH(3178 bytes) + GADSs(approx.1.225 Mbytes) = approx. 1.229 Mbytes

**15.6.14.1 Format**

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

**Table 15.6.14.1-1 - Structure of the Flight Model Reference Cross Sections File**

<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 11 DSD:</b>
<i>DSD pointing to the O3 Reference Spectra (GOME) GADS</i>
<i>DSD pointing to the NO2 Reference Spectra (GOME) GADS</i>
<i>DSD pointing to the Ring Reference Spectra (GOME) GADS</i>
<i>DSD pointing to the O3 Reference Spectra (SCIA) GADS</i>
<i>DSD pointing to the NO2 Reference Spectra (SCIA) GADS</i>
<i>DSD pointing to the BrO Reference Spectra (SCIA) GADS</i>
<i>DSD pointing to the SO2 Reference Spectra (SCIA) GADS</i>
<i>DSD pointing to the HCHO Reference Spectra (SCIA)GADS</i>
<i>DSD pointing to the OCIO Reference Spectra (SCIA) GADS</i>
<i>DSD pointing to the NO Reference Spectra (SCIA) GADS</i>
DSD pointing to the O2 Reference Spectra (SCIA) GADS
O3 Reference Spectra (GOME) GADS
NO2 Reference Spectra (GOME) GADS
Ring Reference Spectra (GOME) GADS
O3 Reference Spectra (SCIA) GADS
NO2 Reference Spectra (SCIA) GADS
BrO Reference Spectra (SCIA) GADS
SO2 Reference Spectra (SCIA) GADS

HCHO Reference Spectra (SCIA) GADS
OCIO Reference Spectra (SCIA) GADS
NO Reference Spectra (SCIA) GADS
O2 Reference Spectra (SCIA) GADS

#### 15.6.14.1.1 O3 Reference Spectra (GOME) GADS

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

The molecule names in the GADSs below are given in left-justified ASCII characters. Unused characters shall be filled with ASCII blank characters.

N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels (O3, GOME-FM-spectra)	-	2	us	1
3	Number of spectral segments	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
6	Number of temperatures per segment	-	4	us	2
7	Number of coefficients per segment	-	4	us	2
8	Number of spectral entries per segment (O3, GOME-FM-spectra)	-	4	us	2
9	Type of formula for coefficients	-	1	uc	1
10	Type of wavelength information	-	1	uc	1
12	Temperature grid for first segment	K	20	fl	5
13	Wavelength grid for spectral segment (O3, GOME-FM-spectra)	nm	72184	fl	18046
14	Cross-sections for first spectral segment per temperature (O3, GOME-FM-spectra)	cm2/mol	66780	fl	16695
15	Cross-sections coefficients for second spectral segment (O3, GOME-FM-spectra, Hartley-Huggins bands)	-	16212	fl	4053
<i>Size of Component:</i>			<b>155223</b>		

The ozone spectra is specified in two segments in different ways : in the first segment as cross-sections on a temperature grid and in the second segment (called the Hartley-

Huggins bands) by coefficients of a temperature dependent formula. In fact, the second segment is a subset of the first.

The first segment is given at five temperatures between 200 K and 300 K. The wavelength grids cover the spectral range from about 230 nm up to about 800 nm, a total of 3330 to 3339 entries (depending on temperature, see remark in the description of the refspect structure). These spectra are available as a function of wavelength at the five different temperatures. The number of cross-section entries is identical to the number of wavelength entries per block.

In the Hartley-Huggins bands, additional cross-sections coefficients are stored in the data base. Three sets of coefficients are available. The wavelength grid covers the spectral range from 235.0 nm up to 370.0 nm, a total of 1351 entries. Cross-sections coefficients are available as a function of wavelength. The first entry corresponds to the first data set and the first wavelength entry, running over wavelength and then over data set number, a total of 4053 entries (1351\*3).

#### 15.6.14.1.2 NO2 Reference Spectra (GOME) GADS

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

The molecule names in the GADSs below are given in ASCII. Unused characters shall be filled with ASCII blank characters.

Table 15.6.14.1.2-1 GOME - NO2 Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (NO <sub>2</sub> , GOME-FM-spectra)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
6	Number of temperatures	-	2	us	1
8	Number of spectral entries (NO <sub>2</sub> , GOME-FM-spectra)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
12	Temperature grid (NO <sub>2</sub> , GOME-FM-spectra)	K	16	fl	4
13	Wavelength grid per temperature (NO <sub>2</sub> , GOME-FM-spectra)	nm	54528	fl	13632
14	Cross-sections per temperature (NO <sub>2</sub> , GOME-FM-spectra)	cm <sup>2</sup> /mol	54528	fl	13632
<i>Size of Component:</i>		-	<b>109090</b>	-	-

The NO<sub>2</sub> spectra is specified in one segment and four different temperatures between 200 K and 300 K. The wavelength grids cover the spectral range from about 230 nm up to about 800 nm, a total of 3408 entries in one segment. Cross-sections are available for each block as a function of wavelength, representing the four different temperatures. The number of cross-section entries is identical to the number of wavelength entries per block.

### 15.6.14.1.3 Ring Reference Spectra (GOME) GADS

The GADS format is described in the table below.

Table 15.6.14.1.3-1 GOME -Ring Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Spectra type	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segment (channels)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
8	Number of spectral entries (per channel)	-	4	us	2
10	Type of wavelength information	-	1	uc	1
13	Wavelength grid per channel	nm	6408	fl	1602
14	Ring spectrum values per channel	-	6408	fl	1602
<i>Size of Component:</i>			<b>12834</b>		

The FM-derived Ring spectrum has two segments covering the 2 default DOAS fitting windows. The channel 2 segment contains 764 points from 320.189 nm to 405.168 nm. The channel 3 segment contains 838 points from 405.206 nm to 580.985 nm. Other than the literature Ring spectrum the measured Ring spectrum is based on a wavelength grid and therefore the type of wavelength information is 1.

### 15.6.14.1.4 O3 Reference Spectra (SCIA) GADS

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

Table 15.6.14.1.4-1 SCIA - O3 Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5

Table 15.6.14.1.4-1 SCIA - O3 Reference Spectra GADS					
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (O <sub>3</sub> , SCIA-FM-spectra)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
6	Number of temperatures	-	2	us	1
8	Number of spectral entries (O <sub>3</sub> , SCIA-FM-spectra)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
12	Temperature grid	K	20	fl	5
13	Wavelength grid per temperature (O <sub>3</sub> , SCIA-FM-spectra)	nm	47780	fl	11970
14	Cross-sections per temperature (NO <sub>2</sub> , GOME-FM-spectra)	cm <sup>2</sup> /mol	47780	fl	11970
<i>Size of Component:</i>		-	<b>95798</b>	-	-

The O<sub>3</sub> spectrum is specified in one segment and for five different temperatures between 200 K and 300 K (203, 223, 243, 273, 293 K). The wavelength grids cover the spectral range from about 230 nm up to about 600 nm, a total of 2394 entries. Cross-sections are available for each block as a function of wavelength, representing the five different temperatures. The number of cross-section entries is identical to the number of wavelength entries per block.

#### 15.6.14.1.5 NO<sub>2</sub> Reference Spectra (SCIA) GADS

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

Table 15.6.14.1.5-1 SCIA - NO2 Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (NO <sub>2</sub> , SCIA-FM-spectra)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
6	Number of temperatures	-	2	us	1
8	Number of spectral entries (NO <sub>2</sub> , SCIA-FM-spectra)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
12	Temperature grid (NO <sub>2</sub> , SCIA-FM-spectra)	K	16	fl	4

Table 15.6.14.1.5-1 SCIA - NO <sub>2</sub> Reference Spectra GADS					
13	Wavelength grid per temperature (NO <sub>2</sub> , SCIA-FM-spectra)	nm	50320	fl	12580
14	Cross-sections per temperature (NO <sub>2</sub> , SCIA-FM-spectra)	cm <sup>2</sup> /mol	50320	fl	12580
<i>Size of Component:</i>			-	<b>100674</b>	-

The NO<sub>2</sub> spectrum is specified in one segment and four different temperatures between 200 K and 300 K (223, 243, 273, 293 K). The wavelength grids cover the spectral range from about 233 nm up to about 769 nm, a total of 3145 entries. Cross-sections are available for each block as a function of wavelength, representing the five different temperatures. The number of cross-section entries is identical to the number of wavelength entries per block.

#### 15.6.14.1.6 BrO Reference Spectra (SCIA) GADS

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

Table 15.6.14.1.6-1 SCIA - BrO Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (BrO, SCIA-FM-spectra)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
6	Number of temperatures	-	2	us	1
8	Number of spectral entries (BrO, SCIA-FM-spectra)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
12	Temperature grid (BrO, SCIA-FM-spectra)	K	12	fl	3
13	Wavelength grid per temperature (BrO, SCIA-FM-spectra)	nm	88840	fl	22210
14	Cross-sections per temperature (BrO, SCIA-FM-spectra)	cm <sup>2</sup> /mol	88840	fl	22210
<i>Size of Component:</i>			-	<b>177718</b>	-

The BrO spectrum is specified in one segment and five different temperatures between 200 K and 300 K (203, 223, 243, 273, 293 K). The wavelength grids cover the spectral range from about 304 nm up to about 378 nm, a total of 4442 entries. Cross-sections are available for each block as a function of wavelength, representing the three different temperatures. The number of cross-section entries is identical to the number of

wavelength entries per block.

#### 15.6.14.1.7 SCIA -SO2 Reference Spectra GADS

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

Table 15.6.14.1.7-1 SCIA - SO2 Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (SO <sub>2</sub> , SCIA-FM-spectra)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
6	Number of temperatures	-	2	us	1
8	Number of spectral entries (SO <sub>2</sub> , SCIA-FM-spectra)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
12	Temperature grid	K	20	fl	5
13	Wavelength grid per temperature (NO <sub>2</sub> , GOME-FM-spectra)	nm	28040	fl	7010
14	Cross-sections per temperature (SO <sub>2</sub> , SCIA-FM-spectra)	cm <sup>2</sup> /mol	28040	fl	7010
<i>Size of Component:</i>		-	<b>56118</b>	-	-

The SO<sub>2</sub> spectrum is specified in one segment and for five different temperatures between 200 K and 300 K (203, 223, 243, 273, 293 K). The wavelength grids cover the spectral range from about 239 nm up to about 395 nm, a total of 1402 entries in one segment. Cross-sections are available for each block as a function of wavelength, representing the five different temperatures. The number of cross-section entries is identical to the number of wavelength entries per block.

#### 15.6.14.1.8 SCIA -HCHO Reference Spectra GADS

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

Table 15.6.14.1.8-1 SCIA - HCHO Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1

N	Description	Units	Byte Size	Data Type	Dim.
3	Number of spectral segments (HCHO, SCIA-FM-spectra)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
6	Number of temperatures	-	2	us	1
8	Number of spectral entries (HCHO, SCIA-FM-spectra)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
12	Temperature grid	K	4	fl	1
13	Wavelength grid per temperature (HCHO, SCIA-FM-spectra)	nm	5532	fl	1383
14	Cross-sections per temperature (HCHO, SCIA-FM-spectra)	cm <sup>2</sup> /mol	5532	fl	1383
<i>Size of Component:</i>		-	<b>11086</b>	-	-

The HCHO spectrum is specified in one segment and one temperature (293 K). The wavelength grids cover the spectral range from about 247 nm up to about 400 nm, a total of 1383 entries. Cross-sections are available as a function of wavelength. The number of cross-section entries is identical to the number of wavelength entries.

#### 15.6.14.1.9 OCIO Reference Spectra (SCIA) GADS

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

N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (OCIO, SCIA-FM-spectra)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
6	Number of temperatures	-	2	us	1
8	Number of spectral entries (OCIO, SCIA-FM-spectra)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
12	Temperature grid	K	4	fl	1
13	Wavelength grid per temperature (OCIO, SCIA-FM-spectra)	nm	5012	fl	1253



Table 15.6.14.1.9-1 SCIA - OCIO Reference Spectra GADS					
14	Cross-sections per temperature (OCIO, SCIA-FM-spectra)	cm <sup>2</sup> /mol	5012	fl	1253
<i>Size of Component:</i>		-	10046	-	-

The OCIO spectrum is specified in one segment and for one temperature (293 K). The wavelength grids cover the spectral range from about 291 nm up to about 460 nm, a total of 1253 entries. Cross-sections are available as a function of wavelength. The number of cross-section entries is identical to the number of wavelength entries.

#### 15.6.14.1.10 NO Reference Spectra (SCIA) GADS

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

Table 15.6.14.1.10-1 SCIA - NO Reference Spectra GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Molecule name	ascii	5	uc	5
2	Number of atmospheric levels	-	2	us	1
3	Number of spectral segments (NO, SCIA-FM-spectra)	-	2	us	1
4	Maximum number of temperatures	-	2	us	1
5	Maximum number of coefficients	-	2	us	1
6	Number of temperatures	-	2	us	1
8	Number of spectral entries (NO, SCIA-FM-spectra)	-	2	us	1
10	Type of wavelength information	-	1	uc	1
12	Temperature grid	K	4	fl	1
13	Wavelength grid per temperature (NO, SCIA-FM-spectra)	nm	1600	fl	400
14	Cross-sections per temperature (NO, SCIA-FM-spectra)	cm <sup>2</sup> /mol	1600	fl	400
<i>Size of Component:</i>		-	3222	-	-

The NO spectrum is specified in one segment and for one temperature (293 K). The wavelength grids cover the spectral range from about 214 nm up to about 260 nm, a total of 400 entries in one segment. Cross-sections are available as a function of wavelength. The number of cross-section entries is identical to the number of wavelength entries.

#### 15.6.14.1.11 O2 Reference Spectra (SCIA) GADS

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

<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	<b>Molecule name</b>	ascii	5	uc	5
2	<b>Number of atmospheric levels</b>	-	2	us	1
3	<b>Number of spectral segments (O<sub>2</sub>, SCIA-FM-spectra)</b>	-	2	us	1
4	<b>Maximum number of temperatures</b>	-	2	us	1
5	<b>Maximum number of coefficients</b>	-	2	us	1
6	<b>Number of temperatures</b>	-	2	us	1
8	<b>Number of spectral entries (O<sub>2</sub>, SCIA-FM-spectra)</b>	-	2	us	1
10	<b>Type of wavelength information</b>	-	1	uc	1
12	<b>Temperature grid</b>	K	12	fl	3
13	<b>Wavelength grid per temperature (O<sub>2</sub>, SCIA-FM-spectra)</b>	nm	49152	fl	12288
14	<b>Cross-sections per temperature (O<sub>2</sub>, SCIA-FM-spectra)</b>	cm <sup>2</sup> /mol	49152	fl	12288
<i>Size of Component:</i>		-	<b>98334</b>	-	-

The O<sub>2</sub> spectrum is specified in one segment and for three different temperatures between 200 K and 300 K (203, 243, 293 K). The wavelength grids cover the spectral range from about 214 nm up to about 810 nm, a total of 4096 entries. Cross-sections are available for each block as a function of wavelength, representing the three different temperatures. The number of cross-section entries is identical to the number of wavelength entries per block.

### 15.6.15 Undersampling correction spectra File

FILE ID: SCI\_UC2\_AX

TYPE: Auxiliary USE: Level 2 processing

UPDATED: infrequently

SIZE: MPH(1247 bytes) + SPH(378 bytes) + GADS(32832 bytes) = 34457

bytes

#### 15.6.15.1 Format

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

**Table 15.6.15.1-1 - Schematic Structure of the Undersampling correction spectra File**

<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 1 DSD:</b>
<i>DSD pointing to the Undersampling spectra GADS</i>
<b>Undersampling spectra GADS</b>

**15.6.15.1.1 Undersampling correction channel 2 GADS**

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

<b>Table 15.6.15.1.1-1 Undersampling correction channel 2 GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	<b>Spectra type</b>	-	5	uc	5
2	<b>Number of atmospheric levels</b>	-	2	us	1
3	<b>Number of spectral segments (channel)</b>	-	2	us	1
4	<b>Maximum number of temperatures</b>	-	2	us	1
5	<b>Maximum number of coefficients</b>	-	2	us	1
6	<b>Number of spectral entries in channel</b>	-	2	us	1
7	<b>Type of wavelength information</b>	-	1	uc	1
8	<b>Wavelength grid channel</b>	nm	4096	fl	1024
9	<b>Cross-sections for channel</b>	cm <sup>2</sup> /mol	4096	fl	1024
<i>Size of Component:</i>			<b>8208</b>		

The undersampling spectrum is available for the entire channel. There is only one spectral segment.

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 earth-shine 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. The correction spectra cover the spectral regions of interest for DOAS and IAS applications.

**15.6.15.1.2 Undersampling correction channel 3 GADS**

The format of the GADS is identical to that of Undersampling correction channel 2 described in Table 15.6.15.1.1-1.

**15.6.15.1.3 Undersampling correction channel 7 GADS**



The format of the GADS is identical to that of Undersampling correction channel 2 described in Table 15.6.15.1.1-1.

**15.6.15.1.4 Undersampling correction channel 8 GADS**

The format of the GADS is identical to that of Undersampling correction channel 2 described in Table 15.6.15.1.1-1.

**15.6.16 PMD minimum reflectance library File**

FILE ID: SCI\_CC2\_AX

TYPE: Auxiliary USE: Level 2 processing

UPDATED: infrequently

SIZE: MPH(1247 bytes) + SPH(378 bytes) + GADS(3000006 bytes) =

Approx.

3Mbytes

**15.6.16.1 Format**

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

**Table 15.6.16.1-1 - Schematic Structure of the PMD minimum reflectance library File**

<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 1 DSD:</b> <i>DSD pointing to the PMD minimum reflectance data base GADS</i>
<b>PMD minimum reflectance data base GADS</b>

**15.6.16.1.1 PMD minimum reflectance data base GADS**

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

<b>Table 15.6.16.1.1-1 PMD minimum reflectance data base GADS</b>
---

Table 15.6.16.1.1-1 PMD minimum reflectance data base GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Number of PMD-channels used in CCA (n)	-	2	us	1
2	Number of latitude entries	-	2	us	1
4	Number of longitude entries	-	2	us	1
4	Reflectance thresholds	-	n* 1000000	ss	n*500 000
<i>Size of Component:</i>			<b>3000006</b> <sup>a</sup>		

a. Number of PMD-channels may be increased in the future which also increase the number of PMD thresholds.

The reflectance thresholds are given as a function of the geolocation and special coverage of the PMD's. The reference grids for latitude and longitude can be derived from the number of points per latitude (500) and longitude (1000). The first reference latitude corresponds to the interval from -90° to -89.64° and the first longitude corresponds to the interval from 0° to 0.36°. The first reflectance threshold is valid for the first PMD, the first reference latitude and the first reference longitude. The values run over the PMD channel number, then latitude and finally longitude, making a total of 1 500 000 entries (3\*500\*1000). Looping by channel, longitude, latitude being channel the innermost (faster) cycle, latitude the outermost.

The values are in the range (0,100); In fact, they are currently even smaller than 50. To reduce the size of the table, the values in the data base are first scaled by a factor 0.01 and then by a factor of 32768 (the maximum size of a signed short int).

### 15.6.17 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

SIZE: MPH(1247 bytes) + SPH(658 bytes) + GADS approx. 2.621 MB) =  
 approx. 2.623MB



**15.6.17.1 Format**

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

**Table 15.6.17.1-1 - Schematic Structure of the Air Mass Factor Look-Up Table File**

<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 2 DSD:</b>  <i>DSD pointing to the AMF LUT for O3 GADS</i>  <i>DSD pointing to the AMF LUT for NO2 GADS</i>  <i>DSD pointing to the AMC DOAS LUT for H2O GADS</i>
<b>AMF LUT for O3 GADS</b>
<b>AMF LUT for NO2 GADS</b>
<b>AMC DOAS LUT for H2O GADS</b>

Three look-up tables are required. The DS\_NAME field of the DSDs will be specified according to the content of the corresponding GADS. The following keywords are envisaged:

- AMF\_O3
- AMF\_NO2
- AMC\_H2O

The dataset identified by AMC\_H2O is used by the AMC-DOAS algorithm, and has its own format.

**15.6.17.1.1 AMF LUT for O3 GADS**

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

<b>Table 15.6.17.1.1-1 AMF LUT for O3 GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	Number of reference wavelengths	-	2	us	1
2	Number of reference heights	-	2	us	1
3	Number of reference 'scenarios' (see note)	-	2	us	1

Table 15.6.17.1.1-1 AMF LUT for O3 GADS					
4	Number of reference albedos	-	2	us	1
5	Number of reference aerosol types	-	2	us	1
6	Number of coefficients in solar zenith angle parameterisation	-	2	us	1
7	Number of coefficients in line-of-sight nadir angle parameterisation	-	2	us	1
8	Number of azimuths	-	2	us	1
9	Number of reference days	-	2	us	1
10	Reference wavelengths	nm	8	fl	2
11	Reference heights	km	28	fl	7
12	Latitude grid of the reference scenarios	degree	32	fl	8
13	Reference albedos	%	16	fl	4
14	Reference azimuths	degree	20	fl	5
15	Reference days	-	8	us	4
16	Air Mass Factor coefficient O <sub>3</sub>	-	1747200	do	218400
<i>Size of Component:</i>			<b>1747330</b>		

The azimuths are given from 0° to 180° in steps of 45°, a total of 5 entries. The reference heights are given from 0 km up to 8 km, a total of 7 entries. The reference albedos are given from 5% up to 95%, a total of 4 entries. There are two different aerosol types: maritime (1) and rural (2).

The reference scenarios are a combination of latitude zones and season (reference days for a time interpolation), a total of 26 entries. The following scheme is used :

- 1-4 : latitude zone 85 degree in spring (1), summer (2), autumn (3) and winter (4)
- 5-8 : latitude zone -85 degree in spring (7), summer (8), autumn (6) and winter (5)
- 9-12 : latitude zone 50 degree in spring (9), summer (10), autumn (11) and winter (12)
- 13-16 : latitude zone 35 degree in spring (13), summer (14), autumn (15) and winter (16)
- 17-20 : latitude zone -35 degree in spring (19), summer (20), autumn (17) and winter (18)
- 21-24 : latitude zone -60 degree in spring (23), summer (24), autumn (21) and winter (22)
- 25 : latitude zone 10 degree the same for all seasons
- 26 : latitude zone -10 degree the same for all seasons

No seasonal dependency is parameterised in the tropics. thus the total number of entries is 8 (ref. latitude bands) \* 4 (seasons) - 6 (no seasons in the tropics) = 26. To reduce the size of the AMF look-up table, the 3 geometrical angles are not used directly in the database, but they are parameterised using polynomial fits. The parameterisation scheme used for the AMF tables uses a hyperbolic fit (4+1 coefficients out of 14 calculated values, the one extra value is used to handle angles > 90°) for the solar zenith angle, a 2th order polynomial (3 coefficients out of 8 calculated values) for the line-of-sight nadir angle. Total 15 coefficients for the geometry. The fitting order for these coefficients is line-of-sight nadir and then solar zenith.

The Air Mass Factors are given beginning with the first wavelength (for NO<sub>2</sub> there's only one), the first reference scenario, the first azimuth angle, height value (0 km), the first albedo value (5%), the first aerosol scenario (maritime) and the first parameter of the geometrical parameterisation. They run first over the geometrical coefficients, then over aerosol type, then albedo value, then height values, then azimuth angles, then the reference scenarios and finally the wavelengths giving a total of 218400 values ( $2 \times 26 \times 5 \times 7 \times 4 \times 2 \times 15 = 218400$ ) for O<sub>3</sub>.

**15.6.17.1.2 AMF LUT for NO<sub>2</sub> GADS**

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

Table 15.6.17.1.2-1 AMF LUT for NO <sub>2</sub> GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Number of reference wavelengths	-	2	us	1
2	Number of reference heights	-	2	us	1
3	Number of reference 'scenarios' (see note)	-	2	us	1
4	Number of reference albedos	-	2	us	1
5	Number of reference aerosol types	-	2	us	1
6	Number of coefficients in solar zenith angle parameterisation	-	2	us	1
7	Number of coefficients in line-of-sight nadir angle parameterisation	-	2	us	1
8	Number of azimuths	-	2	us	1
9	Number of reference days	-	2	us	1
10	Reference wavelengths	nm	8	fl	2
11	Reference heights	km	28	fl	7
12	Latitude grid of the reference scenarios	degree	32	fl	8
13	Reference albedos	%	16	fl	4
14	Reference azimuths	degree	20	fl	5
15	Reference days	-	8	us	4
16	Air Mass Factor coefficient NO <sub>2</sub>	-	873600	do	109200
<i>Size of Component:</i>			<b>873730</b>		

The azimuths are given from 0° to 180° in steps of 45°, a total of 5 entries. The reference heights are given from 0 km up to 8 km, a total of 7 entries. The reference albedos are given from 5% up to 95%, a total of 4 entries. There are two different aerosol types: maritime (1) and rural (2).

The reference scenarios are a combination of latitude zones and season (reference days for a time interpolation), a total of 26 entries. The following scheme is used :

The reference scenarios are a combination of latitude zones and season (reference days



for a time interpolation), a total of 26 entries. The following scheme is used :

- 1-4 : latitude zone 85 degree in spring (1), summer (2), autumn (3) and winter (4)
- 5-8 : latitude zone -85 degree in spring (7), summer (8), autumn (6) and winter (5)
- 9-12 : latitude zone 50 degree in spring (9), summer (10), autumn (11) and winter (12)
- 13-16 : latitude zone 35 degree in spring (13), summer (14), autumn (15) and winter (16)
- 17-20 : latitude zone -35 degree in spring (19), summer (20), autumn (17) and winter (18)
- 21-24 : latitude zone -60 degree in spring (23), summer (24), autumn (21) and winter (22)
- 25 : latitude zone 10 degree the same for all seasons
- 26 : latitude zone -10 degree the same for all seasons

No seasonal dependency is parameterised in the tropics. thus the total number of entries is 8 (ref. latitude bands) \* 4 (seasons) - 6 (no seasons in the tropics) = 26.

To reduce the size of the AMF look-up table, the 3 geometrical angles are not used directly in the database, but they are parameterised using polynomial fits. The parameterisation scheme used for the AMF tables uses a hyperbolic fit (4+1 coefficients out of 14 calculated values, the one extra value is used to handle angles > 90°) for the solar zenith angle, a 2th order polynomial (3 coefficients out of 8 calculated values) for the line-of-sight nadir angle. Total 15 coefficients for the geometry. The fitting order for these coefficients is line-of-sight nadir and then solar zenith.

The Air Mass Factors are given beginning with the first wavelength (for NO<sub>2</sub> only), the first reference scenario, the first azimuth angle, height value (0 km), the first albedo value (5%), the first aerosol scenario (maritime) and the first parameter of the geometrical parameterisation. They run first over the geometrical coefficients, then over aerosol type, then albedo value, then height values, then azimuth angles, then the reference scenarios and finally the wavelengths giving a total of 109200 values (26\*5\*7\*4\*2\*15 = 109200) for NO<sub>2</sub>.

#### 15.6.17.1.3 AMC LUT for H2O GADS

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

Table 15.6.17.1.3-1 AMC LUT for H2O GADS					
N	Description	Units	Byte Size	Data Type	Dim.
1	Number of reference solar zenith angles	-	2	us	1
2	Number of reference wavelengths	-	2	us	1
3	Reference solar zenith angles	-	72	do	9
4	Reference wavelengths	-	4800	do	600
5	2D matrix of coefficients b	-	43200	do	5400
6	2D matrix of coefficients c	-	43200	do	5400
7	2D matrix of coefficients τO <sub>2</sub>	-	43200	do	5400
<i>Size of Component:</i>			<b>134476</b>		



The coefficients  $b$ ,  $c$  and  $\tau_{O2}$  are needed for the AMC-DOAS algorithm. Coefficients run first over SZAs, then over wavelengths. There is a total of  $9 \times 600 = 5400$  entries for each coefficient.

### 15.6.18 BIAS Slant Path Factor Look-Up Table File

Used for BIAS component of the Level 2 processing.

FILE ID: SCI\_PF2\_AX

TYPE: Auxiliary

USE: Level 2 processing

UPDATED: infrequently

SIZE: MPH(1247 bytes) + SPH(378 bytes) + GADS (1092 bytes) = approx. 2.7kbytes.

#### 15.6.18.1 Format

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

**Table 15.6.18.1-1 - Schematic Structure of the BIAS Slant Path Factor Look-Up Table File**

<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 1 DSDs:</b> <i>DSD pointing to the Slant Path Factors LUT GADS</i>
<b>Slant Path Factors LUT GADS</b>

#### 15.6.18.1.1 Slant Path Factors LUT GADS

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

<b>Table 15.6.18.1.1-1 BIAS Slant Path Factors LUT GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	<b>Number of atmospheric levels</b>	-	2	us	1
2	<b>Number of reference solar zeniths</b>	-	2	us	1
3	<b>Reference solar zenith angles</b>	degrees	64	fl	16
4	<b>Slant path factors</b>	-	1024	fl	256
<i>Size of Component:</i>			<b>1092</b>		

### 15.6.19 AAIA Rayleigh Correction Look-Up Table File

This file contains the Rayleigh Correction 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

SIZE: MPH(1247 bytes) + SPH(378 bytes) + GADS (42336 bytes) = approx. 44kbytes.

#### 15.6.19.1 Format

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

**Table 15.6.19.1-1 - Schematic Structure of the AAIA Rayleigh Correction Look-Up Table File**

<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 1 DSDs:</b> <i>DSD pointing to the AAIA Rayleigh Correction Look-Up Table GADS</i>
<b>AAIA Rayleigh Correction Look-Up Table GADS</b>

#### 15.6.19.1.1 AAIA Rayleigh Correction Look-Up Table GADS

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

<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	Number of reference heights	-	2	us	1
2	Number of reference wavelengths	-	2	us	1
3	Number of reference albedos	-	2	us	1
4	Number of azimuth harmonics	-	2	us	1
5	Number of coefficients in solar zenith angle parameterisation	-	2	us	1
6	Number of coefficients in line-of-sight nadir angle parameterisation	-	2	us	1
7	Reference heights	km	44	fl	11
8	Reference wavelength	nm	8	fl	2
9	Reference albedos	-	32	fl	8

Table 15.6.19.1.1-1 AAIA Rayleigh Correction Look-Up Table GADS					
10	Rayleigh reflectance coefficient, first harmonic	SR -1	33792	do	4224
11	Rayleigh reflectance coefficient, second harmonic	SR -1	4224	do	528
12	Rayleigh reflectance coefficient, third harmonic	SR -1	4224	do	528
<i>Size of Component:</i>			<b>42336</b>		

The reference albedos are given from 0.0 to 0.90, a total of 8 entries. The reference wavelengths are 340 nm and 380 nm.

To reduce the size of the Rayleigh reflectance look-up table, geometric angles are not used directly in the database, but they are parameterised using polynomial fits. The parameterization scheme for this table has a 5th order polynomial (6 coefficients out of 14 calculated values) for the solar zenith cosine dependence and a third order polynomial (4 coefficients out of 8 calculated values) for the line of sight nadir cosine dependence.

The azimuth dependence is in the form of an analytic Fourier series in the cosine of the azimuth angle -- for Rayleigh scattering just three terms in the series are required. Twenty-four zenith angle coefficients are specified for each harmonic; a total of 72 coefficients for the geometry. The fitting order for these coefficients is first line-of-sight nadir polynomial, and then the solar zenith polynomial fitting.

The Rayleigh reflectance coefficients for the first harmonic are given beginning with the first wavelength, the first height and the first parameter of the double zenith-angle parameterisation. They run first over the geometrical coefficients, then over albedo, then over height and then over wavelength giving a total of 4224 values ( $24 \times 8 \times 1 \times 21 = 4224$ ). The second and third harmonics do not have an albedo dependency. The ordering (except for the albedo) is similar to that for the first harmonic, giving a total of 528 values ( $24 \times 11 \times 2 = 528$ ) for harmonic 2 and 3.

### 15.6.20 Static parameters for the level 2 off-line product Initialization file

This SCI\_IN\_AX file is used to specify the following parameters for the level 2 off-line product:

- overall control of the level 1b to 2 processing chain,
- DOAS/IAS fitting specifications (windows, reference spectra, fitting control, etc.),
- parameters controlling the LUTs,
- parameters controlling cloud fitting and aerosol indicator algorithms.
- Limb retrieval specifications.
- etc.

The GADS of the initialisation file for the static parameters is a block of ASCII data formatted with XML representing the static parameters of the level 1b to 2 processing. The position of the parameters in the XML file is arbitrary.

### 15.6.20.1 Format

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

**Table 15.6.20.1-1 - Schematic Structure of the SCI\_IN\_\_AX File**

<b>MPH</b>
<b>SPH -Auxiliary Data SPH (defined in Volume 16) with 1 DSDs:</b>  <i>DSD pointing to the Static Parameter GADS</i>
<b>Static parameter of the Level2 off-line Processor GADS</b>

#### 15.6.20.1.1 Static Parameter of the Level 2 off-line Processor GADS

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

<b>Table 15.6.20.1.1-1 Static parameter of the Level2 off-line Processor GADS</b>					
<b>N</b>	<b>Description</b>	<b>Units</b>	<b>Byte Size</b>	<b>Data Type</b>	<b>Dim.</b>
1	<b>Xml text of the initialisation file which covers the complete range of static parameters (the present size is an estimation)</b>	-	variable	var.	var.
<i>Size of Component:</i>			<b>Variable</b>		

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

### 15.6.21 ECMWF Data Files

The SCIAMACHY processors have been build in a way to use the ECMWF data files. These files are common to many instruments and are hence defined in Volume 16. However SCIAMACHY processors up to level 2 off-line version 5.01 do not use the ECMWF files.

### 15.6.22 Orbit State Vectors

The Orbit State Vectors files available from the FOS or from the DORIS data are defined in Volume 16.

## 15.7 PRODUCT SUMMARY SHEETS

The data on the following pages is extracted from the product summary information contained in the DDT data base.



<b>SCIAMACHY Level 0</b>	
<b>PRODUCT ID</b>	SCI_NL__0P
<b>PRODUCT NAME</b>	SCIAMACHY Level 0
<b>DESCRIPTION</b>	This data consists of time ordered AISPs containing spectra measured from light transmitted, backscattered or reflected by trace gases in the atmosphere.
<b>APPLICATIONS</b>	Archived product forming basis for all higher level processing
<b>DELIVERY TIME</b>	NRT version available from PDHS within 3 hours from data take. OFL (fully consolidated) version available from the LRAC starting 1-2 weeks after data take.
<b>COVERAGE</b>	full orbit, nadir and limb measurements
<b>THROUGHPUT</b>	1 product per orbit (100'); 400 kbps instrument data rate.
<b>PRODUCT SIZE</b>	max: 230 MB per orbit
<b>GEOMETRICAL SAMPLING</b>	Limb: samples atmosphere between 1 and 100 km.
<b>GEOMETRIC RESOLUTION</b>	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
<b>GEOMETRIC ACCURACY</b>	Information not available
<b>RADIOMETRIC RESOLUTION</b>	spectral resolution: 0.24 to 1.5 nm, depends on spectral range coded on 16 or 24 bits/sample
<b>RADIOMETRIC ACCURACY</b>	N/A
<b>AUXILIARY DATA</b>	Orbit State Vectors; SBT/UTC Time conversion parameters
<b>ALGORITHMS USED</b>	Satellite positioning, UTC time conversion
<b>NOTES</b>	produced systematically



<b>SCIAMACHY Geolocated and Calibrated Spectra</b>	
<b>PRODUCT ID</b>	SCI_NL__1P
<b>PRODUCT NAME</b>	SCIAMACHY Geolocated and Calibrated Spectra
<b>DESCRIPTION</b>	This is the base level 1B product for SCIAMACHY and includes calibrated spectra, calibration and housekeeping information. Calibration data has been 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.
<b>APPLICATIONS</b>	Calibrated product is basis for Level 2 generation
<b>DELIVERY TIME</b>	NRT product available from PDHS within 3 hours from data take. OFL (fully consolidated) product available from the D-PAC starting 2 weeks after data take ( not LRAC anymore since Dec 2004)
<b>COVERAGE</b>	full orbit, nadir and limb measurements
<b>THROUGHPUT</b>	1 product per orbit
<b>PRODUCT SIZE</b>	max. size approx 400 MBytes per orbit
<b>GEOMETRICAL SAMPLING</b>	Limb: samples atmosphere between 1 and 100 km.
<b>GEOMETRIC RESOLUTION</b>	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
<b>GEOMETRIC ACCURACY</b>	information not available
<b>RADIOMETRIC RESOLUTION</b>	coded on 16 or 24 bits/sample spectral resolution: 0.24 to 1.5 nm, depends on spectral range
<b>RADIOMETRIC ACCURACY</b>	Sun normalized radiometric accuracy: 2-3 % (unpolarized light); 3-4% polarized light. Relative radiometric accuracy < 1%. Spectral accuracy 0.005 to 0.035 nm.
<b>ALGORITHMS USED</b>	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);
<b>NOTES</b>	produced systematically from Level 0 data





<b><u>SCIAMACHY Vertical Column Amounts</u></b>	
<b>PRODUCT ID</b>	SCI_NL__2P
<b>PRODUCT NAME</b>	SCIAMACHY Vertical Column Amounts
<b>DESCRIPTION</b>	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 SCI_NL__1P product measurements.
<b>APPLICATIONS</b>	Measurement of ozone and other atmospheric constituents for meteorology and climatology
<b>DELIVERY TIME</b>	NRT product available from PDHS within 3 hours from data take. OFL (fully consolidated) product available from the PAC starting 3 to 4 weeks after data take.
<b>COVERAGE</b>	full orbit, nadir and limb measurements
<b>THROUGHPUT</b>	1 product per orbit
<b>PRODUCT SIZE</b>	max. size of approx. 6 MBytes per orbit
<b>GEOMETRICAL SAMPLING</b>	N/A
<b>GEOMETRIC RESOLUTION</b>	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
<b>GEOMETRIC ACCURACY</b>	information not available
<b>RADIOMETRIC RESOLUTION</b>	N/A
<b>RADIOMETRIC ACCURACY</b>	N/A
<b>AUXILIARY DATA</b>	Summary Quality ADS (SQADS) Geolocation ADS (LADS) Geolocation of the Ground Pixels ADS
<b>ALGORITHMS USED</b>	Preprocessing of a priori information Processing of atmospheric initial guess profile data; Processing of observing geometry data Preparation of input data for fitting process Retrieval of geophysical target qualities Noise assessment
<b>NOTES</b>	produced systematically from Level 1B data

<b><u>SCIAMACHY Level-2 Off-line product</u></b>	
<b>PRODUCT ID</b>	SCI_OL__2P
<b>PRODUCT NAME</b>	SCIAMACHY Level-2 Off-line product
<b>DESCRIPTION</b>	This product contains geophysical trace gas columns and profiles, and other geophysical parameters including their 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.
<b>APPLICATIONS</b>	Measurement of ozone and other atmospheric constituents for meteorology and climatology
<b>DELIVERY TIME</b>	Fully consolidated product available from the PAC starting 1-2 weeks after data take.
<b>COVERAGE</b>	full orbit, nadir, limb and occultation measurements
<b>THROUGHPUT</b>	1 product per orbit
<b>PRODUCT SIZE</b>	max. size of approx. 20 MBytes per orbit
<b>GEOMETRICAL SAMPLING</b>	N/A
<b>GEOMETRIC RESOLUTION</b>	Nadir spatial resolution = typically 60 km (across track) x 30 km (along track) --depends on scan speed and integration time Nadir spatial resolution = 920 m along track Limb spatial resolution = 3 km vertical Occultations = 3 km vertical
<b>GEOMETRIC ACCURACY</b>	information not available
<b>RADIOMETRIC RESOLUTION</b>	N/A
<b>RADIOMETRIC ACCURACY</b>	N/A
<b>AUXILIARY DATA</b>	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
<b>ALGORITHMS USED</b>	Preprocessing of a priori information , Processing of atmospheric initial guess profile data;  Processing of observing geometry data, Preparation of input data for fitting process Retrieval of geophysical target qualities, Noise assessment
<b>NOTES</b>	produced off-line from Level 1B data



<b><u>SCIAMACHY Selected Vertical Column Amounts for Meteo Users</u></b>	
<b>PRODUCT ID</b>	SCI_RV_2P
<b>PRODUCT NAME</b>	SCIAMACHY Selected Vertical Column Amounts for Meteo Users
<b>DESCRIPTION</b>	This Level 2 SCIAMACHY product contains selected vertical column amounts of the NRT Vertical Column Amounts product.
<b>APPLICATIONS</b>	For NRT environmental monitoring
<b>DELIVERY TIME</b>	Available 3 hours after data acquisition from the PDHS.
<b>COVERAGE</b>	full orbit
<b>THROUGHPUT</b>	1 product per orbit (approx. 100 minutes)
<b>PRODUCT SIZE</b>	approx. 200 kB per orbit
<b>GEOMETRICAL SAMPLING</b>	Limb: samples atmosphere between 1 and 100 km.
<b>GEOMETRIC RESOLUTION</b>	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
<b>GEOMETRIC ACCURACY</b>	information not available
<b>RADIOMETRIC RESOLUTION</b>	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
<b>RADIOMETRIC ACCURACY</b>	N/A
<b>AUXILIARY DATA</b>	Orbit State Vectors; SBT/UTC time conversion parameters; Geolocation of the Ground Pixels ADS
<b>ALGORITHMS USED</b>	information not available
<b>NOTES</b>	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.



## 15.8 ANNEX – PRODUCTS DISCONTINUED

### 15.8.1 SCIAMACHY Vertical Column Amounts Level 2 Product – SCI\_NL\_\_2P

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

This Level 2 SCIAMACHY product contains geophysical Trace Gas Column Densities, Cloud Top Height and cover, as well as Aerosol Absorption Indicator resulting from the processing of the SCI\_NL\_\_1P product measurements. The NRT version of this product is available within 3 hours of data acquisition and is intended for NRT atmospheric modeling. A fully consolidated version is processed systematically off-line and is available after 1 to 2 weeks from the PAC.

Level 2 products of nadir measurements may include the following trace gas columns and geophysical parameters, as indicated in the following list. This list shows the different trace gases and geophysical parameters which may be retrieved from SCIAMACHY. The amount of trace gas constituents to be retrieved is related to the availability of processing power and the availability of corresponding reference cross sections.

O3:	Column using DOAS and pre-calculated AMF look-up table in UV and visible wavelength range
NO2:	same as O <sub>3</sub> , but only in the visible wavelength range
BrO	slant column retrieval from DOAS only
SO2:	same as BrO, but only for volcanic eruptions
OCIO:	same as BrO, but only for ozone hole conditions
HCHO:	same as BrO, but only for bio mass burning
SO2:	same as BrO, but only for volcanic eruptions
Cloud:	Cloud clearing algorithm using PMDs to determine the fractional cloud cover cloud top height from database
Aerosol:	aerosol absorbing indicator algorithm
H <sub>2</sub> O:	column using BIAS
N <sub>2</sub> O:	same as H <sub>2</sub> O
CO:	same as H <sub>2</sub> O
CH <sub>4</sub> :	same as H <sub>2</sub> O, but reduced quality, because it will be a by-product of the CO retrieval



### 15.8.1.1 Input Data

Level 1B product plus auxiliary data.

### 15.8.1.2 Auxiliary Data Used

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

Table 15.8.1.2-1 - Auxiliary Data Files for SCIAMACHY Level 2 Processing	
Description	Auxiliary File ID
Level 2 Initialization file	SCI_LI2_AX
Atmospheric Climatologies Data file (Profile Data Bases)	SCI_PR2_AX
Cloud Parameters Data file	SCI_CL2_AX
Surface Data Base file	SCI_SF2_AX
Literature Cross-Sections Data Base file	SCI_CS2_AX
Flight-Model Reference Cross Spectra Data file	SCI_FM2_AX
Undersampling correction spectra file (Undersampling Data bases)	SCI_UC2_AX
PMD minimum reflectance library	SCI_CC2_AX
Air Mass Factor Look-Up-Table file	SCI_MF2_AX
BIAS slant path factor look-up table	SCI_PF2_AX
AAIA Rayleigh scattering correction look-up table	SCI_RC2_AX
Line by Line Absorption cross sections	SCI_BL2_AX

### 15.8.1.3 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.

### 15.8.1.4 Product Structure

The high level product structure is shown below:



Table 15.8.1.4-1 - SCIAMACHY Level 2 Product Structure
<b>MPH</b>
<b>SPH</b>
<b>Summary Quality ADS (SQADS)</b>
<b>Geolocation ADS (LADS)</b>
<b>States of the Product ADS</b>
<b>Geolocation of the Ground Pixels ADS</b>
<b>Cloud and Aerosol MDS</b>
<b>DOAS Trace Gas MDSs (up to 22)</b>
<b>BIAS Trace Gas MDSs (up to 10)</b>

**15.8.1.5 Main Product Header**

The Main Product Header is described in Volume 5.

**15.8.1.6 Specific Product Header**

The SPH is an ASCII header which conforms to the ASCII conventions defined in Volume 5. The Ø symbol indicates the position of an ASCII blank space character.

Table 15.8.1.6-1 Specific Product Header of Level 2 Product					
N	Description	Units	Byte Length	Data Type	Dim.
1	<b>SPH_DESCRIPTOR=</b>	keyword	15	uc	15
	quotation mark (“)	-	1	uc	1
	<b>SPH descriptor</b> (Set to SCI_NL_2P SPECIFIC HEADER)	-	28	uc	28
	quotation mark(“)	-	1	uc	1
	newline character	terminator	1	uc	1
2	<b>STRIPLINE_CONTINUITY_INDICATOR=</b>	keyword	31	uc	31
	Value: +000 = No stripline continuity, the product is a complete segment Other: Stripline Counter	-	4	Ac	1
	newline character	terminator	1	uc	1
3	<b>SLICE_POSITION=</b>	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	<b>NUM_SLICES=</b>	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
	<i>Product Location Information</i>				
5	<b>START_TIME=</b>	keyword	11	uc	11

**Table 15.8.1.6-1 Specific Product Header of Level 2 Product**

N	Description	Units	Byte Length	Data Type	Dim.
	quotation mark (“)	-	1	uc	1
	<b>Start time of the measurement data in this product</b> UTC time of the first MDSR	utc	27	uc	27
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
6	<b>STOP_TIME=</b>	keyword	10	uc	10
	quotation mark (“)	-	1	uc	1
	<b>Time of the end of the measurement data in this product (last MDSR time)</b> UTC time of the last MDSR	utc	27	uc	27
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
7	<b>START_LAT=</b>	keyword	10	uc	10
	<b>Latitude of the satellite nadir at the START_TIME</b> WGS84 latitude, positive = North	1e-6 deg	11	Al	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
8	<b>START_LONG=</b>	keyword	11	uc	11
	<b>Longitude of the satellite nadir at the START_TIME</b> 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	<b>STOP_LAT=</b>	keyword	9	uc	9
	<b>Latitude of the satellite nadir at the STOP_TIME</b> WGS84 latitude, positive = North	1e-6 deg	11	Al	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
10	<b>STOP_LONG=</b>	keyword	10	uc	10
	<b>Longitude of the satellite nadir at the STOP_TIME</b> 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	<b>Spare (blank characters (Ø))</b>	-	50	uc	50
	newline character	terminator	1	uc	1
<i>Other Product Information</i>					
12	<b>FITTING_ERROR_SUM=</b>	keyword	15	uc	15
	quotation mark (“)	-	1	uc	1
	Quality summary of the fitting errors: GOOD or FAIR or BADØ	-	28	uc	28

**Table 15.8.1.6-1 Specific Product Header of Level 2 Product**

N	Description	Units	Byte Length	Data Type	Dim.
	quotation mark(“)	-	1	uc	1
	newline character	terminator	1	uc	1
13	<b>NO_OF_DOAS_FITTING_WINDOWS=</b>	keyword	15	uc	15
	Number of DOAS fitting windows	-	28	uc	28
	newline character	terminator	1	uc	1
14	<b>DOAS_FITTING_WINDOW_0=</b>	keyword	15	uc	15
	quotation mark (“)	-	1	uc	1
	Wavelength range of fitting window given as a pattern of two wavelengths like: xxxx-yyyy e.g., 0325-0335	-	28	uc	28
	quotation mark(“)	-	1	uc	1
	newline character	terminator	1	uc	1
15-20	<b>The field above is repeated for DOAS_FITTING_WINDOW_1 to DOAS_FITTING_WINDOW_6</b>	-	204	uc	204
21	<b>NO_OF_BIAS_FITTING_WINDOWS=</b>	keyword	27	uc	27
	Number of BIAS fitting windows	-	4	Ac	1
	newline character	terminator	1	uc	1
22	<b>BIAS_FITTING_WINDOW_0=</b>	keyword	22	uc	22
	quotation mark (“)	-	1	uc	1
	Wavelength range of fitting window given as a pattern of two wavelengths like: xxxx-yyyy e.g., 0325-0335	-	9	uc	9
	Number of microwindows in this fitting window. Possible values: 00000: no microwindows are used in this fitting window 0+002: two microwindows are used in this fitting window 0+003: three microwindows are used in this fitting window	-	5	uc	5
	Wavelength range of first microwindow. Same convention as previous wavelength range but with a leading blank space 0xxxx-yyyy. Set to blank spaces if not used.	-	10	uc	10
	Wavelength range of second microwindow. Same convention as previous range of microwindow: 0xxxxyyyy. Set to blank spaces if not used.	-	10	uc	10
	Wavelength range of third microwindow. Same convention as previous range of microwindow: 0xxxx-yyyy. Set to blank spaces if not used.	-	10	uc	10
	quotation mark (“)	-	1	uc	1
	Newline character	terminator	1	uc	1
23-25	<b>The field above is repeated for BIAS_FITTING_WINDOW_1 to BIAS_FITTING_WINDOW_3</b>	-	207	uc	207



**Table 15.8.1.6-1 Specific Product Header of Level 2 Product**

N	Description	Units	Byte Length	Data Type	Dim.
26	<b>NO_OF_DOAS_MOLECULES=</b>	keyword	21	uc	21
	Number of molecules to be retrieved with DOAS	-	4	Ac	1
	Newline character	terminator	1	uc	1
27	<b>DOAS_MOLECULE_00=</b>	keyword	17	uc	17
	quotation mark (“)	-	1	uc	1
	Fitting window ID and acronym of the molecule to be retrieved given as the following pattern: W_xxxxxx e.g., 1_NO20000 note unused characters set to the ascii blank space character (Ø). Number of the fitting window corresponds to the list above.	-	8	uc	8
	quotation mark(“)	-	1	uc	1
	newline character	terminator	1	uc	1
28-49	<b>The field above is repeated for DOAS_MOLECULE_01 to DOAS_MOLECULE_21</b>	-	588	Uc	588
50	<b>NO_OF_BIAS_MOLECULES=</b>	keyword	21	uc	21
	Number of molecules to be retrieved with BIAS	-	4	Ac	1
	Newline character	terminator	1	uc	1
51	<b>BIAS_MOLECULE_0=</b>	keyword	16	uc	16
	quotation mark (“)	-	1	uc	1
	Fitting window ID and acronym of the molecule to be retrieved given as the following pattern: W-xxxxxx e.g., 1-NO20000 note unused characters set to the ascii blank space character (Ø). Number of the fitting window corresponds to the list above.	-	8	uc	8
	quotation mark (“)	-	1	uc	1
	Newline character	terminator	1	uc	1
52-60	<b>The above field is repeated for BIAS_MOLECULE_1 to BIAS_MOLECULE_9.</b>	-	243	uc	243
	<i>DSDs for Attached Data Sets</i>				
61	<i>DSD (A) for the SQ ADS</i>	-	280	dsd	1
62	<i>DSD (A) for the Geolocation ADS (L ADS)</i>	-	280	dsd	1
63	<i>DSD (A) for the States of the Product ADS</i>	-	280	dsd	1
64	<i>DSD(A) for the Geolocation of the Ground Pixels ADS</i>	-	280	dsd	1
65	<i>DSD (M) Clouds and Aerosol MDS</i>	-	280	dsd	1
66	<i>DSD (M) for the DOAS Fitting Window Trace Gas #0 -21 MDSs (unused entries set to NOT USED as described in Volume 5).</i>	-	6160	dsd	21
67	<i>DSD (M) for the BIAS Fitting Window Trace Gas #0 -9 MDSs (unused entries set to NOT USED as described in Volume 5).</i>	-	2800	dsd	10
	<i>DSDs for reference files</i>				
68	<i>DSD (R) -Level 1B product from which this product is produced</i>	-	280	dsd	1

Table 15.8.1.6-1 Specific Product Header of Level 2 Product					
N	Description	Units	Byte Length	Data Type	Dim.
69	<i>DSD (R) -Level 2 Initialization file</i>	-	280	dsd	1
70	<i>DSD (R) -Atmospheric Climatologies Data file</i>	-	280	dsd	1
71	<i>DSD (R) -Cloud Parameters Data file</i>	-	280	dsd	1
72	<i>DSD (R) -Surface Data Base file</i>	-	280	dsd	1
73	<i>DSD (R) -Literature Cross-Sections Data Base file</i>	-	280	dsd	1
74	<i>DSD (R) -Line by Line Absorption Cross-Sections file</i>	-	280	dsd	1
75	<i>DSD (R) -Flight-Model Reference Cross Spectra Data file</i>	-	280	dsd	1
76	<i>DSD (R) -Undersampling correction spectra file</i>	-	280	dsd	1
77	<i>DSD (R) -PMD minimum reflectance library file</i>	-	280	dsd	1
78	<i>DSD (R) -Air Mass Factor Look-Up-Table file</i>	-	280	dsd	1
79	<i>DSD (R) -BIAS slant path factor look-up table file</i>	-	280	dsd	1
80	<i>DSD (R) -AAIA Rayleigh scattering correction look-up table file</i>	-	280	dsd	1
81	<i>DSD -Spare (279 blank space characters followed by 1 newline character)</i>	-	280	dsd_s p	1
	<b>size (in bytes)</b>	-	<b>16199</b>	-	-

The following ASCII strings are used to fill the DS\_NAME field in the DSDs (refer to Volume 5).

Table 15.8.1.6-2 - DS_NAME Field Strings	
DSD	DS_NAME
<i>DSD (A) for the SQ ADS</i>	SUMMARY_QUALITY
<i>DSD (A) for the Geolocation ADS (L ADS)</i>	STATE_GEOLOCATION
<i>DSD (A) for the States of the Product ADS</i>	STATES
<i>DSD(A) for the Geolocation of the Ground Pixels ADS</i>	GEOLOCATION
<i>DSD (M) Clouds and Aerosol MDS</i>	CLOUDS_AEROSOL
<i>DSD (M) for the DOAS Fitting Window Trace Gas #0 MDS</i>	DOAS_0_O3
<i>DSD (M) for the DOAS Fitting Window Trace Gas #1 MDS</i>	DOAS_1_NO2
<i>DSD (M) for the DOAS Fitting Window Trace Gas #2 MDS</i>	DOAS_1_H2O
<i>DSD (M) for the DOAS Fitting Window Trace Gas #3 MDS</i>	DOAS_1_O3
<i>DSD (M) for the DOAS Fitting Window Trace Gas #4 MDS</i>	DOAS_2_BRO
<i>DSD (M) for the DOAS Fitting Window Trace Gas #5 MDS</i>	DOAS_2_O3_L
<i>DSD (M) for the DOAS Fitting Window Trace Gas #6 MDS</i>	DOAS_2_O3_H
<i>DSD (M) for the DOAS Fitting Window Trace Gas #7 MDS</i>	DOAS_2_NO2
<i>DSD (M) for the DOAS Fitting Window Trace Gas #8 MDS</i>	DOAS_2_OCLO
<i>DSD (M) for the DOAS Fitting Window Trace Gas #9 MDS</i>	DOAS_3_OCLO



<b>Table 15.8.1.6-2 - DS_NAME Field Strings</b>	
<b>DSD</b>	<b>DS_NAME</b>
<i>DSD (M) for the DOAS Fitting Window Trace Gas #10 MDS</i>	DOAS_3_NO2
<i>DSD (M) for the DOAS Fitting Window Trace Gas #11 MDS</i>	DOAS_3_O4
<i>DSD (M) for the DOAS Fitting Window Trace Gas #12 MDS</i>	DOAS_4_SO2
<i>DSD (M) for the DOAS Fitting Window Trace Gas #13 MDS</i>	DOAS_4_O3
<i>DSD (M) for the DOAS Fitting Window Trace Gas #14 MDS</i>	DOAS_5_HCHO
<i>DSD (M) for the DOAS Fitting Window Trace Gas #15 MDS</i>	DOAS_5_BRO
<i>DSD (M) for the DOAS Fitting Window Trace Gas #16 MDS</i>	DOAS_5_O3_L
<i>DSD (M) for the DOAS Fitting Window Trace Gas #17 MDS</i>	DOAS_5_O3_H
<i>DSD (M) for the DOAS Fitting Window Trace Gas #18 MDS</i>	DOAS_5_NO2
<i>DSD (M) for the DOAS Fitting Window Trace Gas #19 MDS</i>	DOAS_5_O4
<i>DSD (M) for the DOAS Fitting Window Trace Gas #20 MDS</i>	DOAS_SPARE_1
<i>DSD (M) for the DOAS Fitting Window Trace Gas #21 MDS</i>	DOAS_SPARE_2
<i>DSD (M) for the BIAS Fitting Window Trace Gas #0 MDS</i>	BIAS_0_H2O
<i>DSD (M) for the BIAS Fitting Window Trace Gas #1 MDS</i>	BIAS_0_CO2
<i>DSD (M) for the BIAS Fitting Window Trace Gas #2 MDS</i>	BIAS_1_N2O
<i>DSD (M) for the BIAS Fitting Window Trace Gas #3 MDS</i>	BIAS_1_H2O
<i>DSD (M) for the BIAS Fitting Window Trace Gas #4 MDS</i>	BIAS_1_CH4
<i>DSD (M) for the BIAS Fitting Window Trace Gas #5 MDS</i>	BIAS_2_CO
<i>DSD (M) for the BIAS Fitting Window Trace Gas #6 MDS</i>	BIAS_2_H2O
<i>DSD (M) for the BIAS Fitting Window Trace Gas #7 MDS</i>	BIAS_2_CH4
<i>DSD (M) for the BIAS Fitting Window Trace Gas #8 MDS</i>	BIAS_SPARE_1
<i>DSD (M) for the BIAS Fitting Window Trace Gas #9 MDS</i>	BIAS_SPARE_2
<i>DSD (R) -Level 1B product from which this product is produced</i>	LEVEL_1B_PRODUCT
<i>DSD (R) -Level 2 Initialization file</i>	INITIALISATION_FILE
<i>DSD (R) -Atmospheric Climatologies Data file</i>	CLIMA_DBPR_FILE
<i>DSD (R) -Cloud Parameters Data file</i>	CLIMA_DBCL_FILE
<i>DSD (R) -Surface Data Base file</i>	CLIMA_DBSF_FILE
<i>DSD (R) -Literature Cross-Sections Data Base file</i>	CLIMA_DBCS_FILE
<i>DSD (R) -Line by Line Absorption Cross-Sections file</i>	CLIMA_DBLB_FILE
<i>DSD (R) -Flight-Model Reference Cross Spectra Data file</i>	CLIMA_DBFM_FILE
<i>DSD (R) -Undersampling correction spectra file</i>	CLIMA_DBSL_FILE
<i>DSD (R) -PMD minimum reflectance library file</i>	CLIMA_DBCC_FILE
<i>DSD (R) -Air Mass Factor Look-Up-Table file</i>	AMF_LOOK_UP_FILE
<i>DSD (R) -BIAS slant path factor look-up table</i>	BSPF_LOOK_UP_FILE
<i>DSD (R) -AAIA Rayleigh scattering correction look-up table</i>	AIRC_LOOK_UP_FILE



**15.8.1.7 Data Sets**

The following sub-sections describe the individual data sets which together form the 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.

**15.8.1.7.1 Summary Quality ADS**

The SQ ADS provides a summary of the quality flags set for a given state. There is one ADSR per state, each preceded with a time stamp to indicate which portion of the product the ADSR pertains to. The format of each ADSR is identical.

Table 15.8.1.7.1-1 - SQ ADSR Format					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start time of the scan phase of the state	-	12	MJD	1
2	Attachment Flag indicating if MDS DSRs are attached to the current ADS DSR (1 = no MDSRs, 0 otherwise)	-	1	uc	1
3	Summary of quality for the different geophysical parameters (cloud and trace gas concentration) of the entire state (see comment below, some spare)	-	152	uc	152
<i>Size:</i>			<b>165</b>		

To support the Product Quality Facility a summary of all quality flags for each state is given in this SQADS. It is anticipated there will be approximately 27 ADSRs for a typical product.

The quality flags are given as unsigned characters having a range from 0 to 10. '0' represents the best and '10' the worst quality which is envisaged for the mean value of all quality parameters of a certain kind which are encountered during one state. A quality range for each individual parameter will be defined. Following quality parameters are envisaged:

- ❑ error on the cloud fraction (1)
- ❑ aerosol parameter diagnostic (1)
- ❑ error on the vertical column densities (32)
- ❑ error on the DOAS slant column densities (22)
- ❑ RMS of the DOAS/BIAS fitting algorithm (32)
- ❑  $\chi^2$  of the DOAS/BIAS fitting algorithm (32)
- ❑ goodness of fit of the DOAS/BIAS fitting algorithm (32)

Quality flags which are not existing in the data due to a smaller number of trace gas data sets shall be set to zero.

**15.8.1.7.2 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 nadir state. The number of DSRs is estimated at 27.

Table 15.8.1.7.2-1 - Geolocation ADSR					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start time of the scan phase of the state	-	12	MJD	1
2	Flag indicating if MDS DSRs are attached to the current ADS DSR (1 = no MDSRs, 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			45		

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

#### 15.8.1.7.3 States of the Product ADS

Each ADSR 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 of the Ground Pixels ADS).

Table 15.8.1.7.3-1 - States of the Product ADSR					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start Time of DSR	-	12	MJD	1
2	Flag indicating if MDS DSRs are attached to the current ADS DSR (1: no, 0: yes)	-	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 observations in the state	-	2	us	1
Size:			23		

#### 15.8.1.7.4 Geolocation of the Ground Pixels ADS

This ADS provides the detailed geolocation for the shortest integration time

of the corresponding measurements. In the case where a fitting window application (DOAS or BIAS) 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 timestamped to allow cross-reference to the MDSRs. The format of each ADSR is defined below.

Table 15.8.1.7.4-1 - Geolocation of the Ground Pixels ADSR					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start Time of DSR	-	12	MJD	1
2	Flag indicating if MDS DSRs are attached to the current ADS DSR (always set to zero for this ADSR)	-	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	degree	12	fl	3
5	Line-of-sight nadir angles of start, middle and end of the integration time at TOA	degree	12	fl	3
6	Relative azimuth angles of start, middle and end of the integration time at TOA	degree	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	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 first in flight direction and the fourth the last in time and flight direction)	-	32	Coord	4
10	Centre coordinate of the nadir ground pixel	-	8	Coord	1
<i>Size:</i>			<b>99</b>		

**15.8.1.7.5 Clouds and Aerosol MDS**

This MDS receives one record per observation. Cloud fraction data and cloud-top pressure will be present in each record, they refer to the shortest integration time. AAI data will be present only if the observation contains a cluster covering an AAI window.

Table 15.8.1.7.5-1 - Clouds and Aerosol MDSR Format					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start Time of DSR	-	12	MJD	1

Table 15.8.1.7.5-1 - Clouds and Aerosol MDSR Format					
2	Length of DSR	-	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 PMD sub-pixels for this DSR	-	2	us	1
6	Cloud fraction of PMD sub-pixel	%	nPMD	fl	4* nPMD
7	Average cloud fraction of footprint	%	4	fl	1
8	Quality of fractional cloud cover	-	1	uc	1
9	Cloud-top pressure	hPa	4	fl	1
10	Absorbing aerosol indicator	-	4	fl	1
11	Equivalent Lambertian albedo	-	4	fl	1
12	Flag describing the output above	flags	2	us	1
Size:			variable		

The flag describing the output (field 10) has to be interpreted bit-wise. It will contain the following information reflecting the same important settings in the initialization file. The definition of each bit is as follows (when the bit is set the underlined condition is true, bits are counted from 0 to 15) : The bit numbering convention is defined in Volume A.

- 0 : no -yes all sub-pixel cloud fraction values are reliable
- 1 : no - yes at least one sub-pixel had no entry in data base
- 2 : no - yes at least one sub-pixel had sun-glint
- 3 : no - yes at least one sub-pixel had snow-ice flag set
- 4 : no -yes AAIA computation successfully ended
- 5-15 : not used

#### 15.8.1.7.6 DOAS Fitting Window Trace Gas MDS

There are up to 21 DOAS Fitting Window Trace Gas MDSs in a product. The contents of each MDS is identified in the SPH. Each MDS contains several MDSRs. All MDSRs for all MDSs share a common format which is defined below.

Table 15.8.1.7.6-1 - DOAS Fitting Window Trace Gas MDSR Format					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start Time of DSR	-	12	MJD	1
2	Length of DSR	-	4	ul	1
3	Quality indicator (-1 if empty DSR)	-	1	sc	1
4	Number of fitting parameters, nfit	-	2	us	1

5	<b>Integration time for this DSR</b>	1/16 s	2	us	1
6	<b>Vertical column density (VCD)</b>	mol/cm2	4	fl	1
7	<b>Error on the VCD above</b>	%	4	fl	1
8	<b>Flag describing the VCD output above</b>	flags	2	uc	2
9	<b>Slant column density</b>	mol/cm2	4	fl	1
10	<b>Error on slant column density</b>	%	4	fl	1
11	<b>RMS, <math>\chi^2</math>, goodness of fit for the fitting window</b>	-	12	fl	3
12	<b>Iteration number for the fitting window</b>	-	2	us	1
13	<b>Cross correlation parameters</b>	-	$n_{cross}$	fl	4* $n_{cross}$
14	<b>Flag describing the output above</b>	flags	2	uc	2
15	<b>AMF to ground for species</b>	-	4	fl	1
16	<b>AMF to cloud-top for species</b>	-	4	fl	1
17	<b>Calculated reflectance from ground</b>	sr -1	4	fl	1
18	<b>Calculated reflectance from cloud-top</b>	sr -1	4	fl	1
19	<b>Measured reflectance</b>	sr -1	4	fl	1
20	<b>Flag describing the output above</b>	flags	2	uc	2
<i>Size:</i>			<b>variable</b>		

The format component above is repeated for each trace gas constituent retrieved.

The flags describing the output are interpreted bit-wise. They contain the following information (when the bit is set the underlined condition is true, bits are counted from 0 to 15). The bit numbering convention is defined in Volume A.

Field 6 describes the VCD calculation. Each bit is defined as follows:

- 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
- 5-15: not used

Field 11 describes the slant column density calculation (DOAS/BIAS). Each bit is defined as follows:

- 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 8-15 not





used

Field 20 describes the AMF look-up scheme. Each bit is defined as follows:

- 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

**15.8.1.7.7 BIAS Fitting Window Trace Gas MDS**

There are up to 10 BIAS Fitting Window Trace Gas MDSs in a product. The contents of each MDS is identified in the SPH. Each MDS contains several MDSRs. All MDSRs for all MDSs share a common format which is defined below.

Table15.8.1.7.7-1 - BIAS Fitting Window Trace Gas MDSR Format					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start Time of DSR	-	12	MJD	1
2	Length of DSR	-	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 geophysical parameters fitted	-	2	us	1
6	Number of segments in fitting window	-	2	us	1
7	Height value and error	km	8	fl	2
8	Flag describing height variable usage	flags	4	us	2
9	Trace gas vertical column density	mol/cm2	4	fl	1
10	Error on vertical column density	%	4	fl	1
11	Fitted first-closure parameter	sr <sup>-1</sup>	4	fl	1
12	Error on fitted first-closure parameter	%	4	fl	1
13	RMS, chi-squared, goodness of fit, transmittance cut-off for the fitting window	-	16	fl	4
14	Iteration number for the fitting window	-	2	us	1
15	Cross correlation parameters	-	ncross	fl	4* ncross
16	Flag describing the output above	flags	2	uc	2
Size:			variable		

The format component above is repeated for each trace gas constituent retrieved. The flags describing the output are interpreted bit-wise. They contain the following information (when the bit is set the underlined



condition is true). The bit numbering convention is defined in Volume A.

Field 7 describes the use of the height value. Each bit is defined as follows:

- 0: no -yes height value was retrieved in this application
- 1: no - yes retrieved from earlier application is used as input in present application
- 2: no - yes height value from climatology
- 3: no -yes use of height uncertainty as a process error in trace gas application
- 4: no -yes height retrieval failed (yes), succeeded (no) 5-15: not used

Field 15 specifies the BIAS vertical column density fitting. Each bit is defined as follows:

- 0: no -yes error weighting of fitting
- 1: no -yes convergence reached
- 2: satisfactory -poor shape of the fit depending on the magnitude of the first closure parameter
- 3: satisfactory -noisy noisiness of the fit depending on magnitude RMS
- 4-15: not used

#### **15.8.1.8 Size Estimate**

The size of the product depends on the number of trace gas species included. The following estimate is provided in R-36:

The size of one level 2 product containing 7 trace gas species (which might be the most probable scenario: UV-O<sub>3</sub>, Vis-O<sub>3</sub>, NO<sub>2</sub>, H<sub>2</sub>O, CO, N<sub>2</sub>O, CH<sub>4</sub>) is approximately 3.7 MB for an optimised nadir/limb timeline scenario (approx. 9030 single observations). A pure nadir scenario would double the number of observations, and retrieval additional species in additional windows might mean another factor of 2 or even 3. However; retrieval of no more 10 simultaneous species is foreseen currently, thus the maximum size of a level 2 product could be about 11MB.



## 15.8.2 SCIAMACHY Selected Vertical Column Amounts for Meteo Users Level 2 Product – SCI\_RV\_\_2P

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

This Level 2 SCIAMACHY product contains selected vertical column amounts from the SCI\_NL\_\_2P product. The product may be converted to BUFR format outside the PDS for distribution to Meteo users.

### 15.8.2.1 Input Data

Level 2 Vertical Profiles product plus auxiliary data.

### 15.8.2.2 Auxiliary Data Used

Extraction only. No further auxiliary data required.

### 15.8.2.3 Processing Performed

Extraction only.

### 15.8.2.4 Product Structure

The high level structure of the product is shown below:

Table 15.8.2.4-1 - SCIAMACHY Level 2 Meteo Product Structure
MPH
SPH
Geolocation of the Ground Pixels ADS
Vertical Column of Ozone MDS

### 15.8.2.5 Main Product Header

The MPH is described in Volume 5.

### 15.8.2.6 Specific Product Header

The SPH is an ASCII header which conforms to the ASCII conventions defined in Volume 5. The Ø symbol indicates the position of an ASCII blank space character.

Table 15.8.2.6-1 - Specific Product Header of Level 2 Meteo Product					
N	Description	Units	Byte Length	Data Type	Dim.

**Table 15.8.2.6-1 - Specific Product Header of Level 2 Meteo Product**

N	Description	Units	Byte Length	Data Type	Dim.
1	<b>SPH_DESCRIPTOR=</b>	keyword	15	uc	15
	quotation mark (“)	-	1	uc	1
	<b>SPH descriptor</b> (Set to SCI_RV_2P SPECIFIC HEADER)	-	28	uc	28
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
2	<b>STRIPLINE_CONTINUITY_INDICATOR=</b>	keyword	31	uc	31
	Value: +000 = No stripline continuity, the product is a complete segment Other: Stripline Counter	-	4	Ac	1
	newline character	terminator	1	uc	1
3	<b>SLICE_POSITION=</b>	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	<b>NUM_SLICES=</b>	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
<i>Product Location Information</i>					
5	<b>START_TIME=</b>	keyword	11	uc	11
	quotation mark (“)	-	1	uc	1
	<b>Start time of the measurement data in this product</b> UTC time of the first MDSR	utc	27	uc	27
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
6	<b>STOP_TIME=</b>	keyword	10	uc	10
	quotation mark (“)	-	1	uc	1
	<b>Time of the end of the measurement data in this product (last MDSR time)</b> UTC time of the last MDSR	utc	27	uc	27
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
7	<b>START_LAT=</b>	keyword	10	uc	10
	<b>Latitude of the satellite nadir at the START_TIME</b> WGS84 latitude, positive = North	1e-6 deg	11	Al	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
8	<b>START_LONG=</b>	keyword	11	uc	11
	<b>Longitude of the satellite nadir at the START_TIME</b> WGS84 longitude, positive = East, 0 = Greenwich	1e-6 deg	11	Al	1
	<10-6degE>	units	10	uc	10
	newline character	terminator	1	uc	1

**Table 15.8.2.6-1 - Specific Product Header of Level 2 Meteo Product**

N	Description	Units	Byte Length	Data Type	Dim.
9	<b>STOP_LAT=</b>	keyword	9	uc	9
	<b>Latitude of the satellite nadir at the STOP_TIME</b> WGS84 latitude, positive = North	1e-6 deg	11	Al	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
10	<b>STOP_LONG=</b>	keyword	9	uc	9
	<b>Longitude of the satellite nadir at the STOP_TIME</b> WGS84 longitude, positive = East, 0 = Greenwich	1e-6 deg	11	Al	1
	<10-6degN>	units	10	uc	10
	newline character	terminator	1	uc	1
11	<b>Spare (blank characters (Ø))</b>	keyword	10	uc	10
	newline character	terminator	1	uc	1
<i>Other Product Information</i>					
12	<b>FITTING_ERROR_SUM=</b>	keyword	18	uc	18
	quotation mark (“)	-	1	uc	1
	Quality summary of the fitting errors: GOOD or FAIR or BADØ	-	4	uc	4
	quotation mark (“)	-	1	uc	1
	newline character	terminator	1	uc	1
	13	<b>DOAS_FITTING_WINDOW_0=</b>	keyword	22	uc
quotation mark (“)		-	1	uc	1
Wavelength range of fitting window given as a pattern of two wavelengths like: xxxx-yyyy e.g., Ø325-Ø335		-	9	uc	9
quotation mark (“)		-	1	uc	1
newline character		terminator	1	uc	1
<i>DSDs for Attached Data Sets</i>					
14	<i>DSD(A) for the Geolocation of the Ground Pixels ADS</i>	-	280	dsd	1
15	<i>DSD (M) for the Column of Ozone MDS</i>	-	280	dsd	1
<i>DSDs for reference files</i>					
16	<i>DSD (R) -Level 2 product from which this product is produced</i>	-	280	dsd	1
	<b>size (in bytes)</b>	-	<b>1277</b>		

The following ASCII strings are used to fill the DS\_NAME field in the



DSDs (refer to Volume 5).

Table 15.8.2.6-2 DS_NAME Field Strings	
DSD	DS_NAME
<i>DSD(A) for the Geolocation of the Ground Pixels ADS</i>	GEOLOCATION
<i>DSD (M) for the Column of Ozone</i>	O3_VERTICAL_COLUMN
<i>DSD (R) -Level2 product from which this product is produced</i>	SCI_NL__2P

### 15.8.2.7 Data Sets

The following sub-sections describe the individual data sets which together form the Level 2 Meteo 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.

#### 15.8.2.7.1 Geolocation ADS

The Geolocation ADS provides geolocation information for the Ozone estimates. There is one ADSR per estimate, each preceded with a time stamp to indicate which portion of the product the ADSR pertains to. The format of each ADSR is identical.

Table 15.8.2.7.1-1 - Geolocation ADSR Format					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start time of the DSR	-	12	MJD	1
2	Attachment Flag indicating if MDS DSRs are attached to the current ADS DSR (1 = no MDSRs, 0 otherwise)	-	1	uc	1
3	Integration time of this geolocation entity	1/16 s	2	us	1
4	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 first in flight direction and the fourth the last in time and flight direction)	-	32	Coord	4
<i>Size:</i>			47		

#### 15.8.2.7.2 Ozone Vertical Column MDS

There is one MDSR per estimate, each preceded with a time stamp. The format of each MDSR is identical. The fields are extracted from the DOAS MDS of the SCI\_NL\_\_2P product corresponding to the UV fitting window DOAS\_0\_O3 MDS assuming index "0" for this window.



Table 15.8.2.7.2-1 - Ozone Vertical Column MDSR Format					
N	Description	Units	Byte Size	Data Type	Dim.
1	Start time of the DSR	-	12	MJD	1
2	quality Indicator (-1 if empty MDSR, 0 otherwise)	-	1	sc	1
3	Integration time for this DSR	1/16 s	2	us	1
4	Ozone Vertical Column Density (VCD)	mol/cm <sup>2</sup>	4	fl	1
5	Error on the VCD above	%	4	fl	1
Size:			23		

### 15.8.2.7.3 Common Structures

The following structures are used in the descriptions of the Level 2 products.

Table 15.8.2.7.3-1 - Coord Structure					
N	Description	Units	Byte Size	Data Type	Dim.
1	Latitude (convention defined in Volume A)	deg	4	fl	1
2	Longitude (convention defined in Volume A)	deg	4	fl	1
Size			8		

### 15.8.2.8 Size Estimate

The size of one Meteo product containing only ozone is approximately 100 kB for an optimised nadir/limb timeline scenario (approx. 1250 single observations). A pure nadir scenario would double the number of observations. This means that the maximum size of a Meteo product could be about 200 kB.



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