ENVISAT

SCIAMACHY

Level 1b to 2 Off-line Processing

Input / Output Data Definition

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Change Record

Issue	*Rev*	*Date*	*Sheet*	*Description of Change*
Draft		30.05.98	all	completely new
1		30.07.98	all	numerous minor changes in several places according to comments from IFE, KNMI and RAL after the ADC Review at June 15th, 1998
2		29.11.99	40 ff.	Inclusion of the Limb MDS record after discussion at SAO in October 1999
2	A	25.04.00		Updates according to working meeting with ESRIN on April 20th, 2000: • addition of ECMWF input file • reference to Data Base version in SPH, deletion of reference DSDs to DB files • change of the identifier of the initialisation file • body of the initialisation file changed to XML • rename the source of external auxiliary data: Data-Base Server
2	B	21.12.00	-	• GADS added for static parameters (e.g. TOA) • Surface pressure added to cloud/aerosol record • DSR length added to Nadir record • Slant column incl. error added to Nadir record • DSR length added to Limb record
3		03. Apr 2001	-	A large amount of inconsistencies has been eliminated. Comments and RIDs received during the DSR meeting (Jan 2001) have been included in this version.
4		02. Oct 2001	-	After further discussions about the content of the Limb MDS internally and with SAO and after the implementation of the operational code for the writing of the level 2 off-line product, a new version of the I/O DD was necessary. The present version is completely re-worked using a data base to keep the definition of the product file formats.
4	A	09. Aug 2002	After iteration with the team which is implementing the level 2 off-line format within EnviView the following changes have been made:	
			20	A remark about variable records has been added
			25ff	The summary table of product components has been expanded to have one row per data set
			28ff	The SPH format table has been expanded to have one row per line in the SPH, additional a notation has been added to describe the number of characters of the various elements of each line

Issue	*Rev*	*Date*	*Sheet*	*Description of Change*
			32ff	A remark has been added to describe the notation in the comments column of the SPH table
			35ff	The DS_NAME notation for Limb and Occultation IR have been put in line with the notation in the SPH
			39	The length field of the static parameter GADS has been removed
			43	A comment has been added before the clouds and aerosol data set to inform about the variable length of the record
			45	A comment has been added before the nadir fitting window application data set to inform about the variable length of the record
			45	A new field (5) has been added to the Nadir record allowing for a variable number of VCDs and their corresponding errors. The VCD and the ERRVCD fields (6 and 7) may have a variable number of elements
			47	A comment has been added before the limb fitting window application data set to inform about the variable length of the record
			47ff	Fields 14 and 15 of the Limb record of Iss. 4 have been removed and replaced by fields 14 to 18 of Issue 4A
			55	The length field of the static parameter GADS has been removed
			58	The Limb Profile Record has been removed from the compound data types
			58	The Limb Profile Layer Record is now used within the Limb Fitting Window Application Data Set
			58	Field 6 of the Measurement Grid Record has been split into two fields (6 and 7)
4	B	07.07.03	47	Integration Time field added to the Limb MDS record
			63ff	A new XML content of a recent initialisation file is given covering additionally limb parameters
4	C	04.06.03	29-32	Level 2 SPH size of fields 15-58 increased to 52
4	D	23.03.04	41f	Geolocation angles unit changed to degrees / float
			50	Initialization file identifier changed to SCI_IN__AX
4	E	17.08.04	30-36	Limb / Occ. windows adapted to DSDs in SPH
		19.08.04	33	SPH example fixed
		25.10.04	41, 42	Satellite height, earth radius, and tangent height changed to float in Nadir/LimbGeolocation
		03.11.04	all	line-of-sight zenith changed to line-of-sight nadir

Issue	*Rev*	*Date*	*Sheet*	*Description of Change*
4	F	23.08.2005	51	Additional information added in the entry „Additional Diagnostics“ of the Limb MDS with respect to profile content in particle density and the full averaging kernel
			23 & 63	Correction of partial column density unit from ppmV to ppV in units description table (p.23) and in entry 1 „TANGVMR“. Partial column density in units of Volume Mixing Ratio can be understood as Tangent Layer Volume Mixing Ratio (p. 63).
4	G	02.05.2006	16	ECMWF file usage defined for current issue
			19	Usage of AMF LUTs removed since of no further usage
			30	SPH Entry 11 changed from „Spare“ to „Decontamination flag“
			45	MDS Cloud&Aerosol Entries 10&11 changed from cloud-top pressure (and error) to cloud-top height (and error). Errors for cloud-top height and cloud optical thickness are given in the disclaimer; instead 99.99 is provided as marker.
			45/46	MDS Cloud&Aerosol Entries 7, 11, 13, 16, and 18 (errors) changed from % to relative fraction
			46	Cloud flag bit 2-6 defined for SACURA
			47/48	MDS Nadir Entries 7, 10, 14, 25, and 27 (errors) changed from % to relative fraction
4	H	15.11.2007	61ff	Subsections “Climatological and Spectroscopic Data Bases”, “Air Mass Factor Look-up Table”, “BIAS Slant Path Factor Look-up Table” and “AAIA Rayleigh Reflectance Look-up Table” (SCR 23) added
		22.11.2007	45/46	MDS Cloud&Aerosol field 24: number of additional aerosol parameters increased to 3; fields 22-24: comments added (SCR 23)
		16.04.2008	61ff	Subsection “Auxiliary Cross-Sections” added (SCR 21, 22)
			138ff	Section “SO_2 Background Data Base” added (SCR 22)
		21.04.2008	38/39	DSD for m-factor file added; 44 applications = clouds and aerosol plus 43 fitting window applications (SCR 19)
			148	New example of an initialization file added (SCR 18, 19, 21, 22)
			62	Section “M-Factor File” added (SCR 19)
			49	MDS Nadir field 23: flags added (bits 8-11)
		24.04.2008	9	Introduction updated
			10	Reference added

Issue	*Rev*	*Date*	*Sheet*	*Description of Change*
			11	Abbreviations added
			14	Section “Measurment Scenarios...” updated
			16	Section “Processing Overview” updated
			18	Subsection on m-factors inserted, item on SO_2 data base added to subsection “Data Base Server” (SCR 19, 22)
			20	Section “Summary of I/O Files” updated
			25/26	Subsection “Description” of section “SCIAMACHY Level 2 Off-line Product” updated (SCR 21, 22, 23)
			54	Remark on document for Limb MDS added
			63	Remark on unused data bases added
		11.07.2008	all	Many minor corrections after proof-reading
			36	Example SPH updated (SCR 21, 22)
		14.07.2008	16	Flow diagram updated (SCR 22)
		04.08.2008	125	Comments on PMD minimum reflectance library shortened
			63	Description of M-Factor File copied from Level 0 to 1 I/O DD, references and abreviations added, TOC page numbers in updated
5		08.08.2008	56	Section Limb Clouds Data Set added (SCR 25)
		29.08.2008	164	Configuration for SCODA (cloud detection from limb measurments) added (SCR 25)
		22.09.2008	138	AMC look-up table for H_2O added (SCR 30)
		10.11.2008	38/39	Changes in DSD: NAD_UV7_H2O and LIM_CLOUDS added, NAD_UV7_SPARE renamed to NAD_UV8_SPARE, SPARE readded, numbers and size updated (SCR 25, 30)
		24.11.2008	50/51	Remarks concerning AMC-DOAS added (SCR 30)
		13.01.2009	27	Product component table updated: H_2O, volcanic SO_2 and limb clouds added (SCR 25, 27, 30)
			31	SPH size updated (SCR 27, 30)
			31-37	SPH example entries updated, especially new nadir fitting windows for H_2O, volcanic SO_2 added (SCR 27-32)
			38/39	Changes in DSD: NAD_UV7_SO2 added NAD_UV7_H2O renamed to NAD_UV8_H2O, numbers and size updated (SCR 27, 30)
		14.01.2009	26/27	Product description updated, new applications inserted (SCR 25, 27-32)
		26.01.2009	9	Introduction updated

Issue	*Rev*	*Date*	*Sheet*	*Description of Change*
			14-16	Typing errors corrected
		20.02.2009	75-79 85-89	New profile climatologies added (BIRA, IFE, CIRA, GLATM)
		20.02.2009	73-77 137/ 138	Key data DB added (ETA, ZETA)
		25.02.2009	54	Comments to fields 9 (NUM_RLEVEL) and 21 (STVEC_SIZE) corrected
		27.03.2009	179	New configuration for BIAS added (SCR 31)
		30.04.2009	53	Comments regarding IAS results in the Nadir MDS added (SCR 31)
			62	SGP_12N changed to SGP_12OL, ’0 to 1a’ replaced by ’1b to 2’
			all	BIAS changed to IAS (SCR 31)
			19	Remarks on the stop of NRT development and replacement of BIAS by BIRRA added (SCR 31)
			14	Abbreviations and Acronyms updated
			20	Limb cloud pre-processing added to initialization file section (SCR 25)
		08.05.2009	all	Page headers updated
		13.05.2009	14	Abbreviation LIDORT added
			20	AMF look up changed to AMF algorithm
			21	Comment on UV/vis cross-sections changed
			28	O3 VCD: AMF calculations by LIDORT
			44	Component size of XML initialization file updated
			75	BL2 removed, comment on UX2 adapted, BIAS changed to IAS (SCR 31)
			76	Example on similar formats for BIAS data deleted
			77	Number of GADS for DBUX updated
			79	New auxiliary cross sections added for OClO (SCR 29)
			80	BIAS reference atmosphere marked as obsolete
			136	BIAS changed to IAS (SCR 31)
		14.05.2009	all	Version numbers changed from 4.00 to 5.00
			11	Introduction updated for Nadir IR (SCR 31)
			15	Abbreviations OCRA and SCODA added
			29	Names of cloud algorithms inserted
			52	Footnote added
			88	Height grid for IFE_BL & IFE_VOLC climatologies changed to 23 entries, sizes and table updated

Issue	*Rev*	*Date*	*Sheet*	*Description of Change*
			167	hydrostatic_profile changed to IFE_BL
			169	New comment on vcd_algorithm = “Standard”
			178	Database SPF deleted from initialization file section
			150-152	BIAS Slant Path Factor Look-up Table (SCI_PF2_AX) is obsolete for SGP_12OL; section has been deleted
			111-115	Line-by-line Absorption Cross-Sections (SCI_BL2_AX) are obsolete for SGP_12OL; section has been deleted
			78	BIAS_REF_CLIMATOLOGY marked as obsolete
			92	BIAS Reference Atmosphere is obsolete for SGP_12OL; section has been deleted
		15.05.2009	131-133	Descriptions of the five new cross-sections used for OClO retrieval inserted (SCR 29)
			119	Components table of Auxiliary Cross-Sections updated
			9	TOC updated
		18.05.2009	16	Wording improved, last remark on automatically generated parts deleted
		27.05.2009	94	Typo fixed
			14	Abbreviation AMC-DOAS added
		15.06.2009	155	Size of SO2 background record fixed
			142	Blank page removed
		16.06.2009	137	TODO remark deleted
			59	Explanation for ice cloud flag = 3 (bad data) and 9 (strange case) added
			49	Grammar fixed
			42	Explanation for 44 applications fixed
			21	Typo fixed
			20	Duplicate word ’Appendix’ deleted
			19	M-factor file added to description of Figure 1
			19	List items joined
			19	’Since 2006’ inserted as stop for NRT development
		17.06.2009	6-8	SCRs inserted to Change Record
			2	J. Frerick deleted from Distribution
			17	Mission extension changed form 2014 to 2013
			19	’prototype’ changed to ’processor’ (three times)
			21	Forward reference to section on m-factors inserted
			29	Typo fixed

Issue	*Rev*	*Date*	*Sheet*	*Description of Change*
			30	'from UV' and 'from IR' added to product components 19 and 21 (both nadir H_2O)
			35	Field 24: Comment changed to NAD_FIT_WINDOW_UV9
			57	Citation of R11 added
			76	Citation fixed
			all	Date changed to 17. June 2009, page numbers and TOC updated
		19.06.09	2	Sum of distributed copies corrected to 12
5	A	19.01.10	54/55	Two remarks added that errors of AMC-DOAS are absolute values (not relative fractions)

Table of Content

1 Introduction

1.1 Purpose and Scope

SCIAMACHY (SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY) is one of the Earth observation research instruments which is part of the payload of the ENVISAT platform of ESA (European Space Agency) which has been launched on March 1st, 2002.

The main scientific objective of SCIAMACHY is to measure distributions of a number of chemically important atmospheric trace gas species on a global basis. SCIAMACHY has a spectrometer and telescope system designed to observe light transmitted through, reflected by and scattered from the Earth´s atmosphere over a spectral range from 240 to 2400 nm. It has an alternating limb and nadir viewing capability, and is able to perform solar and lunar occultation measurements.

Nadir UV/visible measurements provide global column distributions of O_3, NO_2, BrO, SO_2, OClO and H_2O, as well as cloud and aerosol parameters. Nadir infrared measurements are used to generate column distributions of CO. Limb observations provide vertical stratospheric profiles of O_3, NO_2 and BrO for UV/visible wavelength range.

This document provides the specification of the input and output files as generated by version 5.00 of the level 1b to 2 off-line processor and in particular the level 2 off-line product.

1.2 Documents

The following documents are applicable for the SCIAMACHY project:

[A1] ESA Software Engineering Standards, ESA PSS-05-0, Issue 2, 15.2.1991

[A2] ENVISAT Product Specifications, PO-RS-MDA-GS-2009, Issue 3 rev. K, 4.4.2006

[A3] ENVISAT-1 Ground Segment Concept, ESA/PB-EO(94)75, Issue 5, 20.9.1994

The following documents have been provided as reference documentation:

[R1] GOME Level 1 to 2 Algorithms Description, ER-TN-DLR-GO-0025, Issue 2/B, 18.12.2000

[R2] SCIAMACHY Operations Concept - II. Timeline Generation Rules and Reference Timelines (to be issued soon), PO-TN-DLR-SH-0001/2, Issue 3 rev. 0, 0.0.0000

[R3] GOME Software Databases for Level 1 to 2 Processing, ER-TN-IFE-GO-0018, Issue 2/A, 18.12.2000

[R4] SCIAMACHY Operations Concept - III. Instrument States and Onboard Tables (PFM), PO-TN-DLR-SH-0001/3, Issue 3 rev. 1, 30.3.2001

[R5] Scientific Requirements Document for SCIAMACHY Data and Algorithm Development, Issue 1, 15.12.1996

[R6] SCIAMACHY Operations Concept - I. Mission Scenarios, PO-TN-DLR-SH-0001/1, Issue 3

The following documents are relevant project documents used for the generation of the present document:

[R7] SCIAMACHY Level 1b to 2 NRT Processing - Detailed Processing Model / Parameter Data List, ENV-TN-DLR-SCIA-0011, Issue 2, 2003

[R8] SCIAMACHY Level 1b to 2 NRT Processing - Input/Output Data Definition, ENV-TN-DLR-SCIA-0010, Issue 3/B, 29.5.2000

[R9] SCIAMACHY Level 1c to 2 Off-line Processing - Algorithm Theoretical Basis Document, ENV-ATB-SAO-SCI-2200-0003, Issue 2, 21.12.2000

[R10] SCIAMACHY Level 0 to 1b Processing - Input/Output Data Definition, ENV-TN-DLR-SCIA-0005, Issue 6/A, 4.4.2006

[R11] SCIAMACHY Level 1c to 2 Off-line Processing - Instructions for the Usage of the Level 2 Limb MDS, ENV-TN-DLR-SCIA-0077, Issue 1.0, 15.09.2006

[R12] ENVISAT Mission extension scenario description, PE-RP-ESA-SA-205, ESA, EO-PE, 15.10.2007

[R13] SCIAMACHY Calibration Plan, PL-SCIA-1000TP/022, Issue 2, 22.1.96

[R14] Definition of Instrument Characterisation Data Base, PO-ID-DOR-SY-0037, Issue 1, 11.5.94

There are severel scientific documents that serve as additional references:

[S1] Richter A. (2006): SCIAMACHY SO_2 Vertical Columns - Algorithm Description, Institute for Environmental Physics, University of Bremen, www.sciamachy.org/products/SO2/SO2vc_IFE_AD.doc

[S2] Chance K.V. (1998) : Analysis of BrO Measurments from the Global Ozone Monitoring Experiment, Geophys. Res. Lett., 25, 3335-3338.

[S3] Slijkhuis S., A. von Bargen, W. Thomas and K.V. Chance (1999) : Calculation of Undersampling correction spectra for DOAS spectral fitting, ESA WPP-161, 563-569.

[S4] Brühl Ch. and P. Crutzen (1991) : MPI model output climatology from the 2-D chemical-dynamical model, Max-Planck Institute for Chemistry, Mainz, Germany, Private communication.

[S5] Anderson G.P., S.A. Clough, F.X. Kneizys, J.H. Chetwynd and E.P. Shettle (1986) : AFGL Atmospheric constituents profiles (0-120km), Air Force Geophysical Laboratory, Hanscom, Mass., U.S.A., Report AFGL-TR-86-1001, AD175173.

[S6] Loyola D. (1999) : A New Cloud Recognition Algorithm for Optical Sensors, IEEE International Geoscience and Remote Sensing Symposium, IGARSS '98 DIGEST VOLUME II, 572-574.

[S7] Bogumil, K., J. Orphal, T. Homann, S. Voigt, P. Spietz, O. C. Fleischmann, A. Vogel, M. Hartmann, H. Bovensmann, J. Frerik and J.P. Burrows (2003) : Measurements of Molecular Absorption Spectra with the SCIAMACHY Pre-Flight Model: Instrument Characterization and Reference Data for Atmospheric Remote-Sensing in the 230-2380 nm Region, J. Photochem. Photobiol. A., 157, 167-184.

[S8] Vountas, M., V.V. Rozanov and J.P. Burrows (1998) : Ring effect: impact of rotational Raman scattering on radiative transfer in Earth's atmosphere, J. Quant. Spectrosc. Radiat. Transfer 60, 943-961.

[S9] Fleischmann, O.C., M. Hartmann, J.P. Burrows and J. Orphal (2004) : New ultraviolet absorption cross-sections of BrO at atmospheric temperatures measured by time-windowing Fourier transform spectroscopy, J. Photochem. Photobiol. A, 168, 117-132.

[S10] Vandaele, A.C., P.C. Simon, J.M. Guilmot, M. Carleer, R. Colin (1994) : SO2 absorption cross section measurement in the UV using a Fourier transform spectrometer, J. Geophys. Res., 99(D12), 25599-25606.

[S11] Rozanov, V. V., M. Buchwitz, K.-U. Eichmann, R. de Beek, and J. P. Burrows (2002) : SCIATRAN - a new radiative transfer model for geophysical applications in the 240 - 2400 nm spectral region: The pseudo-spherical version, Adv. Space Res., 29, 1831-1835.

[S12] Noël, S., M. Buchwitz, H. Bovensmann, R. Hoogen, and J. P. Burrows (1999) : Atmospheric water vapor amounts retrieved from GOME satellite data, Geophys. Res. Lett., 26, 1841-1844.

1.3 Abbreviations and Acronyms

Please find below the abbreviations and acronyms which are used in the present document:

AAIA	Absorbing Aerosol Index Algorithm
ADS	Annotation Data Set
AMF	Air Mass Factor
AMC-DOAS	Air Mass Corrected DOAS
ASCII	American Standard Code for Information Interchange
BIAS	Basic Infra-red Absorption Spectroscopy
BIRA	Belgisch Instituut voor Ruimte-Aëronomie (Belgian Institute for Space Aeronomy)
BIRRA	Beer Infra-Red Retrieval Algorithm
CIR	Color Index Ratio
DB	Data Base
D-PAC	German Processing and Archiving Centre (as part of the ENVISAT ground segment)
DLR	Deutsches Zentrum für Luft- und Raumfahrt e.V. (German Aerospace Centre)
DOAS	Differential Optical Absorption Spectroscopy
DSD	Data Set Descriptor
DSR	Data Set Record
DTD	Document Type Definition
ECMWF	European Centre for Medium-Range Weather Forecasts
ENVISAT	Environmental Satellite
ESA	European Space Agency
ESFT	Exponential Sum Fitting Transmission
ESC	Effective Slant Column
FWHM	Full Width Half Maximum
GADS	Global Auxiliary Data Set
GOME	Global Ozone Monitoring Experiment
HITRAN	High-resolution Transmission Molecular Absorption Database
HTML	Hypertext Mark-up Language
HWHM	Half Width Half Maximum
I/O	Input/Output
IAS	Infra-red Absorption Spectroscopy
IR	Infra-Red
IEEE	Institute of Electrical and Electronics Engineers
IFOV	Instantaneous Field-of-View
ISCCP	International Satellite Cloud Climatology Project
IUP-UB	Institute of Environmental Physics, University of Bremen (Institut für Umweltphysik, Universität Bremen)
KNMI	Koninklijk Nederlands Meteorologisch Instituut (Royal Netherlands Meteorological Institute)
LADS	Location Annotation Data Set
LBL	Line-by-line
LIDORT	Linearized Discrete Ordinate Radiative Transfer
LOS	Line-Of-Sight
MB	Mega Byte (1024 x 1024 Bytes)
MDS	Measurement Data Set
MDSR	Measurement Data Set Record

MPH	Main Product Header
ND	Neutral Density
NRT	Near Real-Time
NLC	Noctilucent Cloud
OL	Offline
OCRA	Optical Cloud Recognition Algorithm
PMD	Polarisation Measurement Device
PQF	Product Quality Facility
PSC	Polar Stratospheric Cloud
RMS	Root Mean Square
SACURA	Semianalytical Cloud Retrieval Algorithm
SBT	Satellite Binary Time
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
SCODA	SCIAMACHY Cloud Detection Algorithm
SGP	SCIAMACHY Ground Processor
SGP_12OL	SCIAMACHY Level 1b to 2 Off-line Ground Processor
SOS	SCIAMACHY Operations Support
SPH	Specific Product Header
SQADS	Summary of Quality Annotation Data Set
SSAG	SCIAMACHY Scientific Advisory Group
SZA	Solar Zenith Angle
TOMS	Total Ozone Mapping Spectrometer
UTC	Universal Time Coordinate
UV	Ultra-Violet
VCD	Vertical Column Density
WLS	White Light Source
WMO	World Meteorological Organisation
XML	Extensible Mark-up Language

1.4 Document Overview

The present document is divided into the following sections:

- General assumptions

  This section gives an overview about the measurement scenarios, timelines and instrument modes, which are an important prerequisite for the definition of the level 2 off-line product format. Finally a short processing overview is repeated here for completeness.
- Detailed I/O Data Formats

  Starting with a summary of input and output files, which will be defined in the present document and an approach on how the different I/O files are defined, there will be a sub-section for each I/O file. The files are grouped into the following categories:
  - products
  - auxiliary data files
- Generic Data Representations

  The precise format of the basic and compound data types used throughout the data definition is given.
- An appendix covering:
  - a reference timeline which is used for the sizing of the level 2 off-line product
  - an example for the initialisation file.

2 General Assumptions

This section gives an overview about the measurement scenarios, timelines and instrument modes which are an important prerequisite for the definition of the level 2 off-line product format. Finally a short processing overview is repeated here for completeness.

2.1 Measurement Scenarios, Timelines and Instrument States

The operation concept of SCIAMACHY is based on a hierarchy of mission scenarios, time lines and states. A detailed description of the SCIAMACHY operations concept is given in [R6], [R2] and [R4].

The *mission scenarios* describe categories of measurements to be performed and how the various categories are related to each other. The *timelines* represent the implementation of the mission scenarios in the sense that they give a detailed outline of the sequence of individual measurements. Timelines can be generated once scientific and technical mission planning rules have been established. The *states* are the lowest level in the hierarchy; each state represents a single measurement type with a specific set of parameters.

The mission scenarios of SCIAMACHY depend on the time frame of the mission. The extension of the ENVISAT mission until 2010 has recently been confirmed, and a further extension until 2014 is planed. This will result in changing mission scenarios; for instance changing to a lower orbit is required [R12].

A fixed number of SCIAMACHY time lines is be stored on-board; there is the opportunity for updating time lines according to established and configuration-controlled procedures. Consequently, in order to facilitate daily operations, time lining schemes have been developed, which cover most of the envisaged instrument activities (mission scenarios). A reference time lines is described in Appendix A, which was used to calculate the parameters and sizes of the level 2 product, described in section 3.4.

The states are classified according to measurement categories depending on the type of observation e.g. nadir, limb, sun occultation, spectral lamp source, etc. Level 0 to 1b processing picks up the measurements of a complete state of a certain measurement category and routes them through the various processing steps of the level 0 to 1b processor to yield a number of MDSs (Measurement Data Sets) of different measurement categories. Level 1b to 2 processing takes the MDSs of those states of the level 1b product which belong to the Nadir, Limb and Occultation measurement category, and retrieves the anticipated trace gas vertical columns and profiles. The hierarchy of the SCIAMACHY operational concept above the level of these instrument states is (in principle) invisible to a level 2 data user. The type of ground coverage over an orbit full of data depends on the applied timeline; the most common situation consists of an alternating nadir and limb sequence.

2.2 Processing Overview

Level 1b to 2 processing is concerned with the retrieval of atmospheric constituent profiles and column amounts from the calibrated geolocated radiance derived from level 0 to 1b processing.

A number of retrieval algorithms are required in SGP_12OL to generate trace gas and other geophysical products proposed by SSAG (see the SCIAMACHY Operational Processing Baseline for details). Figure 1 is a schematic flow diagram of the SGP off-line level 1b to 2 processor. There are five main algorithm functions (indicated by the rectangular boxes with grey shading); these are:

- A 'climatological pre-processing' algorithm, which compiles reference data and retrieves auxiliary cloud and aerosol parameters;
- A 'DOAS/IAS spectral fitting' algorithm for the retrieval of trace gas total column amounts from SCIAMACHY nadir measurements;
- An 'Limb retrieval' algorithm based on a global fitting approach for the retrieval of a variety of stratospheric profiles from SCIAMACHY limb measurements;
- An 'ozone profile' algorithm for the retrieval of height-resolved ozone from SCIAMACHY nadir measurements (optional);

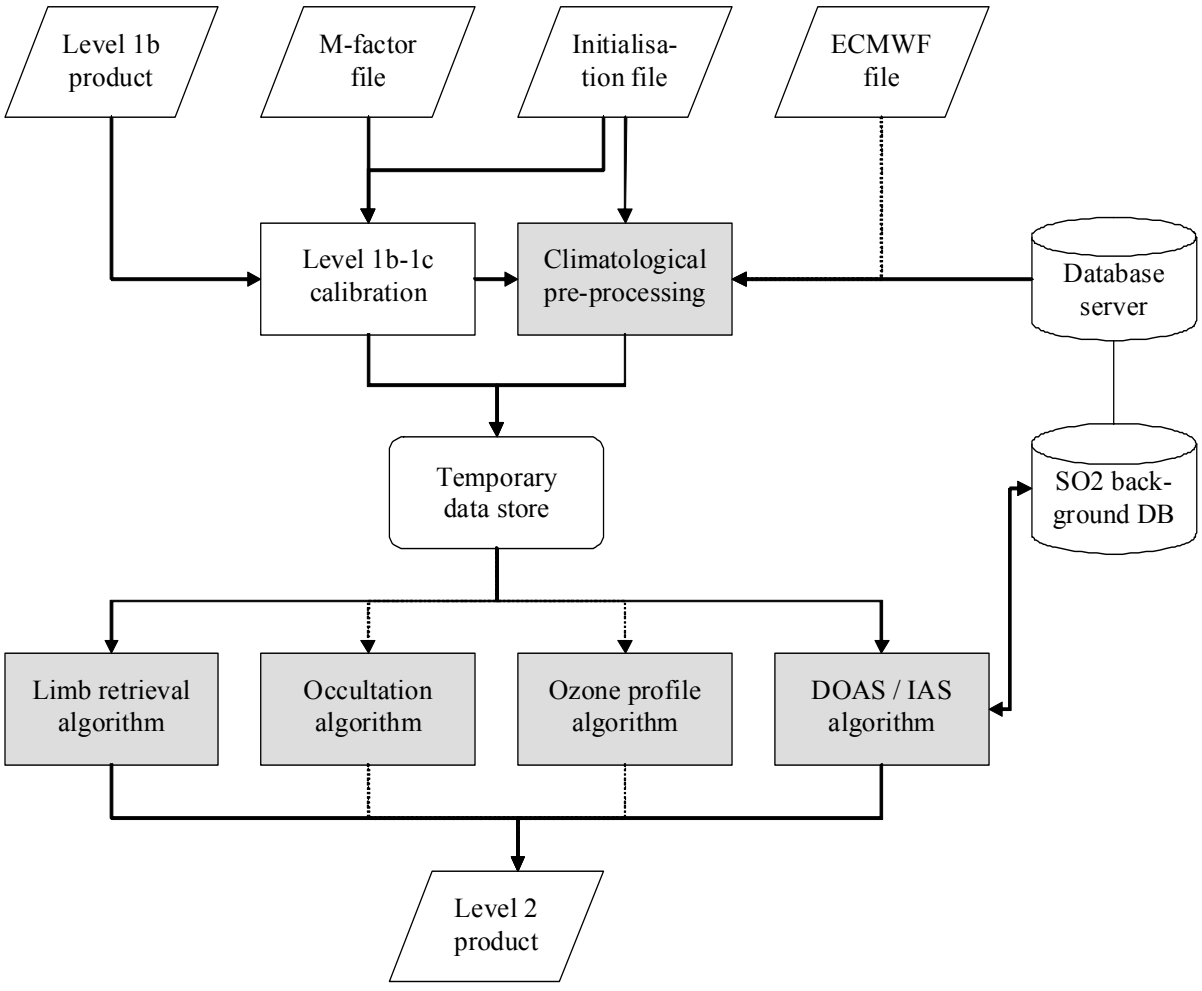

Figure 1: Data Flow Diagram of the complete Level 1b to 2 Off-line Processor

- An ‘occultation’ algorithm for the retrieval of stratospheric profiles from SCIAMACHY occultation measurements (optional).

SCIAMACHY is a complex instrument with an ambitious scientific mission. For the development of the first operational processor, time and resources are severely limited. The baseline requirements on the algorithm content are:

- Only the first three algorithms were implemented in the operational processor. The ‘ozone profile’ and ‘occultation’ algorithms are regarded as options to be implemented at a later date;
- The two main fitting algorithms (DOAS/IAS and Limb retrieval) are stand-alone in the baseline; this means that nadir and limb results are not combined in any way to iterate the retrieval or define new products;
- The ‘pre-processing’ and ‘DOAS/IAS’ algorithms was based closely on their equivalents in the SCIAMACHY NRT processor; processor development at DLR ran in parallel for these algorithms. Since 2006 the development of the NRT processor has been stopped. The previous algorithm for nadir IR retrieval, BIAS, has been replaced by BIRRA.
- It is recognised that the height-resolved ozone retrieval process is a very sophisticated scientific research goal; there has been no recommendation from SSAG concerning its implementation in the first SGP_12OL. Parallel developments for the GOME Data Processor will be influential in the implementation of a height-resolved nadir profile algorithm for both instruments. For now, the nadir column and limb profile algorithms have a higher priority for the development of an operational SGP_12OL.
- Further scientific research is needed to prove the validity of defining tropospheric products from nadir and limb retrieval results in the SCIAMACHY context. There is a higher priority on getting the basic retrievals working satisfactorily. Ultimately however, decisions on the baseline content for SGP_12OL are resource driven.
- There are two additional functions illustrated in Figure 1 regarding the input and output to SGP_12OL. Functions to read level 1b input data and to write the level 2 off-line product are required.
- There will be just one level 2 off-line product with a number of measurement data sets (MDSs) structured according to the results of the corresponding algorithms.

The *Clim. Pre Proc.* function consists of two ancillary algorithms intended to retrieve cloud and aerosol parameters. The cloud detection algorithm generates fractional cloud cover from an examination of PMD data; the cloud-top height is taken from a climatology database. The aerosol indicator algorithm examines Rayleigh-corrected reflectance ratios for an indication of the presence of absorbing aerosols (following the scheme developed by the KNMI). Both auxiliary algorithms are independent from the main 1b to 2 components above.

In Figure 1 there are four input interfaces (Level 1b product, M-factor file, initialisation file, database server), and one output interface (Level 2 off-line product). Some initial requirements on these interface files are presented in the following sections.

2.3 Input Files and Data

The following sub-section gives a short overview about the various input files and other data which is used by the processor.

2.3.1 Level 1b product

In order to generate total columns and ozone profiles from nadir measurements and also limb or occultation profiles from a series of limb or occultation scans, we require all scans from a given SCIAMACHY state, complete with geolocation information. We also require a suitable extraterrestrial solar spectrum to compute reflectance from the radiance data.

Since limb and occultation scan sequences run from the lower levels of the atmosphere upwards, all scans in a limb or occultation state must be extracted before Limb retrieval can begin.

The level 1b requirements are then (we leave out occultation for now):

- A complete set of nadir measurements, to include wavelengths and radiance measurements, errors on these measurements and spectral status;
- A complete set of limb scan measurements from lowest levels to top of the atmosphere, to include wavelengths and radiance measurements, errors on these measurements and spectral status;
- Geolocation information for each limb scan or nadir measurement. This shall include the line-of-sight nadir and azimuth angles at the spacecraft, the solar zenith and azimuth angles at the spacecraft, the height of the spacecraft above the geoid, the earth radius at the sub-satellite point, the latitude and longitude of the sub-satellite point, and the UTC date/time.
- The solar spectrum, to include wavelengths and irradiance values, errors on these measurements and spectral status;
- The PMD data, to include reflectance at each sub-pixel point and for each PMD channel, plus accompanying geolocation information (viewing geometry, and surface locations for nadir footprints);
- Information about the slit function, a complete data set of slit function parameters as delivered from instrument pre-flight calibration, including FWHMs, pixel-to-pixel variations, shape functions, etc.

2.3.2 Initialisation file

The static parameter input file contains variables controlling the execution of the 1b to 2 off-line processing. The file is grouped into various classes reflecting the algorithmic functions (DOAS, IAS, AMF algorithm, cloud pre-processing, aerosol pre-processing, limb cloud pre-processing and limb retrieval). The file is read just once at the beginning of processing, and variables are checked immediately for validity before any further processing. The read of these variables should include the following:

- Overall algorithm control – order of applications in IAS and limb retrieval, use of shifts and squeezes for DOAS, etc.
- Fitting control for the individual retrieval problems, including use of system errors, choice of parameters to be fitted, fitting convergence criteria, fitting window limits, etc.
- Forward model control and data base pointers, including assignation of molecules and aerosol properties, slit function options, line-by-line optimisation options, etc.
- All inputs should be read and then checked at the beginning of the processing; they are assigned to a number of data structures for further use.

Appendix B contains an example of the static parameter part of the initialisation file.

2.3.3 ECMWF files

Currently, the ECMWF data are not used for processing. But there is a strong scientific interest to use ECMWF data as 'a priori' information for the retrieval of geophysical constituents. Therefore, this kind of auxiliary input shall be foreseen for the level 1b to 2 off-line processing chain for coming version.

2.3.4 M-factor files

Due to the degradation within the instrument light path during its stay in orbit the pre-flight calibration data would need to be changed. Instead of actually changing the pre-flight calibration data the so-called m-factors are applied, which are collected in m-factor auxiliary files (SCI_MF1_AX, see Section 3.7).

2.3.5 Data Base Server

Most reference data sets required for SGP_12OL have already been compiled for GOME and SCIAMACHY NRT projects which can be taken over for the off-line processor. These data sets are collected in a so-called Data Base Server which provides a uniform programming interface to this data for all retrieval algorithms. In contradiction to NRT processing these data sets are not defined as individual auxiliary files within the present I/O DD, but are an inherent part of the processor. Nevertheless, there is an unambiguous identification for the content of this Data Base Sever so that data users may known what this data has been.

The outstanding data set required from SCIAMACHY calibration and characterisation activities is the set of slit function parameters. The main new requirement in the limb is for multiple scatter correction factors to the forward model.

- For the infrared, atmospheric profile data sets are those used for SCIAMACHY NRT level 1b to 2 retrievals. The TOMS Version 8 ozone profile climatology should be used at the outset, otherwise for the UV and visible, existing GOME profiles can be taken over.
- The aerosol data set of optical properties and phase functions shall be taken from Lowtran 7 (extension of GOME to infrared). Surface reflection data, and cloud-top reflectance data will be extended to infrared from GOME wavelengths. Global topography shall be that for GOME. Two new surface data sets are required – global sea ice and snow cover data.
- Line spectroscopic data (mainly from HITRAN 96) are common to all infrared retrieval (IAS, limb), as used already in SCIAMACHY NRT to generate LBL cross-section look-ups. Many new UV/visible cross-sections from various sources (IFE, BIRA) have been added.
- Rayleigh cross sections and depolarisation values shall be based on the latest data, along with up to date Ring spectroscopic parameters.
- For the limb retrievals, a data set of multiple scattering correction factors are required to supplement the forward modelling; these cover contributions from tropospheric back-scattered light (especially UV/visible).
- An offset which varies with latitude and time is present in the SO_2 data [S1]. This offset is derived from a reference sector covering the Pacific (180° - 220° longitude). Slant columns from this sector will be retrieved, averaged over latitude bins and put into a newly introduced SO_2 Background Data Base. This compensates most of the effect and also some of the ozone interference.

2.4 Output: Level 2 Off-line Product

The final function of the level 1b to 2 off-line process is the generation of the level 2 off-line product. The latter 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. The product content will be listed next. Depending on the viewing mode (nadir, limb or occultation), different geolocation information is required.

- Product Header Information
- Geolocation Information (a subset of the level 1b geolocation data)
  - Date & Time (all retrievals)
  - Solar zenith and Line-of-Sight nadir at centre of ground pixel (all)
  - 4 Corner Coordinates & Centre of Ground Pixel (nadir only)
  - Coordinates of Tangent Ground Point (limb, occultation)
  - Tangent Height above geoid (limb, occultation)
- Main Result Output

  Profile information and total column amounts of the various trace gases and other geophysical parameters (cloud-top pressure and cloud fractional cover, aerosol parameters). Also output are relative errors on all these parameters.
- A large amount of intermediate output depending on different algorithms:
  - Slant columns from the DOAS module, and extracted AMF values
  - Fitting diagnostics (chi-square, RMS, correlation matrix)

3 Detailed I/O Data Formats

Starting with a summary of input and output files which will be defined in the present document, and an approach on how the different I/O files are defined, there will a sub-section for each I/O file given. The files are grouped into the following categories:

- products
- auxiliary data files

3.1 Summary of I/O Files

A list of all I/O files which can be used within the SCIAMACHY level 1b to 2 off-line processing chain is given in the following table:

Id	Type	Identifier	Name
1	Product	SCI_NL__1P	SCIAMACHY Level 1b Product
2	Product	SCI_OL__2P	SCIAMACHY Level 2 Off-line Product
3	Auxiliary	SCI_IN__AX	Initialisation File
4	Auxiliary	SCI_ECA_AX	ECMWF Analysis Data File
5	Auxiliary	SCI_MF1_AX	M-Factor File

All except the ECMWF analysis file are used in the current version 5.00.

The present I/O DD employs a field identification scheme which may be used in algorithm descriptions. Each field has an unambiguous identification as follows:

$x_1.x_2.x_3$

- x_1 is the identification number of the I/O file, as given in the table above,
- x_2 is the identification number of the individual component of each file. At the beginning of each format description the file component table identifies these components which are described in the following tables,
- x_3 is the field number, as given in the format description tables of each file component.

E.g. the coefficients of the spectral calibration parameters may be given as:

2.9.5

“2” for the level 2 off-line product, “9” for the Limb Geolocation ADS and “5” for the LOS nadir angles field.

3.2 Approach for File Definition

For each file described in this document, the information is classified according to a standardised template. The file description is broken down into the following categories: identifier, name, type, description, format, sizing, data volume, throughput and remarks. In this explanation, each category is defined and the different descriptors used within the categories are presented.

Identifier

An identifier has been defined for each kind of file used and/or generated at the ground segment. This identifier will be used for referring to specific kind of files and for referring to the associated file format. The identifiers are listed in the summary table of the previous section.

Name

This part of the description contains a short descriptive name of the file.

Type

The file type defines the general relation of the file with the ground processor. The following types are defined:

Product: The file is either primary data from the Space Segment or an *output* from a ground processor, to be delivered to the end users.

Auxiliary: The file is an *input* to the ground processor; it contains data external to the space segment and the ground processor. Data of this type may originate from external sources or may be determined analytically.

Description

This section provides details about the contents and purpose of the file.

Format

The format of the product files has been defined according to the guidelines in ENVISAT product specification (volume 5); the relevant details for this document are as follows:

- A file is divided into four main parts: a general header (MPH), a specific header (SPH), data set descriptors (DSD)[1] and specific data sets (DS) of the corresponding input/output file. Each of these parts has a specific structure defined in the following bullets.

1. According to the ENVISAT product specification the DSDs are an integral part of the SPH. For the purpose of the present definition the list of DSDs is handled as an individual product file component.

- The detailed format is given in form of tables containing columns, as described in the following table.

Column	Description
No	Defines the sequence of fields in the DSR
Name	This is a name of the field which may be referred to in algorithm description, etc. Names use capital letters, digits and under score characters only
Comments	Gives a detailed description of the content of the field, sometimes including examples to make it more clear
Unit	Physical unit of the quantity or quantities given in this field; a list of possible units including their description is given hereafter
Type	Data type of the quantities in this field; the possible values including their precise format is given in section 4 on page 156
#	Number of elements described by this field
Size	Complete size of this field; this is a calculated value and is given by the size of the data type multiplied with the number of elements
Offset	Offset of the field within the DSR; this is a calculated field by summing up the sizes in the column before

- Note that for the data definition in the present document, the notation '~' is used to indicate the inclusion of an ASCII blank-space character and the '^' for the newline character.
- The 'Unit' column gives the physical unit or the kind of interpretation of the field. A dash (-) is given for a field corresponding to a flag, a cardinal number or any other unit-less type of information.
- The following units are used:

Notation	Description
%	Percent
-	No unit
1/16 s	1/16 of a second
day	Day of the year
degree	General angle, 360 per cycle
hPa	Pressure (hecto pascal)
K	Temperature (Kelvin)
km	Kilometre
molecule/cm^2	Column density
nm	Nanometre (wavelength)
ppV	Volume mixing ratio (parts per volume)
rel. fraction	Relative fraction
s	Second
us	Microsecond

- The available data types (simple and compound) are defined in section 4 on page 156
- Each component of the format description is preceded by a size entry indicating the number of records in the component, the record size and the complete size of the component.
- The clouds and aerosol, the Nadir and the Limb application measurement data sets are of variable record length. Nevertheless, the format description tables give also explicit numbers for '#', size and offset to allow for the calculation of typical sizes and offsets of the fields, compo-

nents and the whole file. Whenever an element of the format definition is of variable record length the corresponding numbers are given in brackets and italics.

Sizing

Defines the criteria for the sizing product files.

Data Volume

Defines the size for a whole reference data set.

Throughput

The number of data sets per time frame.

Remarks

Additional explanation and comments on top of the standard descriptions.

3.3 SCIAMACHY Level 1b Product

3.3.1 Identifier

SCI_NL__1P

3.3.2 Type

Product

3.3.3 Description

The detailed format description of the level 1b product is given in [R10].

3.3.4 Format

N/A

3.3.5 Sizing

N/A

3.3.6 Volume

N/A

3.3.7 Throughput

N/A

3.3.8 Remarks

The product to be used for level 1b to 2 off-line processing shall be the off-line level 1b product which will be generated at D-PAC.

3.4 SCIAMACHY Level 2 Off-line Product

3.4.1 Identifier

SCI_OL__2P

3.4.2 Type

Product

3.4.3 Description

The level 2 product includes headers (MPH, SPH), annotation data sets (LADS, SQADS and three general ADSs) and several measurement data sets (MDS) depending on the number of fitting window applications. The level 2 product consists of a single file.

The main product header (MPH) has a fixed format (as described in ENVISAT product spec), and includes information about product identification, data acquisition and processing time and position of the measurement data, ENVISAT orbit and position, SBT to UTC conversion, product confidence data and sizes of the following data.

A specific product header (SPH) includes a reference to climatological data base and look-up table versions, product confidence data, fitting window and retrieved molecule specification and the data set description records (DSD).

The annotation data sets (ADS) include condensed quality information (SQADS), geolocation of the states (LADS) and three ADSs with information about the states of the product and the detailed geolocation for nadir and limb.

The first measurement data set (MDS) of the level 2 product includes cloud and aerosol information for each nadir ground pixel. This is followed by the MDSs including the geophysical parameters of several fitting windows and their associated errors, and auxiliary output. The latter contains selected results and diagnostics from the level 1b to 2 off-line algorithms. The MDSs are labelled according to the type of measurement (nadir, limb or occultation); there are two types of MDSs - one for nadir and the other for limb and occultation, with different record structure. The same trace gas may be retrieved from different fitting windows. There is one special MDS planned which contains the result of an ozone profile retrieval algorithm from nadir measurements.

Level 2 off-line products of SCIAMACHY measurements include trace gas columns and profiles as well as other geophysical parameters as indicated in the list below. 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 and profile data, as well as the corresponding algorithm baseline. The current version 5.00 of SGP_12OL implements the following applications:

- O_3 vertical column retrieved from optical absorption spectroscopy fitting in UV and visible wavelength range, using an AMF calculations by LIDORT.
- NO_2, same as O_3, but only in the visible wavelength range.
- BrO, same as O_3.
- SO_2, two different SO_2 vertical columns are retrieved. The first column is calculated for anthropogenic pollution scenario (SO_2 profile with SO_2 peak in the boundary layer); the second one - for volcanic eruption scenario (SO_2 profile with SO_2 peak between 10 and 11 km).
- OClO slant comlumn retrieval.

- H_2O vertical column retrieval by AMC-DOAS.
- CO vertical column retrieved from IR absorption spectroscopy fitting.
- 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.
- AAI, aerosol absorbing indicator algorithm developed by the KNMI.
- O_3 profiles from limb observations for UV/visible wavelength range.
- NO_2 profiles, same as O_3.
- BrO profiles, same as O_3.
- Cloud retrieval from limb measurements (SCODA).

It may be noted that the L2 product is prepared to include results from further fitting window applications that are not yet implemented. Compared to the previous version 4.00, nadir OClO, H_2O, CO and limb BrO are completely new. For nadir BrO the vertival column has been added, and for SO_2 the proper distinction of antropogenic and volcanic scenario regarding VCD is new. Retrieval of clouds from limb measurements and consideration of these clouds in the limb retrieval is available for the first time in version 5.00.

Geographical Coverage

Nominal: global

The measured ground pattern depends on the scanning mode. Only the largest swath width yields global coverage at the equator after three days. If SCIAMACHY is operating in the most probable combined nadir/limb mode, there are gaps in the nadir MDSs when the instrument is operating in limb or occultation scanning mode and there are also gaps in the limb MDSs when the instrument is operating in nadir scanning mode. The various calibration and monitoring modes leave gaps in both types of MDSs.

Spatial Resolution

SCIAMACHY has a number of viewing modes for nadir, limb and occultation measurements with different resolutions. The along-track length of a nadir ground pixels is given by the fixed Instantaneous Field Of View (IFOV) of 1.8 degree, which corresponds to approximately 25 km on the Earth's surface. The default swath width is ~1000 km.

3.4.4 Format

The detailed format description is divided into several tables representing the hierarchy of product content. The calculation of the product size is based on the reference timeline as given in appendix A and the assumption that all traces gas parameters are included, as discussed for the operational processing guideline. The product consists of the following components:

Id	Product Component	Comp. Type
1	Main Product Header of the Level 2 Off-line Product	MPH
2	Specific Product Header of the Level 2 Off-line Product	SPH
3	Data Set Description of the Level 2 Off-line Product	DSD
4	Summary of Quality Flags per State	ADS
5	Geolocation of the State	ADS
6	Static Parameter of the Level 2 off-line Processor	GADS
7	States of the Product	ADS
8	Nadir Geolocation	ADS
9	Limb Geolocation	ADS
10	Clouds and Aerosol Data Set	MDS
11	Nadir Fitting Window Application Data Set - O_3 from UV	MDS
12	Nadir Fitting Window Application Data Set - NO_2	MDS
13	Nadir Fitting Window Application Data Set - O_3 from visible	MDS
14	Nadir Fitting Window Application Data Set - BrO	MDS
15	Nadir Fitting Window Application Data Set - HCHO	MDS
16	Nadir Fitting Window Application Data Set - SO_2 (anthropogenic)	MDS
17	Nadir Fitting Window Application Data Set - OClO	MDS
18	Nadir Fitting Window Application Data Set - SO_2 (volcanic)	MDS
19	Nadir Fitting Window Application Data Set - H_2O from UV	MDS
20	Nadir Fitting Window Application Data Set - UV/Vis Spare	MDS
21	Nadir Fitting Window Application Data Set - H_2O from IR	MDS
22	Nadir Fitting Window Application Data Set - CH_4	MDS
23	Nadir Fitting Window Application Data Set - N_2O	MDS
24	Nadir Fitting Window Application Data Set - CO	MDS
25	Nadir Fitting Window Application Data Set - CO_2	MDS
26	Nadir Fitting Window Application Data Set - IR Spare	MDS
27	Limb/Occultation Fitting Window Application Data Set - Limb - pTH	MDS
28	Limb/Occultation Fitting Window Application Data Set - Limb - O_3 from UV	MDS
29	Limb/Occultation Fitting Window Application Data Set - Limb - NO_2	MDS
30	Limb/Occultation Fitting Window Application Data Set - Limb - O_3 from visible	MDS
31	Limb/Occultation Fitting Window Application Data Set - Limb - BrO	MDS
32	Limb/Occultation Fitting Window Application Data Set - Limb - H_2CO	MDS
33	Limb/Occultation Fitting Window Application Data Set - Limb - SO_2	MDS
34	Limb/Occultation Fitting Window Application Data Set - Limb - OClO	MDS
35	Limb/Occultation Fitting Window Application Data Set - Limb - UV/Vis Spare	MDS
36	Limb/Occultation Fitting Window Application Data Set - Limb - H_2O	MDS
37	Limb/Occultation Fitting Window Application Data Set - Limb - CH_4	MDS
38	Limb/Occultation Fitting Window Application Data Set - Limb - N_2O	MDS

Id	Product Component	Comp. Type
39	Limb/Occultation Fitting Window Application Data Set - Limb - CO	MDS
40	Limb/Occultation Fitting Window Application Data Set - Limb - IR Spare	MDS
41	Limb/Occultation Fitting Window Application Data Set - Occultation - pTH	MDS
42	Limb/Occultation Fitting Window Application Data Set - Occultation - O_3 from UV	MDS
43	Limb/Occultation Fitting Window Application Data Set - Occultation - NO_2	MDS
44	Limb/Occultation Fitting Window Application Data Set - Occultation - O_3 from visible	MDS
45	Limb/Occultation Fitting Window Application Data Set - Occultation - BrO	MDS
46	Limb/Occultation Fitting Window Application Data Set - Occultation - H_2CO	MDS
47	Limb/Occultation Fitting Window Application Data Set - Occultation - SO_2	MDS
48	Limb/Occultation Fitting Window Application Data Set - Occultation - OClO	MDS
49	Limb/Occultation Fitting Window Application Data Set - Occultation - UV/Vis Spare	MDS
50	Limb/Occultation Fitting Window Application Data Set - Occultation - H_2O	MDS
51	Limb/Occultation Fitting Window Application Data Set - Occultation - CH_4	MDS
52	Limb/Occultation Fitting Window Application Data Set - Occultation - N_2O	MDS
53	Limb/Occultation Fitting Window Application Data Set - Occultation - CO	MDS
54	Limb/Occultation Fitting Window Application Data Set - Occultation - IR Spare	MDS
55	Ozone Profile from Nadir Measurements (tbd)	MDS
56	Limb Clouds Data Set	MDS

The following paragraphs present the detailed definition of the components listed above:

Main Product Header of the Level 2 Off-line Product (MPH)

No of Records: 1
Record Size: 1247
Component Size: 1247 Bytes

No	Name	Comments	Unit	Type	#	Size	Offset
1	MPH	The main product header is described in the ENVISAT product specification ([A2] volume 5)	-	tx	1247	1247	0

Specific Product Header of the Level 2 Off-line Product (SPH)

No of Records: 1
Record Size: 2875
Component Size: 2.81 kB

No	Name	Comments	Unit	Type	#	Size	Offset
1	DESCRIP-TOR	SPH_DESCRIPTOR="SCI_OL__2P~~~~~~~~~~~~~~~"^ (14/28/4) 28*uc	-	tx	46	46	0
2	STRIPCNT	STRIPLINE_CONTINUITY_INDICATOR=+000^ (30/4/2) Ac Strip-line counter or +000, if the product is a complete segment	-	tx	36	36	46
3	SLICEPOS	SLICE_POSITION=+001^ (14/4/2) Ac value: +001 to NUM_SLICES or +001 if no strip-line continuity	-	tx	20	20	82
4	NUMSLICES	NUM_SLICES=+001^ (10/4/2) Ac number of slices in this strip-line or +001 if no strip-line continuity	-	tx	16	16	102
5	STARTTIME	START_TIME="10-FEB-2002~13:32:54.000000"^ (10/27/4) 27*uc time of the first MDSR in the product, UTC format	-	tx	41	41	118
6	STOPTIME	STOP_TIME="10-FEB-2002~14:22:54.000000"^ (9/27/4) 27*uc time of the end of the measurement data in the product, UTC format	-	tx	40	40	159
7	STARTLAT	START_LAT=+0048000000<10-6degN>^ (9/21/2) AI with unit latitude of the satellite nadir at start time, the example above shows 48× North	-	tx	32	32	199
8	STARTLONG	START_LONG=-0120000000<10-6degE>^ (10/21/2) AI with unit latitude of the satellite nadir at start time, the example above shows 120× West	-	tx	33	33	231
9	STOPLAT	STOP_LAT=+0048000000<10-6degN>^ (8/21/2) AI with unit latitude of the satellite nadir at stop time	-	tx	31	31	264
10	STOPLONG	STOP_LONG=-0120000000<10-6degE>^ (9/21/2) AI with unit latitude of the satellite nadir at stop time	-	tx	32	32	295
11	DECONT	DECONT="nnnnnnnn "^ (6/41/4)8*char plus 33*blank Decontamination flag for each detector channel	-	tx	51	51	327

No	Name	Comments	Unit	Type	#	Size	Offset
12	DBSERVER	DB_SERVER_VER="05.00"^ (13/5/4) 5*uc Version number of the database server	-	tx	22	22	378
13	ERRORSUM	FITTING_ERROR_SUM="GOOD"^ (17/4/4) 4*uc quality summary of the fitting errors, may also be "FAIR" or "BAD~"	-	tx	25	25	400
14	NOOFNADIR	NO_OF_NADIR_FITTING_WINDOWS=+008^ (27/4/2) Ac number of nadir fitting windows	-	tx	33	33	425
15	NADIRWIN01	NAD_FIT_WINDOW_UV0="~325-~335~O3~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - O_3 from UV with rough wavelength range and acronym of driving parameter, if a fitting window application is not applied for this product the field shall be filled with the blank-padded and left-adjusted string 'EMPTY', see example in some other fields, this comment is valid for all window specifications below	-	tx	52	52	458
16	NADIRWIN02	NAD_FIT_WINDOW_UV1="~427-~452~NO2~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - NO_2	-	tx	52	52	510
17	NADIRWIN03	NAD_FIT_WINDOW_UV2="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - O_3 from visible	-	tx	52	52	562
18	NADIRWIN04	NAD_FIT_WINDOW_UV3="~336-~351~BRO~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - BrO	-	tx	52	52	614
19	NADIRWIN05	NAD_FIT_WINDOW_UV4="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - HCHO	-	tx	52	52	666
20	NADIRWIN06	NAD_FIT_WINDOW_UV5="~315-~327~SO2~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - anthropogenic SO_2	-	tx	52	52	718
21	NADIRWIN07	NAD_FIT_WINDOW_UV6="~365-~369~OClO~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - OClO	-	tx	52	52	770
22	NADIRWIN08	NAD_FIT_WINDOW_UV7="~315-~327~SO2~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - volcanic SO_2	-	tx	52	52	822

No	Name	Comments	Unit	Type	#	Size	Offset
23	NADIRWIN09	NAD_FIT_WINDOW_UV8="~688-~700~H2O~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications H_2O	-	tx	52	52	874
24	NADIRWIN10	NAD_FIT_WINDOW_UV9="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - UV Spare	-	tx	52	52	926
25	NADIRWIN11	NAD_FIT_WINDOW_IR0="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - H_2O	-	tx	52	52	978
26	NADIRWIN12	NAD_FIT_WINDOW_IR1="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - CH_4	-	tx	52	52	1030
27	NADIRWIN13	NAD_FIT_WINDOW_IR2="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - N_2O	-	tx	52	52	1082
28	NADIRWIN14	NAD_FIT_WINDOW_IR3="2324-2335~CO~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - CO	-	tx	52	52	1134
29	NADIRWIN15	NAD_FIT_WINDOW_IR4="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - CO_2	-	tx	52	52	1186
30	NADIRWIN16	NAD_FIT_WINDOW_IR5="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc nadir fitting window specifications - IR Spare	-	tx	52	52	1218
31	NOOFLIMB	NO_OF_LIMB_FITTING_WINDOWS=+003^ (26/4/2) Ac number of limb fitting windows	-	tx	32	32	1270
32	LIMBWIN00	LIM_FIT_WINDOW_PTH="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - pTH	-	tx	52	52	1322
33	LIMBWIN01	LIM_FIT_WINDOW_UV0="~520-~590~O3~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - O_3 from UV	-	tx	52	52	1374
34	LIMBWIN02	LIM_FIT_WINDOW_UV1="~420-~450~NO2~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - NO_2	-	tx	52	52	1426
35	LIMBWIN03	LIM_FIT_WINDOW_UV2="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - O_3 from visible	-	tx	52	52	1478

No	Name	Comments	Unit	Type	#	Size	Offset
36	LIMBWIN04	LIM_FIT_WINDOW_UV3="~337-~357~BRO~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - BrO	-	tx	52	52	1530
37	LIMBWIN05	LIM_FIT_WINDOW_UV4="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - H_2CO	-	tx	52	52	1582
38	LIMBWIN06	LIM_FIT_WINDOW_UV5="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - SO_2	-	tx	52	52	1634
39	LIMBWIN07	LIM_FIT_WINDOW_UV6="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - OClO	-	tx	52	52	1686
40	LIMBWIN08	LIM_FIT_WINDOW_UV7="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - UV Spare	-	tx	52	52	1738
41	LIMBWIN09	LIM_FIT_WINDOW_IR0="2030-2040~H2O~~~~~~~~~~~~~~~~"^ (18/14/4) 14*uc limb fitting window specifications - H_2O	-	tx	52	52	1790
42	LIMBWIN10	LIM_FIT_WINDOW_IR1="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - CH_4	-	tx	52	52	1842
43	LIMBWIN11	LIM_FIT_WINDOW_IR2="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - N_2O	-	tx	52	52	1894
44	LIMBWIN12	LIM_FIT_WINDOW_IR3="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - CO	-	tx	52	52	1946
45	LIMBWIN13	LIM_FIT_WINDOW_IR4="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc limb fitting window specifications - IR Spare	-	tx	52	52	1978
46	NOOFOCCL	NO_OF_OCCL_FITTING_WINDOWS=+000^ (26/4/2) Ac number of occultation fitting windows	-	tx	32	32	2030
47	OCCLWIN00	OCC_FIT_WINDOW_PTH="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - pTH	-	tx	52	52	2082
48	OCCLWIN01	OCC_FIT_WINDOW_UV0="EMPTY~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - O_3 from UV	-	tx	52	52	2134

No	Name	Comments	Unit	Type	#	Size	Offset
49	OCCLWIN02	OCC_FIT_WINDOW_UV1="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - NO_2	-	tx	52	52	2186
50	OCCLWIN03	OCC_FIT_WINDOW_UV2="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - O_3 from visible	-	tx	52	52	2238
51	OCCLWIN04	OCC_FIT_WINDOW_UV3="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - BrO	-	tx	52	52	2290
52	OCCLWIN05	OCC_FIT_WINDOW_UV4="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - H_2CO	-	tx	52	52	2342
53	OCCLWIN06	OCC_FIT_WINDOW_UV5="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - SO_2	-	tx	52	52	2394
54	OCCLWIN07	OCC_FIT_WINDOW_UV6="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - OClO	-	tx	52	52	2446
55	OCCLWIN08	OCC_FIT_WINDOW_UV7="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - UV Spare	-	tx	52	52	2498
56	OCCLWIN09	OCC_FIT_WINDOW_IR0="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - H_2O	-	tx	52	52	2550
57	OCCLWIN10	OCC_FIT_WINDOW_IR1="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - CH_4	-	tx	52	52	2602
58	OCCLWIN11	OCC_FIT_WINDOW_IR2="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - N_2O	-	tx	52	52	2654
59	OCCLWIN12	OCC_FIT_WINDOW_IR3="EMPTY~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - CO	-	tx	52	52	2706

No	Name	Comments	Unit	Type	#	Size	Offset
60	OCCLWIN13	OCC_FIT_WINDOW_IR4="EMPTY~~~ ~~~~~~~~~~~~~~~~~~~~~~~~"^ (18/14/20) 14*uc occultation fitting window specifications - IR Spare	-	tx	52	52	2758
61	SPARE2	Spare blank characters and one newline	-	tx	65	65	2810

In the field descriptions above the '~' character represents a blank character and the '^' a newline character. Fields 1 to 11 are pre-defined by the ENVISAT product specification (GS-2009). According to this specification all fields of this record shall consist of a parameter name and value separated by an equal sign. Text values are additionally enclosed with quotation marks. Each field in the component description above covers one line including the newline character. The comments column contains for each field a bracket pair with 3 numbers, as follows:

(a/b/c) t

where "a" is the number of characters for the parameter name, "b" the number of characters for the parameter value "c" the number of additional characters (like equal sign, quotes, newline) and "t" the type of parameter value according to GS-2009.

A relative realistic example of this SPH starting from line 12 is the following:

```
DB_SERVER_VER="05.00"
FITTING_ERROR_SUM="GOOD"
NO_OF_NADIR_FITTING_WINDOWS=+008
NAD_FIT_WINDOW_UV0=" 325- 335 O3                "
NAD_FIT_WINDOW_UV1=" 427- 452 NO2               "
NAD_FIT_WINDOW_UV2="EMPTY                       "
NAD_FIT_WINDOW_UV3=" 336- 351 BRO               "
NAD_FIT_WINDOW_UV4="EMPTY                       "
NAD_FIT_WINDOW_UV5=" 315- 327 SO2               "
NAD_FIT_WINDOW_UV6=" 365- 389 OCLO              "
NAD_FIT_WINDOW_UV7=" 315- 327 SO2               "
NAD_FIT_WINDOW_UV8=" 688- 700 H2O               "
NAD_FIT_WINDOW_UV9="EMPTY                       "
NAD_FIT_WINDOW_IR0="EMPTY                       "
NAD_FIT_WINDOW_IR1="EMPTY                       "
NAD_FIT_WINDOW_IR2="EMPTY                       "
NAD_FIT_WINDOW_IR3="2324-2335 CO                "
NAD_FIT_WINDOW_IR4="EMPTY                       "
NAD_FIT_WINDOW_IR5="EMPTY                       "
NO_OF_LIMB_FITTING_WINDOWS=+003
LIM_FIT_WINDOW_PTH="EMPTY                       "
LIM_FIT_WINDOW_UV0=" 520- 590 O3                "
LIM_FIT_WINDOW_UV1=" 420- 470 NO2               "
LIM_FIT_WINDOW_UV2="EMPTY                       "
LIM_FIT_WINDOW_UV3=" 337- 352 BRO               "
LIM_FIT_WINDOW_UV4="EMPTY                       "
LIM_FIT_WINDOW_UV5="EMPTY                       "
LIM_FIT_WINDOW_UV6="EMPTY                       "
LIM_FIT_WINDOW_UV7="EMPTY                       "
LIM_FIT_WINDOW_IR0="EMPTY                       "
LIM_FIT_WINDOW_IR1="EMPTY                       "
LIM_FIT_WINDOW_IR2="EMPTY                       "
```

```
LIM_FIT_WINDOW_IR3="EMPTY                       "
LIM_FIT_WINDOW_IR4="EMPTY                       "
NO_OF_OCCL_FITTING_WINDOWS=+000
OCC_FIT_WINDOW_PTH="EMPTY                       "
OCC_FIT_WINDOW_UV0="EMPTY                       "
OCC_FIT_WINDOW_UV1="EMPTY                       "
OCC_FIT_WINDOW_UV2="EMPTY                       "
OCC_FIT_WINDOW_UV3="EMPTY                       "
OCC_FIT_WINDOW_UV4="EMPTY                       "
OCC_FIT_WINDOW_UV5="EMPTY                       "
OCC_FIT_WINDOW_UV6="EMPTY                       "
OCC_FIT_WINDOW_UV7="EMPTY                       "
OCC_FIT_WINDOW_IR0="EMPTY                       "
OCC_FIT_WINDOW_IR1="EMPTY                       "
OCC_FIT_WINDOW_IR2="EMPTY                       "
OCC_FIT_WINDOW_IR3="EMPTY                       "
OCC_FIT_WINDOW_IR4="EMPTY                       "
```

Data Set Description of the Level 2 Off-line Product (DSD)

No of Records: 58
Record Size: 280
Component Size: 15.86 kB

No	Name	Comments	Unit	Type	#	Size	Offset
1	DSD	The data set descriptor record is described in the ENVISAT product spe-ification ([A2] volume 5)	-	tx	280	280	0

The general structure of the DSD records is defined in the ENVISAT product spec. The first field in these DSDs is the DS_NAME. This field allows to attach a name to each DS in the product; this name serves as a marker by which extraction programmes can identify a specific product content quickly and locate it immediately. A good example for the usage of this field is the extraction of a single trace gas column. The field allows for a maximum length of 28 characters. If a trace gas or geophysical parameter is not fitted, its MDS will not be present and the FILENAME field of the corresponding DSD record shall be filled with NOT USED. The following definitions will be included into the DSDs (ADSs first):

- SUMMARY_QUALITY
- STATE_GEOLOCATION
- STATIC_PARAM
- STATES
- GEOLOCATION_NADIR
- GEOLOCATION_LIMB

MDSs follow:

- CLOUDS_AEROSOL
- NAD_UV0_O3
- NAD_UV1_NO2
- NAD_UV2_O3
- NAD_UV3_BRO
- NAD_UV4_H2CO
- NAD_UV5_SO2
- NAD_UV6_OCLO
- NAD_UV7_SO2
- NAD_UV8_H2O
- NAD_UV9_SPARE
- NAD_IR0_H2O
- NAD_IR1_CH4
- NAD_IR2_N2O
- NAD_IR3_CO
- NAD_IR4_CO2
- NAD_IR5_SPARE
- LIM_PTH

- LIM_UV0_O3
- LIM_UV1_NO2
- LIM_UV2_O3
- LIM_UV3_BRO
- LIM_UV4_H2CO
- LIM_UV5_SO2
- LIM_UV6_OCLO
- LIM_UV7_SPARE
- LIM_IR0_H2O
- LIM_IR1_CH4
- LIM_IR2_N2O
- LIM_IR3_CO
- LIM_IR4_SPARE
- OCC_PTH
- OCC_UV0_O3
- OCC_UV1_NO2
- OCC_UV2_O3
- OCC_UV3_BRO
- OCC_UV4_H2CO
- OCC_UV5_SO2
- OCC_UV6_OCLO
- OCC_UV7_SPARE
- OCC_IR0_H2O
- OCC_IR1_CH4
- OCC_IR2_N2O
- OCC_IR3_CO
- OCC_IR4_SPARE
- NAD_PROFILE_O3
- LIM_CLOUDS

For reference of auxiliary files the following DSD records will be included:

- LEVEL_1B_PRODUCT
- INITIALISATION_FILE
- ECMWF_FILE
- M_FACTOR_FILE
- SPARE

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 Occulation and Ozone profiles from Nadir) one general MDS about clouds from Limb, 4 reference DSD for the input files and one spare record.

Summary of Quality Flags per State (ADS)

No of Records: 60
Record Size: 193
Component Size: 11.31 kB

No	Name	Comments	Unit	Type	#	Size	Offset
1	STARTTIME	Start time of the scan phase of the state	-	MJD	1	12	0
2	ATTACHED	Flag indicating if MDSR is attached to the current ADSR	-	uc	1	1	12
3	QUALITY	Summary of quality for the different geophysical parameters (cloud parameters, trace gas concentrations, etc.) of the complete state	-	uc	180	180	13

To support a product quality facility, a summary of quality flags for each state is given in this SQADS. (The number 60 of records is derived from the reference timeline, as described in chapter 5).

The quality flags are specified as unsigned characters having a range from 0 to 10. `1' represents the best and `10' the worst quality assigned to the mean value of quality parameters of a certain kind which are encountered during one state. Quality ranges will be defined for the following individual parameters:

- error on the cloud parameters (2)
- aerosol parameter diagnostic (2)
- quality of the driving geophysical parameter in each application (44)
- RMS of the retrieval algorithm (44)
- chi-square of the retrieval algorithm (44)
- goodness of fit of the retrieval algorithm (44)

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'.

Geolocation of the State (ADS)

No of Records: 60
Record Size: 45
Component Size: 2.64 kB

No	Name	Comments	Unit	Type	#	Size	Offset
1	STARTTIME	Start time of the scan phase of the state	-	MJD	1	12	0
2	ATTACHED	Flag indicating if MDSR is attached to the current ADSR	-	uc	1	1	12
3	CORNERS	4 corner coordinates of the ground scene which is covered by the state(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)	-	Coord	4	32	13

To support the extraction of SCIAMACHY data according to a given geolocation this ADS gives the geolocation (4 corner coordinates) of the scene on ground which is covered by each state. The number of 60 DSRs is resulting form the example in section 5.

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

No of Records: 1
Record Size: 60000
Component Size: 85.6 kB

No	Name	Comments	Unit	Type	#	Size	Offset
1	XMLPARAMS	XML text of the initialisation file which covers the complete range of static parameters (the present size is an estimation)	-	tx	60000	60000	0

States of the Product (ADS)

No of Records: 60
Record Size: 23
Component Size: 1.35 kB

No	Name	Comments	Unit	Type	#	Size	Offset
1	STARTTIME	Start time of the scan phase of the state	-	MJD	1	12	0
2	ATTACHED	Flag indicating if MDSR is attached to the current ADSR	-	uc	1	1	12
3	STATEID	State ID	-	us	1	2	13
4	DURATION	Duration of scan phase of the state	1/16 s	us	1	2	15
5	LONGEST	Longest integration time	1/16 s	us	1	2	17
6	SHORTEST	Shortest integration time	1/16 s	us	1	2	19
7	NOOFOBS	Number of geolocation records for this state	-	us	1	2	21

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 DSRs 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). The number of 60 DSRs is resulting form the example in section 5.

Nadir Geolocation (ADS)

No of Records: 3600
Record Size: 107
Component Size: 376.17 kB

No	Name	Comments	Unit	Type	#	Size	Offset
1	STARTTIME	Start time of the geolocation entity	-	MJD	1	12	0
2	ATTACHED	Flag indicating if MDSR is attached to the current ADSR	-	uc	1	1	12
3	INTTIME	Integration time for this geolocation entity	1/16 s	us	1	2	13
4	SOLARZEN	Solar zenith angles of the start, middle and end of the integration time at TOA	degree	fl	3	12	15
5	LOSZEN	Line-of-sight nadir angles of the start, middle and end of the integration time at TOA	degree	fl	3	12	27
6	RELAZI	Relative azimuth angles of the start, middle and end of the integration time at TOA	degree	fl	3	12	39
7	HEIGHT	Satellite geodetic height at the middle of the integration time	km	fl	1	4	51
8	RADIUS	Earth radius at the middle of the integration time	km	fl	1	4	55
9	SUBSAT	Sub-satellite point at the middle of the integration time	-	Coord	1	8	59
10	CORNERS	4 corner coordinates of the nadir ground pixel	-	Coord	4	32	67
11	CENTER	Center coordinates of the nadir ground pixel	-	Coord	1	8	99

In contradiction to the 'Geolocation of the States' component before, this ADS provides the detailed geolocation in steps of the shortest integration time of the corresponding observation. In case a fitting window application is using a detector cluster with a larger integration time the geolocation for this observation has to 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

The number of 3600 records assumes 30 minutes (1800 seconds) of Nadir observations with an average shortest integration time of 0.5 seconds.

Limb Geolocation (ADS)

No of Records: 2625
Record Size: 103
Component Size: 264.04 kB

No	Name	Comments	Unit	Type	#	Size	Offset
1	STARTTIME	Start time of the geolocation entity	-	MJD	1	12	0
2	ATTACHED	Flag indicating if MDSR is attached to the current ADSR	-	uc	1	1	12
3	INTTIME	Integration time for this geolocation entity	1/16 s	us	1	2	13
4	SOLARZEN	Solar zenith angles of the start, middle and end of the integration time at TOA	degree	fl	3	12	15
5	LOSZEN	Line-of-sight nadir angles of the start, middle and end of the integration time at TOA	degree	fl	3	12	27
6	RELAZI	Relative azimuth angles of the start, middle and end of the integration time at TOA	degree	fl	3	12	39
7	HEIGHT	Satellite geodetic height at the middle of the integration time	km	fl	1	4	51
8	RADIUS	Earth radius at the middle of the integration time	km	fl	1	4	55
9	SUBSAT	Sub-satellite point at the middle of the integration time	-	Coord	1	8	59
10	TANGGRD-POINT	Coordinates of tangent ground point at the start, middle and end of integration time	-	Coord	3	24	67
11	TANGHEIGHT	Tangent height at the start, middle and end of integration time	km	fl	3	12	91

For Limb the complete geolocation record is given here, as it is available from the level 1b product, even if the Limb results of a certain fitting application are not given for all tangent height levels. The attachment flag indicates which levels are at least once available in the Limb MDSs.

These records provide the detailed geolocation in steps of the shortest integration time of the corresponding observation. The shortest integration time is not constant over the whole product, but depends on the different states and may vary accordingly.

The number of 2625 records assumes 75 vertical scans having 35 measurement grid levels.

Clouds and Aerosol Data Set (MDS)

This component is of **variable record length**. The actual length is given in the DSRLEN field (the second field). Typical values of variable numbers are given in italic and brackets which are used for the calculation of typical sizes and offsets of the file, components and fields.

No of Records: 3600
Record Size: variable *(96)*
Component Size: variable *(337.5 kB)*

No	Name	Comments	Unit	Type	#	Size	Offset
1	STARTTIME	Start time of the clouds and aerosol record	-	MJD	1	12	0
2	DSRLEN	Data set record length (DSR) (required because this record may have a variable record length)	-	ul	1	4	12
3	QUALITY	Quality indicator (-1 if DSR is empty)	-	sc	1	1	16
4	INTTIME	Integration Time of DSR	1/16 s	us	1	2	17
5	SURFPRESS	Surface Pressure	hPa	fl	1	4	19
6	CLOUDFRAC	Cloud Fraction	-	fl	1	4	23
7	ERRCLD-FRAC	Error on cloud Fraction	rel. fraction	fl	1	4	27
8	NUMPMDPIX	Number of PMD sub-pixels for this DSR	-	us	1	2	31
9	FULLFREE	Number of PMD sub-pixels determined to be totally cloudy or totally cloud-free	-	us	2	4	33
10	TOPHEIGHT	Could-top height	km	fl	1	4	37
11	ERRTOPHEIGHT	Error on could-top height (currently set to -99.99), see product disclaimer	rel. fraction	fl	1	4	41
12	CLDOPT-DEPTH	Cloud optical depth	km	fl	1	4	45
13	ERRCLDOPT-DEP	Error on cloud optical depth (currently set -99.99), see disclaimer	rel. fraction	fl	1	4	49
14	CLOUDTYPE	Cloud type	-	us	1	2	53
15	CLOUDBRDF	Cloud-top bi-directional reflectance	-	fl	1	4	55
16	ERRCLOUD-BRDF	Error on cloud-top bi-directional reflectance	rel. fraction	fl	1	4	59
17	EFFSUR-FREFL	Effective Lambertian surface reflectance	-	fl	1	4	63
18	ERREFFS-REFL	Error on Effective Lambertian surface reflectance	rel. fraction	fl	1	4	67
19	CLOUDFLAG	Flag describing the cloud parameter output	-	us	1	2	71
20	AAI	Absorbing aerosol indicator	-	fl	1	4	73
21	AAIDIAG	Diagnostic of the absorbing aerosol indicator	-	fl	1	4	77
22	AAIFLAG	Flag describing the absorbing aerosol indicator output	-	us	1	2	81
23	NUMAERO-PARS	Number of additional aerosol parameters (n_a)	-	us	1	2	83
24	AEROPARS	Additional aerosol parameters	-	fl	n_a *(3)*	*(12)*	*(85)*

Cloud-top height and error are written per observation and are valid for the shortest integration time.

The flags describing the cloud type (field 14) have to be interpreted bit-wise. They contain the classification of clouds according to the WMO scheme (when the bit is set the italic condition is true; bits are counted from 0 to 15). The following is defined:

- 0: *low* or high cloud
- 1: *ice* or water cloud
- 2: *thick* or thin cloud
- 3-15: not used

The flags describing the output (field 19 and 22) have to be interpreted bit-wise. They will contain information reflecting some important settings in the initialisation file (when the bit is set the italic condition is true; bits are counted from 0 to 15).

For the cloud components, the definition is:

- 0: source of cloud fraction *PMD* - fitting
- 1: source of cloud-top pressure *in VCD algorithm* - ISCCP
- 2: source of cloud-top height fitting - SACURA: *full convergence*
- 3: source of cloud-top height fitting - SACURA:
  number of iterations exceeded, average of neighboured values taken
- 4: source of cloud-top height fitting - SACURA: *cloud layer size set to constraint*
- 5: source of cloud-top height fitting - SACURA: *cloud-bottom height set to constraint*
- 6: source of cloud-top height fitting - SACURA: *cloud-top height set to constraint*
- 7-15: not used at present

Note that SACURA provides a sophisticated flagging at output which mirrors if a constraint is set for a quantity during the fitting. This may happen if cloud-bottom height, cloud-top height, or cloud layer size exceed pre-defined constraints. In that case, each quantity can be individually set to the contraint value. In case SACURA exceeds the number of iterations, the arithmetic average of the neighbour values is taken. If cloud-clear condition is reflected from the PMD algorithm, cloud-top height and cloud optical thickness are set to 0.

In case of SACURA, an error of 0.25 km can be expected for full convergence; otherwise 0.5 km.

For the aerosol components (field 22), the current definition is:

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

In case AAI values are not computed, but just copied from observations with longer integration times, AAI flags remain unset.

For the current version the number of additional aerosol parameters (field 23) is 3. Additional aerosol parameters (field 24) are:

- 0: the residue calculated in the AAIA
- 1: the retrieved surface albedo at 380 nm
- 2: the ground height used in the AAIA

The number of records is taken from the number of records of the Nadir geolocation.

Nadir Fitting Window Application Data Set (MDS)

This component is of **variable record length**. The actual length is given in the DSRLEN field (the second field). Typical values of variable numbers are given in italic and brackets which are used for the calculation of typical sizes and offsets of the file, components and fields.

No of Records: 36000
Record Size: variable *(157)*
Component Size: variable *(5.39 MB)*

No	Name	Comments	Unit	Type	#	Size	Offset
1	STARTTIME	Start time of the nadir record	-	MJD	1	12	0
2	DSRLEN	Data set record length (DSR) (required because this record may have a variable record length)	-	ul	1	4	12
3	QUALITY	Quality indicator (-1 if DSR is empty)	-	sc	1	1	16
4	INTTIME	Integration Time of DSR	1/16 s	us	1	2	17
5	NUMOFVCD	Number of vertical column densities (n_V)	-	us	1	2	19
6	VCD	Vertical column density (VCD) of the main parameter	molecule/ cm^2	fl	n_V *(1)*	*(4)*	*(21)*
7	ERRVCD	Error on the vertical column density	relative fraction	fl	n_V *(1)*	*(4)*	*(25)*
8	VCDFLAG	Flag describing the VCD output	-	us	1	*(2)*	*(29)*
9	ESC	Effective slant column (ESC) density of the main parameter	molecule/ cm^2	fl	1	*(4)*	*(31)*
10	ERRESC	Error on the effective slant column (ESC) density above	relative fraction	fl	1	*(4)*	*(35)*
11	NUMLINFITP	Number of linear fitted parameters (n_1)	-	us	1	*(2)*	*(39)*
12	NUMNLIN-FITP	Number of non-linear fitted parameters (n_2)	-	us	1	*(2)*	*(41)*
13	LINPARS	Linear fitted parameters	-	fl	n_1 *(4)*	*(16)*	*(43)*
14	ERRLINPARS	Error on the linear fitted parameters	relative fraction	fl	n_1 *(4)*	*(16)*	*(59)*
15	LINCORRM	Cross-correlation matrix entries of the linear fit ($m_1 = 1/2 * n_1 * (n_1 - 1)$)	-	fl	m_1 *(6)*	*(24)*	*(75)*
16	NLINPARS	Non-linear fitted parameters	-	fl	n_2 *(2)*	*(8)*	*(99)*
17	ERRNLIN-PARS	Error on the non-linear fitted parameters	relative fraction	fl	n_2 *(2)*	*(8)*	*(107)*
18	NLINCORRM	Cross-correlation matrix entries of the non-linear fit ($m_2 = 1/2 * n_2 * (n_2 - 1)$)	-	fl	m_2 *(1)*	*(4)*	*(115)*
19	RMS	RMS of the fit	-	fl	1	*(4)*	*(119)*
20	CHI2	Chi-square of the fit	-	fl	1	*(4)*	*(123)*
21	GOODNESS	Goodness of the fit	-	fl	1	*(4)*	*(127)*
22	NUMITER	Number of Iterations for the non-linear fit	-	us	1	*(2)*	*(131)*
23	FITFLAG	Fitting output flag	-	us	1	*(2)*	*(133)*
24	AMFGRD	AMF to ground	-	fl	1	*(4)*	*(135)*

No	Name	Comments	Unit	Type	#	Size	Offset
25	ERRAMFGRD	Error on the AMF to ground	relative fraction	fl	1	*(4)*	*(139)*
26	AMFCLD	AMF to cloud-top	-	fl	1	*(4)*	*(143)*
27	ERRAMFCLD	Error on the AMF to cloud-top	relative fraction	fl	1	*(4)*	*(147)*
28	AMFFLAG	AMF output flag	-	us	1	*(2)*	*(151)*
29	TEMPERA-TURE	Temperature of reference spectrum	K	fl	1	*(4)*	*(153)*

The format component above is repeated for each fitting window. Therefore the number of records is taken from the Nadir geolocation record multiplied by the number of fitting window applications given in this product (example: 10).

Field 5 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 6 and 7:

- For H_2O [S12] fields 6 and 7 consist of two entries. The first entry of field 6 gives the VCD in molecules/cm^2, the second in g/cm^2. The latter unit is more convenient in the meteorological community. Field 7 contains for both entries the absolute error in g/cm^2.
- For CO fields 6 and 7 consist of two entries. The first entry contains xCO (= $VCD_{CO,ref}$ * α_{CO}/α_{CH4}), the second VCD_{CO} (= $VCD_{CO,ref}$ * α_{CO}).[1]

Flags describing the output will be interpreted bit-wise (conventions as above), and the following are the current baseline. 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).

Field 8 describes the VCD calculation. 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 H_2O) 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-nn: α between bounds and $|\alpha_{err}|$ < limit, a pair of flags for each gas (α_{err} currently 0.5)

1. This is only valid if the first gas in the intitialisation file is CO and the second gas is CH_4.

α is the fitted scaling factor, nn = 2 * number of gases + 5, i.e 11 for CO. The sequence of gases is defined by the initialization file.

Fields 11/12, 13/14 and 16/17 require some special treatment for IAS. Field 11 will contain the number of linear fit parameters, which is currently 1, and Field 12 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 13 and 14 show value and error of the reflectance in the IAS case. Fields 16 and 17 have currently five entries each, containing the values and errors of the scaling factors of gases (i.e. α_{CO}, α_{CH4}, α_{H2O}) and HWHM. The last entry of Field 16 and 17 is empty (i.e. filled with 0) , because value and error of the linear fit parameter are already given in Field 13 and 14, respectively.

Field 23 specifies the slant column density fitting. 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 on measurement grid
- 6: literature - *SCIAMACHY* cross-sections used
- 7: linear - *non-linear fitting*
- 8: no - *yes* use of SO_2 correction
- 9-11: quality, to be interpreted as 3 bit integer, 0 lowest quality, 7 highest quality
- 12-15: not used at present

Field 28 flags options used in the AMF look-up scheme. 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 at present

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 9 and 10 (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 13-15) are absent. In the field 24 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 25 its error. Fields 26 and 27 are left empty as well, because no AMF to cloud-top is calculated in the AMC-DOAS algorithm. All errors for AMC-DOAS (fields 7, 17, 25) are absolute values.

Limb/Occultation Fitting Window Application Data Set (MDS)

This component is of **variable record length**. The actual length is given in the DSRLEN field (the second field). Typical values of variable numbers are given in italic and brackets which are used for the calculation of typical sizes and offsets of the file, components and fields.

No of Records: 750
Record Size: variable *(33163)*
Component Size: variable *(23.72 MB)*

No	Name	Comments	Unit	Type	#	Size	Offset
1	STARTTIME	Start time of the profile record	-	MJD	1	12	0
2	DSRLEN	Data set record length (DSR) (required because this record may have a variable record length)	-	ul	1	4	12
3	QUALITY	Quality indicator (-1 if DSR is empty)	-	sc	1	1	16
4	INTTIME	Integration Time of each indiviual step in the measurement gird	1/16 s	us	1	2	17
5	METHOD	Retrieval method 'O' = optimal estimation, 'N' = non-linear least squares fitting, etc.	-	uc	1	1	19
6	REFH	Height of the reference pressure	km	fl	1	4	20
7	REFP	Reference pressure for hydrostatic equilibrium	hPa	fl	1	4	24
8	REFPSRC	Reference pressure source 'E' = ECMWF, 'C' = climatology, etc.	-	uc	1	1	28
9	NUM_RLEVEL	Number of profile entries (n_{main})	-	uc	1	1	29
10	NUM_MLEVEL	Number of used measurement levels (n_{meas})	-	uc	1	1	30
11	NUM_SPECIES	Number of fitted main gas species (n_1, on the retrieval grid,)	-	uc	1	1	31
12	NUM_CLOSURE	Number of fitted closure parameters (n_2, on the measurement grid)	-	uc	1	1	32
13	NUM_OTHER	Number of fitted other parameters (n_3)	-	uc	1	1	33
14	NUM_SCALE	Number of fitted scaling parameters for auxiliary gases (n_4, just one value per profile, n_4 is contained in n_3)	-	uc	1	1	34
15	TANGH	Tangent height at the lower layer boundary	km	fl	n_{main} *(30)*	*(120)*	*(35)*
16	TANGP	Tangent layer pressure at the lower layer boundary	hPa	fl	n_{main} *(30)*	*(120)*	*(155)*
17	TANGT	Tangent layer temperature (mean)	K	fl	n_{main} *(30)*	*(120)*	*(275)*
18	MAINREC	Main species which have been fitted on the coarse forward model grid	-	LayerRec	$n_{main} * n_1$ *(60)*	*(960)*	*(395)*
19	SCALEDREC	Scaled profiles which have been used for the fit on the coarse forward model grid	-	LayerRec	$n_{main} * n_4$ *(60)*	*(960)*	*(1355)*
20	MGRID	Measurement Grid	-	Meas-Grid	n_{meas} *(13)*	*(429)*	*(2315)*
21	STVEC_SIZE	State vector size ($n_{StVec} = n_1 * n_{main} + n_2 + n_3$)	-	us	1	*(2)*	*(2744)*

No	Name	Comments	Unit	Type	#	Size	Offset
22	STATEVEC	State Vector	-	StateVec	n_{StVec} *(117)*	*(1404)*	*(2746)*
23	CMATRIX-SIZE	Correlation matrix size (m_f = 1/2 * n_{StVec} * (n_{StVec} - 1))	-	us	1	*(2)*	*(4150)*
24	CORRMA-TRIX	Correlation matrix of the fit	-	fl	m_f *(6786)*	*(27144)*	*(4152)*
25	RMS	RMS of the fit	-	fl	1	*(4)*	*(31296)*
26	CHI2	chi-square of the fit	-	fl	1	*(4)*	*(31300)*
27	GOODNESS	Goodness of the fit	-	fl	1	*(4)*	*(31304)*
28	ITERATION	Number of iterations for the fit (n_I)	-	us	1	*(2)*	*(31308)*
29	SUMMARY	Measurement summary: number of used and rejected wavelengths	-	us	2	*(4)*	*(31310)*
30	CRITERIA	Convergency criteria	-	b	1	*(1)*	*(31314)*

No	Name	Comments	Unit	Type	#	Size	Offset
31	RESSIZE	Residuals size ($n_{res} = n_{StVec} * n_I$)	-	us	1	*(2)*	*(31315)*
32	RESIDUALS	Iteration step state vector residuals	-	fl	n_{res} *(461)*	*(1844)*	*(31317)*
33	NUM_ADDDIAG	Number of additional diagnostics (n_{ad})	-	us	1	*(2)*	*(33161)*
34	ADDDIAG	Additional diagnostics. This entry is dynamical and contains additional information provided to the user in following order: Degree of freedom, Information content (not computed and set 1.0), Diagonal of averaging kernel (in partial columns), Retrieved profile(s) in number density, Initial profile(s) in number density, Scaling factor multiplied on profile(s) in partial columns to calculate profile(s) in volume mixing ratio, Scaling factor multiplied on profile(s) in partial columns to calculate profile(s) in number densities, and Averaging kernel in partial columns. Note that the scaling factors are dimensioned in the size of the profiles. Following relations hold between scaling factors and averaging kernel: $Avg.kernel_{num.dens.}(k,m) = Avg.kernel_{partial\ columns} * (scaling\ factor_{num.dens.}(k) / scaling\ factor_{num.dens.}(m))$ and $Avg.kernel_{VMR}(k,m) = Avg.kernel_{partial\ columns} * (scaling\ factor_{VMR}(k) / scaling\ factor_{VMR}(m))$ Number of elements are calculated from $n_{ad} = 2 + n_{stvec} + n_1*n_{main} + n_1*n_{main} + n_{main} + n_{main} + n_1*n_{main}*n_{main}$	-	fl	n_{ad} *(0)*	*(0)*	*(33163)*

The limb measurement data set consists of several records containing the retrieval result of one vertically sorted sequence of limb measurements. A complete limb scan, given by one limb state, may consist of more than one limb profile depending on the integration time during one azimuth sweep of the corresponding channels from which the fitting window parts were taken. Therefore, the number of records of the 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 25 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 MDS per fitting window application (example: 75) multiplied by the number of fitting window applications (example: 10).

Convergency criteria is a flag which is not defined, currently.

Detailed instructions on the usage of the Limb MDS can be found in [R11].

Limb Clouds Data Set (MDS)

This component is of **variable record length**. The actual length is given in the DSRLEN field (the second field). Typical values of variable numbers are given in italic and brackets.

No of Records: 100
Record Size: variable *(66)*
Component Size: variable *(6 kB)*

No	Name	Comments	Unit	Type	#	Size	Offset
1	STARTTIME	Start time of the limb clouds record	-	MJD	1	12	0
2	DSRLEN	Data set record length (DSR) (required because this record may have a variable record length)	-	ul	1	4	12
3	QUALITY	Quality indicator (-1 if DSR is empty)	-	sc	1	1	16
4	INTTIME	Integration time of DSR	1/16 s	us	1	2	17
5	CLOUDDIAG	Diagnostics of the cloud detection algorithm, details see below	-	b	1	1	19
6	FLAG_WCL	Flag for normal water clouds	-	uc	1	1	20
7	MAXVAL_WCL	Maximium value of CIR for normal water clouds	-	fl	1	4	21
8	MAXHEIGHT_WCL	Height of maximum value of CIR for normal water clouds	km	fl	1	4	25
9	MAXHEIGHTIDX_WCL	Height index of maximum value of CIR for normal water clouds	-	uc	1	1	29
10	FLAG_ICL	Flag for ice clouds	-	uc	1	1	30
11	MAXVAL_ICL	Maximium value of CIR for ice clouds	-	fl	1	4	31
12	MAXHEIGHT_ICL	Height of maximum value of CIR for normal water clouds	km	fl	1	4	35
13	MAXHEIGHTIDX_ICL	Height index of maximum value of CIR for ice clouds	-	uc	1	1	39
14	FLAG_PSC	Flag for polar stratospheric clouds	-	uc	1	1	40
15	MAXVAL_PSC	Maximium value of CIR for polar stratospheric clouds	-	fl	1	4	41
16	MAXHEIGHT_PSC	Height of maximum value of CIR for polar stratospheric clouds	km	fl	1	4	45
17	MAXHEIGHTIDX_ICL	Height index of maximum value of CIR for ice clouds	-	uc	1	1	49
18	FLAG_NLC	Flag for noctilucent clouds	-	uc	1	1	50
19	MAXVAL_NLC	not used at present	-	fl	1	4	51
20	MAXHEIGHT_NLC	Maximum height of strictly monotonically increasing radiances for noctilucent clouds	km	fl	1	4	55
21	MAXHEIGHTIDX_NLC	Maximum height index of strictly monotonically increasing radiances for noctilucent clouds	-	uc	1	1	59
22	NUMTANH	Number of tangent heights for CIR (m_1)	-	us	1	2	60

No	Name	Comments	Unit	Type	#	Size	Offset
23	TANH	Tangent heigths for CIR	km	fl	m_1 (0)	(0)	62
24	NUMCIR	Number of CIR (m_2)	-	us	1	2	62
25	CIR	CIR ($m = m_1 * m_2$)	-	fl	m (0)	(0)	64
26	NUMCLOUD-PARS	Number of additional limb cloud parameters (n)	-	us	1	2	64
27	CLOUDPARS	Additional limb cloud parameters	-	fl	n *(0)*	*(0)*	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 assignemt of bits is

- 0: retrieval of normal water clouds succeded
- 1: retrieval of ice clouds succeded
- 2: retrieval of polar stratospheric clouds succeded
- 3: retrieval of noctilucent clouds succeded
- 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.

3.4.5 Sizing

A product will be sized to one orbit of measurements.

3.4.6 Volume

The precise size of one level 2 off-line product is calculated using the assumptions given in the text above. These assumptions yield the following size: 30.15 MB

3.4.7 Throughput

There will be one product per orbit.

3.4.8 Remarks

Detailed instructions on the usage of the Limb MDS can be found in [R11].

3.5 Initialisation File

3.5.1 Identifier

SCI_IN__AX

3.5.2 Type

Auxiliary

3.5.3 Description

In principle static parameters may be inserted directly into the processor's code as constants, but the use of an initialisation file improves the maintainability of SGP_12OL. The GADS of the initialisation file for the static parameters is a block of ASCII data formated with XML representing the static parameters of the level 1b to 2 processing. The position of the parameters in the XML file is arbitrary. The structure of the ASCII block is defined by the DTD given in the format section. The initialisation file is used to specify the following parameters:

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

The static parameters are divided into several main sections, which reflect major components in the SGP_12OL chain.

The initialisation file will include headers and one GADS. The main product header (MPH) has a fixed format, as described in ENVISAT product spec., and includes information about product identification and sizes of the following data. Other fields in the general MPH (such as data acquisition and processing time, position of the measurement data, ENVISAT orbit and position, SBT to UTC conversion and product confidence data) have no real meaning for this product type and will be left blank. A specific product header (SPH) will include the identification of the version of this initialisation file and the data set description record (DSD) for the following GADS. The GADS of this initialisation file will have a single DSR described below.

The detailed list of parameters will be given in the GADS.

The size of this component is variable.

In general, XML is a near relative of HTML, the language of the web. There are following differences:

- The names of tags are not pre-defined. Custom tag definitions may be provided by the use of a DTD, as given below.
- XML is very strict, e.g. it requires always end tags, attribute values have to be enclosed by double quotes and the nesting of tags needs to be done properly.
- XML always requires a DTD, either it is provided within the XML file or by the use on an external file which is the preferred solution, if more than one file shall follow these definitions.

An example of the proposed initialisation file content is given in the appendix.

3.5.4 Format

The detailed format description is divided into several tables representing the hierarchy of product content. The product consists of the following components:

Id	Product Component	Comp. Type
1	Main Product Header of an auxiliary file	MPH
2	Specific Product Header of an auxiliary file	SPH
3	Data Set Description of an auxiliary file	DSD
4	Static Parameter of the Level 2 off-line Processor	GADS

The following paragraphs present the detailed definition of the components listed above:

Main Product Header of an auxiliary file (MPH)

No of Records: 1
Record Size: 1247
Component Size: 1247 Bytes

No	Name	Comments	Unit	Type	#	Size	Offset
1	MPH	The main product header is described in the ENVISAT product specification ([A2] volume 5)	-	tx	1247	1247	0

Specific Product Header of an auxiliary file (SPH)

No of Records: 1
Record Size: 98
Component Size: 98 Bytes

No	Name	Comments	Unit	Type	#	Size	Offset
1	SPH	The specific product header of auxiliary file is described in the ENVISAT product specification ([A2] volume 5)	-	tx	98	98	0

The general structure of the SPH record for auxiliary files is defined in the ENVISAT product specification document ([A2] volume 5).

Data Set Description of an auxiliary file (DSD)

No of Records: 1
Record Size: 280
Component Size: 280 Bytes

No	Name	Comments	Unit	Type	#	Size	Offset
1	DSD	The data set descriptor record is described in the ENVISAT product specification (volume 5)	-	tx	280	280	0

The general structure of the DSD records is defined in the ENVISAT product specification document. The DS_NAME field will contain:

- STATIC_PARAM

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

No of Records: 1
Record Size: 60000
Component Size: 58.59 kB

No	Name	Comments	Unit	Type	#	Size	Offset
1	XMLPARAMS	XML text of the initialisation file which covers the complete range of static parameters (the present size is an estimation)	-	tx	60000	60000	0

3.5.5 Sizing

There is in principle just one initialisation file for one processor version. Modifications or versions of this file are expected after software changes and validation campaigns and recognized in processor version number.

3.5.6 Volume

The size of the (example) initialisation file is approx.: 60.18 kB

3.5.7 Throughput

N/A

3.5.8 Remarks

N/A

3.6 ECMWF Analysis Data File

3.6.1 Identifier

SCI_ECA_AX

3.6.2 Type

Auxiliary

3.6.3 Description

ECMWF data files contain Meteo information. They are ingested into the PDS ground segment on a regular basis and are used by various instrument processors during the generation of products. SCIAMACHY level 1b to 2 off-line processing is designed to input this kind of data as a priori information for the retrieval of geophysical parameters, but makes currently no usage of this opportunity.

There are two kinds of ECMWF data: Forecast and Analysis data. Forecast data is used in NRT processing, while Analysis data is used during off-line product generation. Both types of data have the same format.

The detailed format description of the ECMWF data is given in [A2].

3.6.4 Format

N/A

3.6.5 Sizing

N/A

3.6.6 Volume

N/A

3.6.7 Throughput

N/A

3.6.8 Remarks

N/A

3.7 M-Factor File

3.7.1 Identifier

SCI_MF1_AX

3.7.2 Type

Auxiliary

3.7.3 Description

The m-factor files are an extension to the characterisation data base of SCIAMACHY to describe the degradation of the instrument light path during flight. Currently m-factors are applied as a calibration step in the level 1b to 2 processor. The following parameters are envisaged by the calibration plan [R13]:

- Ratio of sun diffuser measurements
  - ratio of the detector array signals
- Ratios of sun occultation measurements
  - ratio of the detector array signals
  - ratio of the regular PMD signals
  - ratio of the 45° PMD signal
- Ratios of sub-solar calibration measurements
  - ratio of the detector array signals
  - ratio of the regular PMD signals
  - ratio of the 45° PMD signal (additional compared to Calibration Plan)
- Ratio of WLS measurements with and without ND filter
  - ratio of the detector array signals
- Spare ratios of an arbitrary calibration measurements (additional compared to Calibration Plan)
  - ratio of the detector array signals
  - ratio of the regular PMD signals
  - ratio of the 45° PMD signal

3.7.4 Format

The m-factor file will include headers and a set of MDSs. The main product header (MPH) has a fixed format, as described in [A2] and includes information about product identification and sizes of the following data. Other fields in the general MPH like data acquisition and processing time and position of the measurement data, ENVISAT orbit and position, SBT to UTC conversion and product confidence data have no real meaning for this product type and will be left blank. A specific product header (SPH) will include a SPH descriptor and the data set description records (DSD) for the following MDSs. The MDSs of this m-factor file will have just one DSR which consist of one complete file out of the list of different m-factor files as delivered by the SOS team. The header layout may be described as follows:

Main Product Header (MPH)

No of Records: 1
Record Size: 1247
Component Size: 1247 Bytes

Id	Name	Comments	Unit	Type	#	Size	Offset
1	MPH	The main product header is described in the ENVISAT product specification (volume 5)	-	tx	1247	1247	0

Specific Product Header of Auxiliary Data (SPH)

No of Records: 1
Record Size: 98
Component Size: 98 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	SPH_DESCRIPTOR=	keyword	tx	15	15	0
2	"M_FACTOR_FILE~~~~~~~~~~~~~~~~~"	variable	tx	30	30	15
3	Newline character	terminator	tx	1	1	45
4	Spare	-	tx	51	51	46
5	Newline character	terminator	tx	1	1	97

Data Set Descriptior Records (DSD)

No of Records: 11
Record Size: 280
Component Size: 3080

Id	Name	Comments	Unit	Type	#	Size	Offset
1	DSD	The data set descriptor record is described in the ENVISAT product specification (volume 5)	-	tx	280	280	0

For the time being 10 m-factor parameters in the same number of m-factor files are expected by the SOS team [R13]. 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
  1. M_CAL
- from sun occultation
  2. M_DL
  3. M_PL
  4. M_QL
- from sub-solar calibration
  5. M_DN
  6. M_PN
  7. M_QN
- from WLS measurements

8. M_NDF

- spare m-factor set (e.g. from moon occultation)
  9. M_DS
  10. M_PS
  11. M_QS

The general format description of these files is defined in [R14]. For a format description of a specific characterisation data base this general definition has to be extended by a set of acronyms, parameter name definitions and dimensions of the different correction factors. A first version of this information will be given here, because the characterisation activity was even not yet started and it is very likely that also this information (like the characterisation data base) is subject to change.

The following list defines the acronyms specific of the individual m-factors in the files mentioned above:

- Sun viewing via diffuser with ND filter ratio
  1. Parameter name: _M_FACTOR_CAL
     Comment = Ratio of the array detector signals between a reference sun diffuser measurement with the neutral density filter inserted and a corresponding measurement at a certain time
     Accuracy = tbd.
     Unit = <none>
     Dimensions = 1
     Dim_1 = 8192
     Dim_1_Argument = Wavelength
     Dim_1_Unit = nm
     Dim_1_List = 240-2400
     Data_Type = _R4
- Sun occultation measurement ratio
  2. Parameter name: _M_FACTOR_DL
     Comment = Ratio of the array detector signals between a reference sun occultation measurement and a corresponding measurement at a certain time
     Accuracy = tbd.
     Unit = <none>
     Dimensions = 1
     Dim_1 = 8192
     Dim_1_Argument = Wavelength
     Dim_1_Unit = nm
     Dim_1_List = 240-2400
     Data_Type = _R4
  3. Parameter name: _M_FACTOR_PL
     Comment = Ratio of the regular PMD signals between a reference sun occultation measurement and a corresponding measurement at a certain time
     Accuracy = tbd.
     Unit = <none>
     Dimensions = 1
     Dim_1 = 6
     Dim_1_Argument = PMD number
     Dim_1_Unit = <none>

Dim_1_Start = 1
Dim_1_Step = 1
Data_Type = _R4

4. Parameter name: _M_FACTOR_QL
   Comment = Ratio of the 45° PMD signal between a reference sun occultation measurement and a corresponding measurement at a certain time
   Accuracy = tbd.
   Unit = <none>
   Dimensions = 1
   Dim_1 = 1
   Dim_1_Unit = <none>
   Data_Type = _R4

- Sub-solar calibration measurement ratio

5. Parameter name: _M_FACTOR_DN
   Comment = Ratio of the array detector signals between a reference sub-solar calibration measurement and a corresponding measurement at a certain time
   Accuracy = tbd.
   Unit = <none>
   Dimensions = 1
   Dim_1 = 8192
   Dim_1_Argument = Wavelength
   Dim_1_Unit = nm
   Dim_1_List = 240-2400
   Data_Type = _R4
6. Parameter name: _M_FACTOR_PN
   Comment = Ratio of the regular PMD signals between a reference sub-solar calibration measurement and a corresponding measurement at a certain time
   Accuracy = tbd.
   Unit = <none>
   Dimensions = 1
   Dim_1 = 6
   Dim_1_Argument = PMD number
   Dim_1_Unit = <none>
   Dim_1_Start = 1
   Dim_1_Step = 1
   Data_Type = _R4
7. Parameter name: _M_FACTOR_QN
   Comment = Ratio of the 45° PMD signal between a reference sub-solar calibration measurement and a corresponding measurement at a certain time
   Accuracy = tbd.
   Unit = <none>
   Dimensions = 1
   Dim_1 = 1
   Dim_1_Unit = <none>
   Data_Type = _R4

- WLS with / without ND filter ratio

8. Parameter name: _M_FACTOR_NDF
   Comment = (tbd)

Accuracy = tbd.
Unit = <none>
Dimensions = 1
Dim_1 = 8192
Dim_1_Argument = Wavelength
Dim_1_Unit = nm
Dim_1_List = 240-2400
Data_Type = _R4

- Spare ratio

9. Parameter name: _M_FACTOR_DS
   Comment = Ratio of the array detector signals between a reference spare calibration measurement and a corresponding measurement at a certain time
   Accuracy = tbd.
   Unit = <none>
   Dimensions = 1
   Dim_1 = 8192
   Dim_1_Argument = Wavelength
   Dim_1_Unit = nm
   Dim_1_List = 240-2400
   Data_Type = _R4
10. Parameter name: _M_FACTOR_PS
    Comment = Ratio of the regular PMD signals between a reference spare calibration measurement and a corresponding measurement at a certain time
    Accuracy = tbd.
    Unit = <none>
    Dimensions = 1
    Dim_1 = 6
    Dim_1_Argument = PMD number
    Dim_1_Unit = <none>
    Dim_1_Start = 1
    Dim_1_Step = 1
    Data_Type = _R4
11. Parameter name: _M_FACTOR_QS
    Comment = Ratio of the 45° PMD signal between a reference spare calibration measurement and a corresponding measurement at a certain time
    Accuracy = tbd.
    Unit = <none>
    Dimensions = 1
    Dim_1 = 1
    Dim_1_Unit = <none>
    Data_Type = _R4

3.7.5 Sizing

All m-factors will be put into one file.

3.7.6 Volume

approx. 1.0 MB

3.7.7 Throughput

Major calibration measurements are planned every month during normal operation of SCIAMACHY. Therefore, it is expected that a new set of m-factors may be generated once per month.

3.7.8 Remarks

N/A

3.8 Climatological and Spectroscopic Data Bases

3.8.1 Common properties

Identifier

SCI_PR2_AX

SCI_CL2_AX

SCI_SF2_AX

SCI_CS2_AX

SCI_FM2_AX

SCI_UX2_AX

SCI_UC2_AX

SCI_KEY_AX

SCI_ES2_AX

SCI_CC2_AX

Type

Auxiliary

Description

The SCIAMACHY Climatological and Spectroscopic Data Base is divided into 10 general classes as follows:

1. Profile data bases (PR2): Pressure, temperature, trace gas concentration profiles;
2. Cloud data bases (CL2): ISCCP data base, Cloud-top albedo;
3. Surface data bases (SF2): Global surface albedo, global vegetation index, global topography and other surface reflectance data;
4. Cross-section data bases (CS2): Absorption cross-sections from literature appropriate for SCIAMACHY;
5. Flight-model data bases (FM2): Absorption cross-sections for trace gases measured with the SCIAMACHY flight-model during the PI-period;
6. Auxiliary cross-section data (UX2): Absorption cross-sections from GOME and literature sources, especially used for SO_2, BrO and OClO retrieval
7. Undersampling data bases (UC2): Calculated undersampling spectra for DOAS and IAS applications;
8. Key data base (KEY): ETA & ZETA key data;
9. ESFT spectral data (ES2): ESFT Hitran spectral inputs for SACURA cloud algorithm;
10. Cloud clearing data (CC2): PMD minimum reflectance data base.

The current initialisation file of SGP_12OL, version 5.00, 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. For this reason they are included in the I/O DD.

The scientific content and source references for most of these level 1b to 2 data bases have been described for the GOME data processor in [R3]. For the origin of undersampling correction spectra see [S2], [S3].

The Climatological and Spectroscopic Data Bases are divided into several files; each combines logically related information and parameters. Each of these files will include a header and a small number of GADS records. The main product header (MPH) has a fixed format, as described in [R2], and includes information about product identification and sizes of the data. Other fields in the general MPH (such as data acquisition, processing time and position of the measurement data, ENVISAT orbit and position, SBT to UTC conversion and product confidence data) have no real meaning for this product type and will be left blank. A specific product header (SPH) will include the identification of the version of this specific element of the Climatological and Spectroscopic Data Base and the data set description records (DSD) for the following GADS records. The GADS records of these Climatological and Spectroscopic Data Bases will always have one DSR per parameter type, as described below.

Format

The detailed format description is divided into several tables representing the hierarchy of product content. All DB files consists of the following components:

Id	Product Component	Comp. Type
1	Main Product Header of an auxiliary file	MPH
2	Specific Product Header of an auxiliary file	SPH
3	Data Set Description of an auxiliary file	DSD
4+	Data content (several records in each file)	GADS

The MPH, SPH and DSD formats are the same for all the data base files, and these are described first for all the data sets. Then follows a series of format specifications for the individual GADS.

Main Product Header (MPH)

No of Records: 1
Record Size: 1247
Component Size: 1247 Bytes

Id	Name	Comments	Unit	Type	#	Size	Offset
1	MPH	The main product header is described in the ENVISAT product specification (volume 5)	-	tx	1247	1247	0

Specific Product Header (SPH)

No of Records: 1
Record Size: 98
Component Size: 98 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	SPH_DESCRIPTOR=	keyword	tx	15	15	0
2	"CLIMA_xxxx_FILE~~~~~~~~~~~~~~~~"	variable	tx	30	30	15
3	Newline character	terminator	tx	1	1	45
4	Spare	-	tx	51	51	46
5	Newline character	terminator	tx	1	1	97

The "xxxx" in field 2 of this shall be replaced by the following acronyms for the various data base files:

Data base file	Acronym	Number of GADS
Atmospheric climatologies	DBPR	13
Cloud data bases	DBCL	2
Surface data bases	DBSF	7
Literature cross-sections	DBCS	13
Line-by-line absorption cross-sections	DBLB	5
Flight-model cross-sections	DBFM	12
Auxiliary cross sections	DBUX	25
Undersampling correction spectra	DBUS	4
ETA & ZETA key data	KEY_DATA	2
ESFT HITRAN spectral data	DBES	1
Cloud clearing minimum reflectance values	DBCC	1

Data Set Description (DSD)

No of Records: <# of GADS above>
Record Size: 280
Component Size: <according to No of Records above>

Id	Name	Comments	Unit	Type	#	Size	Offset
1	DSD	The data set descriptor record is described in the ENVISAT product specification (volume 5)	-	tx	280	280	0

The number of records of the data set descriptor for a specific data file corresponds to the number of GADS records given in the table above. The DS_NAME field of the DSDs will be determined according to the content of the corresponding GADS. The following keywords are envisaged:

- Atmospheric climatologies
  1. MPI_CLIMATOLOGY
  2. USA_CLIMATOLOGY
  3. TOMS_ CLIMATOLOGY
  4. KNMI_ CLIMATOLOGY
  5. HALOE_ CLIMATOLOGY
  6. BIRA_ CLIMATOLOGY
  7. IFE_BL_ CLIMATOLOGY
  8. IFE_VOLC_ CLIMATOLOGY
  9. CIRA_ CLIMATOLOGY
  10. GLATM_ CLIMATOLOGY
  11. GLATM_US_ CLIMATOLOGY
  12. BIAS_REF_CLIMATOLOGY (obsolete)
  13. WMO_AEROLSOLS
- Cloud data bases
  1. ISCCP_DATA_BASE
  2. CLOUD_REFL_CLIMATOLOGY
- Surface data bases
  1. GLOBAL_TOPOGRAPHY
  2. GLOBAL_ALBEDO_CLIMATOLOGY
  3. SPEC_REFLEC_DATA_BASE
  4. GLITTER_ALBEDO
  5. GLOBAL_REFL_DATA_BASE
  6. TOMS_ALBEDO_DATA_BASE
  7. REFINED_GLOBAL_TOPOGRAPHY
- Literature cross-sections
  1. LITERATURE_CS_O3
  2. LITERATURE_CS_NO2
  3. VANDAELE_CS_NO2
  4. LITERATURE_CS_H2O
  5. LITERATURE_CS_BRO
  6. WILMOUTH_CS_BRO
  7. LITERATURE_CS_SO2
  8. LITERATURE_CS_HCHO
  9. CANTRELL_CS_HCHO
  10. LITERATURE_CS_OCLO
  11. KROMMINGA_CS_OCLO
  12. LITERATURE_CS_O4
  13. THEORETICAL_RING
- Line-by-line absorption cross-sections
  1. LITERATURE_LBL_H2O
  2. LITERATURE_LBL_CO2
  3. LITERATURE_LBL_N2O
  4. LITERATURE_LBL_CO
  5. LITERATURE_LBL_CH4
- Flight-model cross-sections
  1. FM_GOME_CS_O3
  2. FM_GOME_CS_NO2

3. FM_GOME_RING
4. FM_SCIA_CS_O3
5. FM_SCIA_CS_NO2
6. FM_SCIA_CS_BRO
7. FM_SCIA_CS_SO2
8. FM_SCIA_CS_HCHO
9. FM_SCIA_CS_OCLO
10. FM_SCIA_CS_NO
11. M_SCIA_CS_O2
12. FM_SCIA_CS_O3D

- Auxiliary cross-sections
  1. Hitran_H2O_BIRA
  2. SCIA_FM_NO2_243K_BIRA
  3. GREENBLATT_SHIFT_O4
  4. SOL_KITT_PEAK_CONV_CH2
  5. SOL_KITT_PEAK_CONV_CH3
  6. SCIA_FM_O3D_BIRA_S0020
  7. SCIA_FM_O3_243K_BIRA_S0025
  8. SCIA_FM_O3_243K_BIRA_S0020
  9. SCIA_RING_KPNO_ch2_BIRA
  10. SCIA_RING_KPNO_ch3_BIRA
  11. LIT_NO2_BOGUMIL_243K
  12. RING1_BIRA_CH2
  13. RING2_BIRA_CH2
  14. RING_IFE_SO2
  15. LIT_BRO_FLEISCHMANN_223K
  16. LIT_SO2_BIRA_VAC
  17. USAMP_SO2_BREMEN
  18. O3_BOGUMIL_243K_SO2
  19. O3_DIFF_SO2
  20. ETA_NADIR_BREMEN_2
  21. HERMANS_O4_BREMEN
  22. KROMMINGA_OCLO_BREMEN
  23. MAGIC_CORRECTION
  24. RING_IFE_OCLO
  25. USAMP_OCLO_BREMEN
- Undersampling correction spectra
  1. US_CS_CH2
  2. US_CS_CH3
  3. US_CS_CH7
  4. US_CS_CH8
- ETA & ZETA key data
  1. ETA_NADIR_KEY
  2. ZETA_NADIR_KEY
- ESFT HITRAN spectral data
  1. ESFT_O2

- Cloud clearing minimum reflectance values
  1. CCA_PMD

Sizing

N/A

Volume

The climatological and spectroscopic data base will consist of 11 files with a total size of about 65 MB.

Throughput

There is just one set of climatological and spectroscopic data base files for the entire mission.

Remarks

N/A

3.8.2 Atmospheric Climatologies

An atmospheric climatology gives reference information about pressure, temperature and trace gas concentration profiles. There are various standard climatologies and one reference atmosphere in this data base.

- MPI model output climatology from the 2-D chemical-dynamical model developed by the Max-Planck Institute for Chemistry, Mainz, Germany [S4]. DOAS trace species only;
- AFGL US reference atmospheres, provided by Air Force Geophysical Laboratory (AFGL), Hanscom, Mass., U.S.A. [S5], DOAS application only;
- TOMS V8 temperature and O_3 conc. profile;
- KNMI O_3 conc. profile;
- HALOE NO_2 conc. profile;
- BIRA temperature, pressure and BrO conc. profile;
- Boundary layer and volcanic SO2 profiles from IFE Bremen;
- CIRA temperature profiles (for new IR retrieval algo.)
- GLATM temperature, pressure and conc. profiles for several molecules
- Single BIAS reference atmosphere (derived from the AFGL US Standard atmosphere) with trace species for BIAS applications (obsolete);
- WMO Aerosol coefficients.

The data base consists of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	MPI Climatology	GADS
5	USA Climatology	GADS

Id	Product Components	Component Type
6	TOMS Climatology	GADS
7	KNMI Climatology	GADS
8	HALOE Climatology	GADS
9	BIRA Climatology	GADS
10	IFE_BL Climatology	GADS
11	IFE_VOLC Climatology	GADS
12	CIRA Climatology	GADS
13	GLATM Climatology	GADS
14	GLATM_US Climatology	GADS
15	BIAS reference atmosphere	GADS
16	WMO aerosol data base	GADS

The GADS structure for atmospheric climatologies is unified now (some entries may be empty or doubled for special profiles):

Id	Name	Comments	Unit	Type	Size	#
1	nLayer	Number of atmospheric layers/levels	-	us	2	1
2	nLat	Number of reference latitudes	-	us	2	1
3	nSeasonsPT	Number of seasons/months for PT-profiles	-	us	2	1
4	nSeasonsConc	Number of seasons/months for concentration profiles	-	us	2	1
5	nMols	Number of molecules	-	us	2	1
6	nDaysPT	Cumulative days for PT- profiles	-	us	2	nSeasonsPT
7	nDaysConc	Cumulative days for concentration profiles	-	us	2	nSeasonsConc
8	molNames	Molecule names	-	tx	5	nMols
9	nProfilePT	Number of PT-profiles	-	us	2	1
10	nProfileConc	Number of concentration profiles per molecule	-	us	2	1
11	latitude	Reference latitudes	degree	do	8	nLat
12	layers	Atmospheric layers (altitude or pressure)	km or hPa	do	8	nLayer
13	pressure	Pressure profiles	hPa	do	8	nLayer * nProfilePT
14	temperature	Temperature profiles	K	do	8	nLayer * nProfilePT
15	concentration	Molecule conc. profiles	various	do	8	nMols * nLayer * nProfileConc
16	(reserved for special cases)	(see special profiles)	various	do	8	nMols * nLayer * nProfileConc

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

The following 6 components in this sub-section describe the GADS records for the file of atmospheric climatologies. For the header components of this product refer to section 3.8.1 above.

Component: MPI Climatology (GADS)

No of Records: 1
Record Size: 274678
Component Size: 274678 Bytes

Id	Comments	Unit	Type	# (Value)	Size	Offset
1	Number of atmospheric layers	-	us	1 (34)	2	0
2	Number of reference latitudes	-	us	1 (18)	2	2
3	Number of months for PT-profiles	-	us	1 (12)	2	4
4	Number of seasons for concentration profiles	-	us	1 (4)	2	6
5	Number of molecules	-	us	1 (8)	2	8
6	Cumulative days for PT- profiles	-	us	12	24	10
7	Cumulative days for concentration profiles	-	us	4	8	34
8	Molecule names	-	tx	40	40	42
9	Number of PT-profiles	-	us	1 (216)	2	82
10	Number of concentration profiles per molecule	-	us	1 (72)	2	84
11	Reference latitudes	degree	do	18	144	86
12	Atmospheric layer altitudes	km	do	34	272	230
13	Pressure profiles	hPa	do	7344	58752	502
14	Temperature profiles	K	do	7344	58752	59254
15	Molecule concentration profiles	ppV	do	19584	156672	118006
16	Unused	-	do	0	0	274678

All profiles are defined at a height grid 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, a total of 18 entries.

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:

$1 = O_3$, $2 = NO_2$, 3 = NO, 4 = ClO, 5 = HCHO, 6 = BrO, $7 = NO_3$, 8 = OClO

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 degree), 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 latitude zone and the by the month, making a total of 7344 profile entries (12*18*34 = 7344)[1].

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, autum:3, winter:4). The ordering of the concentration profiles is as follows. The first profile value is valid for the first molecule number (8 molecules are provided in this MPI climatology, see below), the first reference latitude (-85.0 degree), the first season of the year (spring) and the first height grid value (60.6 km). Profiles run first over height grid, then over latitude zone, then over the season and finally over the molecule number, making a total of 19584 profile entries (8*4*18*34 = 19584).

1. Wording "runs over x, then over y" means that the index of x runs fastest i.e. the loop over x has to be the innermost one.

Component: USA Climatology (US standard atmosphere) (GADS)

No of Records: 1
Record Size: 22558
Component Size: 22558 Bytes

Id	Comments	Unit	Type	# (Value)	Size	
1	Number of atmospheric layers	-	us	1 (46)	2	0
2	Number of reference latitudes	-	us	1 (6)	2	2
3	Number of seasons for PT-profiles	-	us	1 (2)	2	4
4	Number of seasons for conc.-profiles	-	us	1 (2)	2	6
5	Number of molecules	-	us	1 (8)	2	8
6	Cumulative days for PT-profiles	-	us	2	4	10
7	Cumulative days for conc.-profiles	-	us	2	4	14
8	Molecule names	-	tx	40	40	18
9	Number of profiles per category for PT	-	us	1 (6)	2	58
10	Number of profiles per category for conc.	-	us	1 (6)	2	60
11	Reference latitudes	degree	do	6	48	62
12	Atmospheric layer altitudes	km	do	46	368	110
13	Pressure profiles	hPa	do	276	2208	478
14	Temperature profiles	K	do	276	2208	2686
15	Molecule concentration profiles	ppV	do	2208	17664	4894
16	Unused	-	do	0	0	22558

All profiles are defined at a height grid given from 100 km down to 0 km, a total of 46 entries.

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

1 = H_2O, 2 = O_2, 3 = O_3, 4 = NO_2, 5 = NO, 6 = ClO, 7 = HCHO, 8 = SO_2

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

Nevertheless, the number of reference latitudes (=6, field 2) and the number of seasons (=2, field 3 and 4) is given in the table above. Temperature and pressure profiles are stored as function of height (w.r.t. the 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 height grid and then over profile category, making a total of 276 profile entries (6*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 (8 molecules are provided in the USA climatology), the first profile category (’tropic for all seasons’) and the first height grid value (100 km). Profiles run over height grid, profile category and finally molecule number, making a total of 2208 profile entries (8*6*46 = 2208).

Component: TOMS Climatology (O_3) (GADS)

No of Records: 1
Record Size: 181055
Component Size: 181055 Bytes

Id	Comments	Unit	Type	# (Value)	Size	Offset
1	Number of atmospheric levels	-	us	1 (14)	2	0
2	Number of reference latitudes	-	us	1 (18)	2	2
3	Number of months	-	us	1 (12)	2	4
4	Number of elements in field 7 (numTc)	-	us	1 (18)	2	6
5	Number of molecules	-	us	1 (1)	2	8
6	Cumulative days (used for day->month conversion)	-	us	12	24	10
7	Number of total columns per latitude (numTc)	-	us	18	36	34
8	Molecule names	-	tx	5 ("O3")	5	70
9	Number of profiles for PT (only for T)	-	us	1 (216)	2	75
10	Number of profiles for conc.	-	us	1 (1512)	2	77
11	Reference latitudes	degree	do	18	144	79
12	Pressure grid (per level)	hPa	do	14	112	223
13	Total Column	DU	do	126	1008	335
14	Temperature profiles (per layer)	K	do	2808	22464	1343
15	Molecule profiles (per layer)	mol./cm^2	do	19656	157248	23807
16	Unused	-	do	0	0	181055

The profiles are defined at a pressure grid given from 0.03 hPa (top) to 1013 hPa (bottom), a total of 13 layers given by 14 grid points (pressure at upper and lower bound of each layer). Reference latitudes are given from -85.0 degrees in steps of 10.0 degrees up to +85.0, a total of 18 entries.

Temperature profiles are stored as function of the pressure layers, latitude zone and month of the year. The ordering of the temperature profiles is as follows: The first profile value is valid for the first month of the year (January), the first reference latitude (-85.0 degree) and the first pressure layer (0.03 .. 0.247 hPa). Profiles then run over the pressure layers, followed by the latitude zone and then by month, making a total of 2808 profile entries (12*18*13 = 2808).

Trace gas concentrations (for O_3 only) depend additionally on a different number (per latitude zone) of total column entries.

Concentration profiles are stored as function of month, latitude, total column and pressure, where dependency from latitude is by means of total column(latitude). The ordering of the concentration profiles is as follows: The first profile value is valid for the first month (January), the first total column value of the first latitude zone (tc=125 at -85.0 degree) and the first pressure layer (1013 .. 506.5 hPa). Profiles run first over pressure layers, then over latitude and total col-umn, and finally over the month, making a total of 19656 profile entries (ΣnTc(lat) = 126, 12*126*13 = 19656).

Some additional conversion steps are included in the data already:

-The original 11 base layers of the TOMS V8 profile DB are expanded to 13 layers.
-Concentrations are converted from original Dobson units (DU) and stored as mol/cm^2 units.
-Optional "doubling" of the base layers have to do after data reading on request.

Component: KNMI Climatology (O_3) (GADS)

No of Records: 1
Record Size: 62347
Component Size: 62347 Bytes

Id	Comments	Unit	Type	# (Value)	Size	Offset
1	Number of atmospheric layers	-	us	1 (19)	2	0
2	Number of reference latitudes	-	us	1 (17)	2	2
3	Number of months for PT-profiles	-	us	1 (0)	2	4
4	Number of months for concentration profiles	-	us	1 (12)	2	6
5	Number of molecules	-	us	1 (1)	2	8
6	Cumulative days for PT- profiles (empty)	-	us	0	0	10
7	Cumulative days for concentration profiles	-	us	12	24	10
8	Molecule names	-	tx	5 ("O3")	5	34
9	Number of PT-profiles	-	us	1 (0)	2	39
10	Number of concentration profiles per molecule	-	us	1 (204)	2	41
11	Reference latitudes	degree	do	17	136	43
12	Atmospheric layer pressure grid	hPa	do	19	152	179
13	Pressure profiles (empty)	hPa	do	0	0	331
14	Temperature profiles (empty)	K	do	0	0	331
15	Molecule concentration profiles	ppV	do	3876	31008	331
16	Standard deviation for conc. profiles	ppV	do	3876	31008	31339

The profiles are defined at a pressure grid given from 0.3 hPa (top layer) to 1000 hPa (bottom layer), a total of 19 entries. Reference latitudes are given from -80.0 degrees in steps of 10.0 degrees up to +80.0, a total of 17 entries.

Molecule concentrations for O_3 only, no PT-profiles.

Trace gas concentration profiles are stored as function of pressure, latitude zone and month of the year. The ordering of the concentration profiles is as follows. The first profile value is valid for the first month of the year, the first reference latitude (-80.0 degree) and the first pressure grid value (0.03 hPa). Profiles run first over pressure grid, then over latitude zone and finally over the month, making a total of 3876 profile entries (12*17*19 = 3876).

The storage order for standard deviation is the same as for concentration profiles.

Component: HALOE Climatology (NO_2) (GADS)

No of Records: 1
Record Size: 90621
Component Size: 90621 Bytes

Id	Comments	Unit	Type	# (Value)	Size	Offset
1	Number of atmospheric layers	-	us	1 (44)	2	0
2	Number of reference latitudes	-	us	1 (17)	2	2
3	Number of months for PT-profiles	-	us	1 (0)	2	4
4	Number of seasons for conc. profiles (unused)	-	us	1 (1)	2	6
5	Number of molecules	-	us	1 (1)	2	8
6	Cumulative days for PT- profiles (empty)	-	us	0	0	10
7	Cumulative days for conc. profiles (unused)	-	us	1 (0)	2	10
8	Molecule names	-	tx	5("NO2")	5	12
9	Number of PT-profiles	-	us	1 (0)	2	17
10	Number of concentration profiles per molecule	-	us	1 (16)	2	19
11	Reference latitudes	degree	do	17	136	21
12	Atmospheric layer altitudes	km	do	44	352	157
13	Pressure profiles (empty)	hPa	do	0	0	509
14	Temperature profiles (empty)	K	do	0	0	509
15	Molecule concentration coefficients "sunrise"	-	do	5632	45056	509
16	Molecule concentration coefficients "sunset"	-	do	5632	45056	45565

The profiles are defined at a height grid given from 60 km down to 17 km, a total of 44 entries. Reference latitudes are given from -85.0 degrees up to +85.0, in steps of 20, 5, 10, ..., 10, 5, 20 degrees a total of 17 entries, but profiles are defined for the range covered by each two neighbour latitudes, so there are 16 entries only. For latitude interpolation the centre of each zone is to use.

Molecule concentrations for NO_2 only, one for "sunrise" and one for "sunset", no PT-profiles. Concentrations derived from the coefficients will be in units mol./cm^2.

Trace gas concentration profiles are stored as 7 coefficients plus 1 RMS value for each height and latitude zone. Concentrations will be calculated by a time depending function (day of year) using the coefficients. For height layers 16 km down to 0 km zero concentrations have to use.

The ordering of the concentration coefficients is as follows: The first profile value is valid for the first reference latitude zone (-85.0 .. -65.0 degree) and the first height grid value (60 km). Profiles run first over coefficients, then over height grid and finally over latitude zone, making a total of 5632 coefficients (16*44*(7+1)).

Component: BIRA Climatology (GADS)

No of Records: 1
Record Size: 78299
Component Size: 78299 Bytes

Id	Comments	Unit	Type	# (Value)	Size	Offset
1	Number of atmospheric layers	-	us	1 (45)	2	0
2	Number of reference latitudes	-	us	1 (18)	2	2
3	Number of months for PT-profiles	-	us	1 (4)	2	4
4	Number of seasons for concentration profiles	-	us	1 (4)	2	6
5	Number of molecules	-	us	1 (1)	2	8
6	Cumulative days for PT- profiles	-	us	4	8	10
7	Cumulative days for concentration profiles	-	us	4	8	18
8	Molecule names	-	tx	5 (“BRO“)	5	26
9	Number of PT-profiles	-	us	1 (72)	2	31
10	Number of concentration profiles per molecule	-	us	1 (72)	2	33
11	Reference latitudes	degree	do	18	144	35
12	Atmospheric layer altitudes	km	do	45	360	179
13	Pressure profiles	hPa	do	3240	25920	539
14	Temperature profiles	K	do	3240	25920	26459
15	Molecule concentration profiles	ppV	do	3240	25920	52379
16	Unused	-	do	0	0	78299

All profiles are defined at a height grid given from 50 km down to 6 km, a total of 45 entries. Reference latitudes are given from -85.0 degrees in steps of 10.0 degrees up to +85.0, a total of 18 entries.

There are molecule concentrations for BrO only.

Temperature, pressure and trace gas concentration profiles are stored as function of height (the height grid), latitude zone and season of the year. Four seasons are considered (spring:1, summer:2, autum:3, winter:4). The ordering of the profiles is as follows: The first profile value is valid for the first reference latitude (-85.0 degree), the first season of the year (January) and the first height grid value (50 km). Profiles then run over the height grid, followed by the latitude zone and the by the season, making a total of 3240 profile entries (4*18*45).

Components: IFE_BL & IFE_VOLC Climatology (2 GADS)

No of Records: 1
Record Size: 767
Component Size: 767 Bytes

Id	Comments	Unit	Type	# (Value)	Size	Offset
1	Number of atmospheric layers	-	us	1 (23)	2	0
2	Number of reference latitudes	-	us	1 (1)	2	2
3	Number of months for PT-profiles	-	us	1 (1)	2	4
4	Number of seasons for concentration profiles	-	us	1 (1)	2	6
5	Number of molecules	-	us	1 (1)	2	8
6	Cumulative days for PT- profiles	-	us	1(0)	2	10
7	Cumulative days for concentration profiles	-	us	1(0)	2	12
8	Molecule names	-	tx	5 (“SO2“)	5	14
9	Number of PT-profiles	-	us	1 (1)	2	19
10	Number of concentration profiles per molecule	-	us	1 (1)	2	21
11	Reference latitudes	degree	do	1(0.)	8	23
12	Atmospheric layer altitudes	km	do	23	184	31
13	Pressure profiles	hPa	do	23	184	215
14	Temperature profiles	K	do	23	184	399
15	Molecule concentration profiles	ppV	do	23	184	583
16	Unused	-	do	0	0	767

All profiles are defined at a height grid given from 100 km down to 0 km, a total of 23 entries. They have no latitude and seasonal dependencies.

There are molecule concentrations for SO_2 only. The IFE_BL GADS contains the boundary layer profile, while the IFE_VOLC the volcanic profile. Temperature and pressure profiles are identical in the both GADS.

Components: CIRA Climatology (GADS)

No of Records: 1
Record Size: 226366
Component Size: 226366 Bytes

Id	Comments	Unit	Type	# (Value)	Size	Offset
1	Number of atmospheric layers	-	us	1 (71)	2	0
2	Number of reference latitudes	-	us	1 (33)	2	2
3	Number of months for PT-profiles	-	us	1 (12)	2	4
4	Number of seasons for concentration profiles	-	us	1 (0)	2	6
5	Number of molecules	-	us	1 (0)	2	8
6	Cumulative days for PT- profiles	-	us	12	24	10
7	Cumulative days for concentration profiles	-	us	0	0	34
8	Molecule names	-	tx	0	0	34
9	Number of PT-profiles	-	us	1 (396)	2	34
10	Number of concentration profiles per molecule	-	us	1 (0)	2	36
11	Reference latitudes	degree	do	33	264	38
12	Atmospheric layer altitudes	km	do	71	568	302
13	Pressure grid	hPa	do	71	568	870
14	Temperature profiles	K	do	28116	224928	1438
15	Molecule concentration profiles	ppV	do	0	0	226366
16	Unused	-	do	0	0	226366

All profiles are defined at a height grid given from 119.7 km down to 0.1 km, a total of 71 entries. Reference latitudes are given from -80.0 degrees in steps of 5.0 degrees up to +80.0, a total of 33 entries.

Currently there are no molecule concentrations.

Instead of pressure profiles there is one global pressure grid.

Temperature 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 (-80.0 degree), the first month of the year (January) and the first height grid value (119.7 km). Profiles then run over the height grid, followed by the latitude zone and the by the month, making a total of 28116 profile entries (12*33*71).

Component: GLATM Climatology (GADS)

No of Records: 1
Record Size: 18505
Component Size: 18505 Bytes

Id	Comments	Unit	Type	# (Value)	Size	
1	Number of atmospheric layers	-	us	1 (50)	2	0
2	Number of reference latitudes	-	us	1 (6)	2	2
3	Number of seasons for PT-profiles	-	us	1 (2)	2	4
4	Number of seasons for conc.-profiles	-	us	1 (2)	2	6
5	Number of molecules	-	us	1 (7)	2	8
6	Cumulative days for PT-profiles	-	us	2	4	10
7	Cumulative days for conc.-profiles	-	us	2	4	14
8	Molecule names	-	tx	35	35	18
9	Number of profiles per category for PT	-	us	1 (5)	2	53
10	Number of profiles per category for conc.	-	us	1 (5)	2	55
11	Reference latitudes	degree	do	6	48	57
12	Atmospheric layer altitudes	km	do	50	400	105
13	Pressure profiles	hPa	do	250	2000	505
14	Temperature profiles	K	do	250	2000	2505
15	Molecule concentration profiles	ppV	do	1750	14000	4505
16	Unused	-	do	0	0	18505

All profiles are defined at a height grid given from 120 km down to 0 km, a total of 50 entries.

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

1 = H2O, 2 = CO_2, 3 = O3, 4 = N_2O, 5 = CO, 6 = CH_4, 7 = O_2

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 (like USA climatology, but category 6 is contained in the separate GLATM_US climatology):

1 = tropical 2 = mid-latitude summer 3 = mid-latitude winter
4 = sub-arctic summer 5 = sub-arctic winter

Nevertheless, the number of reference latitudes (=6, field 2) and the number of seasons (=2, field 3 and 4) is given in the table above. Temperature and pressure profiles are stored as function of height (w.r.t. the 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 (’tropical’), and the first height grid value (120 km). Profiles run over height grid and then over profile category, making a total of 250 profile entries (5*50).

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 (7 molecules are provided in the GLATM climatology), the first profile category (’tropical’) and the first height grid value (120 km). Profiles run over height grid, profile category and finally molecule number, making a total of 1750 profile entries (7*5*50).

Component: GLATM_US Climatology (GADS)

No of Records: 1
Record Size: 12566
Component Size: 12566 Bytes

Id	Comments	Unit	Type	# (Value)	Size	
1	Number of atmospheric layers	-	us	1 (50)	2	0
2	Number of reference latitudes	-	us	1 (1)	2	2
3	Number of seasons for PT-profiles	-	us	1 (1)	2	4
4	Number of seasons for conc.-profiles	-	us	1 (1)	2	6
5	Number of molecules	-	us	1 (28)	2	8
6	Cumulative days for PT-profiles	-	us	1	2	10
7	Cumulative days for conc.-profiles	-	us	1	2	12
8	Molecule names	-	tx	140	140	14
9	Number of profiles per category for PT	-	us	1 (5)	2	154
10	Number of profiles per category for conc.	-	us	1 (5)	2	156
11	Reference latitudes	degree	do	1 (0.)	8	158
12	Atmospheric layer altitudes	km	do	50	400	166
13	Pressure profile	hPa	do	50	400	566
14	Temperature profile	K	do	50	400	966
15	Molecule concentration profiles	ppV	do	1400	11200	1366
16	Unused	-	do	0	0	12566

All profiles are defined at a height grid given from 120 km down to 0 km, a total of 50 entries. They have no latitude and seasonal dependencies.

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

1 = H2O, 2 = CO_2, 3 = O3, 4 = N_2O, 5 = CO, 6 = CH_4, 7 = O_2,
8 = NO, 9 = SO_2, 10 = NO_2, 11 = NH_3, 12 = HNO_3, 13 = OH, 14 = HF,
15 = HCl, 16 = HBr, 17 = HI, 18 = ClO, 19 = OCS, 20 = H_2CO, 21 = HOCl,
22 = N_2, 23 = HCN, 24 = CH_3Cl, 25 = H_2O_2, 26 = C_2H_2, 27 = C_2H_6, 28 = PH_3

The first 7 molecules are the same as in the GLATM climatology. Their concentration profiles as well as the pressure and temperature profile comes from the GLATM category 6 (US standard atmosphere). Additional global concentration profiles are contained for the remaining molecules.

Temperature and pressure profiles are stored as function of the height grid, 50 entries each. Trace gas concentration profiles are stored as function of height and molecule number. The ordering of the concentration profiles follows the molecule indexing; total entries 28*50 = 1400.

Component: WMO Aerosol Data Base (GADS)

No of Records: 1
Record Size: 249830
Component Size: 249830 Bytes

Id	Comments	Unit	Type	# (Value)	Size	Offset
1	Number of aerosols	-	us	1 (12)	2	0
2	Number of wavelengths	-	us	1 (15)	2	2
3	Number of phase moments	-	us	1 (50)	2	4
4	Number of humidities per aerosol	-	us	12 (8 / 1)	24	6
5	Humidities per aerosol	%	ss	40	80	30
6	Wavelength	nm	do	15	120	110
7	Scattering coefficients	-	do	600	4800	230
8	Extinction coefficients	-	do	600	4800	5030
9	Phase moments	-	do	30000	240000	9830

Humidity is given from 0 to 99 percent in different steps, a total of 8 entries (for aerosol 0..3) or only one entry "-1" which indicate humidity is not defined (for aerosol 5..11). Wavelengths are given from 225 nm in steps of 25 up to 350 nm and further in steps of 50 up to 800 nm, a total of 15 entries.

Coefficients are given for each aerosol, humidity and wavelength.

Phase moments are vectors with 50 entries for each aerosol, humidity and wavelength.

All arrays start with first aerosol (0), the first humidity (0) and the first wavelength (225.0), running over aerosol, then over humidity and finally wavelength, a total of (4*8+8*1)*15=600 values. Phase moments additional run over phase index, a total of 600*50=30000 values.

3.8.3 Cloud data bases

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

- ISCCP Data Base
- Cloud Albedo Climatology

The product consists of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	ISCCP Data Base	GADS
5	Cloud Reflectance Data Base	GADS

The following 2 components in this sub-section describe the GADS records for the file of cloud parameter climatologies. For the header components of this product refer to section 3.5 above.

Component: ISCCP Data Base (GADS)

No of Records: 1
Record Size: 498534
Component Size: 498534 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of reference latitudes	-	us	1	2	0
2	Number of reference longitudes	-	us	1	2	2
3	Number of months entries in the data base	-	us	1	2	4
4	Reference latitudes	degree	fl	72	288	6
5	Reference longitudes	degree	fl	144	576	294
6	Cloud-top pressures	hPa	fl	124416	497664	870

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 s up to 358.75 degrees, a total of 144 entries.

Cloud-top pressure data starts with the first month (January), the first latitude zone (88.75 degrees) and the first longitude zone (1.25 degrees), running over month then latitude and finally longitude, making a total of 12*72*144 = 124416 values.

Component: Cloud Reflectance Data Base (GADS)

No of Records: 1
Record Size: 40976
Component Size: 40976 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of asymmetry parameters	-	us	1	2	0
2	Number of reference zenith angles	-	us	1	2	2
3	Number of reference azimuths	-	us	1	2	4
4	Number of reference wavelengths for escape function correction	-	us	1	2	6
5	Number of reference zenith angles for escape function correction	-	us	1	2	8
6	Number of different cloud types	-	us	1	2	10
7	Reference wavelengths	nm	fl	25	100	12
8	Reference asymmetry parameters for different cloud types	-	fl	8	32	112
9	Spectral dependent asymmetry parameters for different cloud types	-	fl	200	800	144
10	Reference azimuths	-	fl	12	48	944
11	Cosines of reference zenith angles	-	fl	9	36	992
12	Cosines of reference escape function zenith angles	-	fl	11	44	1028
13	raw data cloud-top reflectance	sr^{-1}	fl	7776	31104	1072
14	raw data escape function	sr^{-1}	fl	2200	8800	32176

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 DB the required cloud-top albedo (independent from viewing geometry) 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 (i.e. the albedo). 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 (originating from photons reflected from the underlying surface). The wavelength dependency of calculated cloud-top albedos comes from the escape function. Thus, the computed escape function depends on the cloud optical depth, the ground albedo and the wavelength.

The spectral dependent asymmetry parameters are ordered first by cloud type and then by wavelength.

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 cloud type, then over azimuth, then over zenith angle of incident radiation and lastly over zenith angle of reflection, giving a total of 7776 entries (8*12*9*9=7776).

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 cloud type, then zenith angle and finally wavelength, giving a total of 2200 entries (8*11*25=2200).

3.8.4 Surface data bases

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

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

The product consists of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	Global Topography	GADS
5	Global Albedo Climatology	GADS
6	Spectral Reflectance Climatology	GADS
7	Glitter Albedo Climatology	GADS
8	Global Reflectance Climatology (GLER)	GADS
9	TOMS Albedo Climatology	GADS
10	Refined Global Topography	GADS

The following 7 components in this sub-section describe the GADS records for the file of surface data sets. For the header components of this product refer to section 3.5 above.

Component: Global topography (GADS)

No of Records: 1
Record Size: 129604
Component Size: 129604 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of reference latitudes	-	us	1	2	0
2	Number of reference longitudes	-	us	1	2	2
3	Height	m	us	64800	129600	4

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

Component: Global albedo climatology (GADS)

No of Records: 1
Record Size: 1166406
Component Size: 1166406 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of reference latitudes	-	us	1	2	0
2	Number of reference longitudes	-	us	1	2	2
3	Number of seasons	-	us	1	2	4
4	Albedo	-	fl	259200	1036800	6
5	Vegetation index	-	us	64800	129600	1036806

The global albedo data base contains the albedo as function of latitude and longitude, with a spatial resolution of 1°x1° degree, 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 latitude -89° and longitude 0°, running first over latitude then longitude and finally over season. The first season given in the data base represents 'winter'.

The vegetation index is a function of latitude and longitude with a spatial resolution of 1°x1°, a total of 64800 (360*180 = 64800) entries. The first entry is valid for a latitude of -89° and a longitude of 0°, running first over latitude then longitude.

Component: Spectral reflectance climatology (GADS)

No of Records: 1
Record Size: 3227
Component Size: 3227 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of surface types	-	us	1	2	0
2	Surface types	-	tx	5	55	2
3	Number of wavelengths	-	us	1	2	57
4	Wavelengths	nm	fl	132	528	59
5	Spectral reflectance	-	fl	660	2640	587

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 blank.

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.

Component: Glitter albedo (GADS)

No of Records: 1
Record Size: 5544
Component Size: 5544 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of glitter albedo sun zenith angles	-	us	1	2	0
2	Number of glitter albedo wavelengths	-	us	1	2	2
3	Glitter albedo reference sun zenith angles	-	fl	32	128	4
4	Glitter albedo reference wavelengths	nm	fl	41	164	132
5	Glitter albedo	-	fl	1312	5248	296

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*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 runs first over wavelength then over sun zenith angle.

Component: Global reflection climatology (GLER) (GADS)

No of Records: 1
Record Size: 17109436
Component Size: 17109436 Bytes

Id	Comments	Unit	Type	# (Value)	Size	Offset
1	Number of reference latitudes	-	us	1 (180)	2	0
2	Number of reference longitudes	-	us	1 (360)	2	2
3	Number of months	-	us	1 (12)	2	4
4	Number of wavelengths	-	us	1 (11)	2	6
5	Cumulated days per months	-	us	12	24	8
6	Reference latitudes	degree	fl	180	720	32
7	Reference longitudes	degree	fl	360	1440	752
8	Reference wavelengths	nm	fl	11	44	2192
9	Albedo	-	ss	8553600	17107200	2236

The wavelength albedo data base contains the albedo as function of latitude and longitude, with a spatial resolution of 1° x 1°, for each month of year and a set of 11 reference wavelengths; a total of 8553600 (180*360*12*11 = 8553600) entries. The first entry is valid for month January, latitude -89.5 and longitude 0.5, and first wavelength, running first over month, then over latitude and longitude and finally over wavelength.

Albedo values are stored as integers using scale factor 1000 (i.e. value 900 means albedo=0.9).

Component: TOMS albedo climatology (GADS)

No of Records: 1
Record Size: 2490222
Component Size: 2490222 Bytes

Id	Comments	Unit	Type	# (Value)	Size	Offset
1	Number of reference latitudes	-	us	1 (180)	2	0
2	Number of reference longitudes	-	us	1 (288)	2	2
3	Number of months	-	us	1 (12)	2	4
4	Cumulated days per months	-	us	12	24	6
5	Reference latitudes	degree	fl	180	720	30
6	Reference longitudes	degree	fl	288	1152	750
7	Albedo	-	fl	622080	2488320	1902

The TOMS albedo data base contains the albedo as function of latitude and longitude, with a spatial resolution of 1° x 1.25°, for each month of year; a total of 622080 (180*288*12 = 622080) entries. The first entry is valid for month January, latitude -89.5 and longitude 0.625, running first over month, then over latitude and finally over longitude.

Component: Refined global topography (GADS)

No of Records: 1
Record Size: 29176206
Component Size: 29176206 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of reference latitudes	-	us	1	2	0
2	Number of reference longitudes	-	us	1	2	2
3	Height	m	us	14588101	29176202	4

The refined global topography data base contains the ground height as function of latitude and longitude, with a spatial resolution of 4' x 4' (ETOPO-4). The first entry is valid for a longitude of -180° and a latitude of 90°, with subsequent entries running first over longitude then latitude. Longitudes range from -180° to 180°, latitudes from -90 to 90°, resulting in a total of 5401*2701 = 14588101 entries.

3.8.5 Literature Reference Cross-Sections

The auxiliary file consists of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	O_3 Reference Spectra (direct from literature)	GADS
5	NO_2 Reference Spectra (direct from literature)	GADS
6	Vandaele NO_2 Reference Spectra	GADS
7	H_2O Reference Spectra (direct from literature)	GADS
8	BrO Reference Spectra (direct from literature)	GADS
9	Wilmouth BrO Reference Spectra	GADS
10	SO_2 Reference Spectra (direct from literature)	GADS
11	HCHO Reference Spectra (direct from literature)	GADS
12	Cantrell HCHO Reference Spectra	GADS
13	OClO Reference Spectra (direct from literature)	GADS
14	Kromminga OClO Reference Spectra	GADS
15	O_4 Reference Spectra (direct from literature)	GADS
16	Theoretical Ring spectrum	GADS

For ease of reading and writing the data bases, all spectral GADS (i.e. those of the next three sections too) have a common structure which looks like this:

Component: *mol* Reference spectra (*type*) (GADS)

No of Records: 1
Record Size: xxxx
Component Size: xxxx Bytes

Field	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
[6]	Number of temperatures per segment	-	us	*n*	2 * *n*	13
[7]	Number of coefficients per segment	-	us	*n*	2 * *n*	
8	Number of spectral entries per segment	-	us	*n*	2 * *n*	
[9]	Type of formula for coefficients	-	uc	1	1	
10	Type of wavelength information	-	uc	1	1	

Field	Comments	Unit	Type	#	Size	Offset
[11]	Atmospheric levels altitudes	km	fl	h	4 * h	
[12]	Temperature grid per spectral segment	K	fl	$t = \Sigma t_n$	4 * t	
13	Wavelength information per spectral segment per temperature	-	wl_inf	$w = \Sigma t_n * w_n$	w * wl_{len}	
[14]	Cross-sections per spectral segment, level, and temperature	cm^2/mol	fl	$w*h*t$	4 * $w*h*t$	
[15]	Cross-section coefficients per spectral segment	-	fl	$c = \Sigma c_n * w_n$	4 * c	

Explanation:

- Fields in brackets are optional; if empty, they are omitted.
- Field 2: The UV and visible spectra have no height dependency; field 11 is empty in that case (h = 0).
- Field 3: Many spectra are available in several wavelength intervals called segments. Temperature dependency and spectral resolution may be different in each segment.
- Field 4: Maximum value of entries in field 6. If this value is 0, field 6 and 12 are empty.
- Field 5: Usually 0. However, in two important cases the temperature dependency is given in an approximation formula. The equation to be used is indicated in field 9, detailed information is given in the appropriate section.
  If 0, fields 7, 9, and 15 are empty.
- Field 6/7/8: The number of temperatures, spectral entries, and coefficients can be different for each segment. Especially, coefficients will be available only in one segment; in the other segments the entry in field 7 will be 0 which means that field 14 has to be taken in this case, while otherwise the appropriate formula has to be applied to the values of field 15 and, eventually, of field 14.
  Entries in field 6 can also be 0: 0 means there is no temperature dependency available (either negligible or unknown) and the corresponding value in field 12 is empty, while 1 means the data is given for exactly the one temperature given in the corresponding entry of field 12.
  Actually there is also a temperature dependency in field 8, but as there are small deviations in number only in some rare cases, the maximum value has been taken and the last entries at those temperatures with fewer values have been set to zero.
- Field 9: Will be explained where it applies, is empty otherwise.
- Field 10: Specifies how field 13 has to be interpreted.
- Field 13: Wavelength information can be available in three forms; in fact, this is a generic field that may cover 1 or 2 fields of elementary data type. Type of wavelength info is invariable for one spectra, however, different wavelength grids may exist for different temperatures in the same segment.

  Type no. 1: Grid

Field	Comments	Unit	Type	#	Size
1	Wavelength	nm	fl	w_n	4 * w_n

Size of Component: $wl_{len} = 4 * w_n$

Type no. 2: Start wavelength and step

Field	Comments	Unit	Type	#	Size
1	Start wavelength (λ_0)	nm	fl	1	4
2	Wavelength step (λ_s)	nm	fl	1	4

Size of Component: $wl_{len} = 8$
In this case the wavelength for cross-section n is calculated by $\lambda = \lambda_0 + (n - 1) * \lambda_s$.

Type no. 3: Start wave number and step

Field	Comments	Unit	Type	#	Size
1	Start wave number (k_0)	cm^{-1}	do	1	8
2	Wave number step (k_s)	cm^{-1}	do	1	8

Size of Component: $wl_{len} = 16$
In this case the wave number for cross-section n is calculated by $k = k_0 + (n - 1) * k_s$.

- Field 14: The cross-section data is organised per segment, then per level (if appropriate), then per temperature (if appropriate), and finally per wavelength (i.e. segments are the outermost loop, wavelengths the innermost). In case that all the data is in the coefficients, the cross section data for that segment is empty.
- Field 15: The cross-section coefficients are organised per segment (not applicable currently, see above), then per coefficient, then per wavelength. No different levels or temperatures are available for parameterised data.

The following 13 components in this sub-section describe the GADS records for the file of literature reference spectral data sets. For the header components of this product refer to section 3.5 above.

The first 12 components contain absorption cross-sections as a function of molecule species, wavelength and, in case of O_3 and NO_2, temperature. For O_3 in the Hartley-Huggins bands, there are additional cross-section coefficients for the temperature dependence parameterisation. Data bases are available from different measurement campaigns, documented in the literature. Seven different species are stored in the data base representing the absorption properties of O_3, NO_2, H_2O, HCHO, SO_2, OClO, BrO and O_4. Most of these sets contain a single segment; the exceptions are O_3 and NO_2, O_4.

The remaining data base entry contains a normalised reference Ring (rotational Raman) which has been calculated using a high resolution solar reference spectrum from literature, and updated O_2 and N_2 Raman spectroscopic parameters.

The molecule names in the GADS records below are given in ASCII. Unused characters are left blank.

Component: O_3 Reference spectra (literature) (GADS)

No of Records: 1
Record Size: 114525
Component Size: 114525 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (O3, BP-spectra and Hartley-Huggins bands)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures per segment	-	us	3	6	13
7	Number of coefficients per segment	-	us	3	6	19
8	Number of spectral entries per segment (O3, BP-spectra, Hartley-Huggins bands)	-	us	3	6	25
9	Type of formula for coefficients	-	uc	1	1	31
10	Type of wavelength information	-	uc	1	1	32
12	Temperature ‘grid’ for first segment	K	fl	1	4	33
13	Wavelength grids for spectral segments (O3, BP-spectra, Hartley-Huggins bands)	nm	fl	11903	47612	37
14	Cross-sections for spectral segments (O3, BP-spectra)	cm^2/mol	fl	11903	47612	47649
15	Cross-section coefficients for spectral segment (O3, BP-spectra) within the Hartley-Huggins bands	-	fl	4816	19264	95261

The first spectral segment of the O_3 Bass-Paur spectra covers the spectral range from 184.9277 nm up to 253.7749 nm, a total of 5122 entries. The data from this spectral segment corresponds to a temperature of 195 K. The second segment is called the Hartley-Huggins bands and covers the wavelength range between 253.7749 nm and 365.3635 nm, a total of 2408 entries. This single segment contains cross-sections and linear (σ_{lin}) and quadratic cross-section coefficients (σ_{quad}) for the spectral range mentioned above. The third segment covers the spectral range from 407.8 nm up to 845.0 nm, a total of 4373 entries (no temperature dependency). Thus the entries in field 6 are 1, 0, 0, the entry in field 12 is 195.0.

Inside the second segment cross-sections (σ_Y) for temperature (T_{BP}) are calculated as follows:

$$\sigma(\lambda) = \sigma_0(\lambda) + \sigma_{lin}(\lambda)(T_{BP} - T_0) + \sigma_{quad}(\lambda)(T_{BP} - T_0)^2 ,$$

where the zero order coefficient σ_0 is taken from the O_3 Bass-Paur spectrum (first segment) and T_{BP} is the Bass-Paur temperature (T_0=273.15K). A formula type of “1” is given in field 9 in this case, 2 coefficients are indicated in field 7 for the second segment, 0 for the other two.

Note: This formula is special in that the 2 coefficients serve only as correction factors for the base cross-sections from field 14 which are valid for 195 K; both fields, 14 and 15, are needed.

Component: NO_2 Reference spectra (literature) (GADS)

No of Records: 1
Record Size: 97934
Component Size: 97934 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (NO2, Harwood-Jones spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures (NO2, Harwood-Jones spectra)	-	us	1	2	13
8	Number of spectral entries (NO2, Harwood-Jones spectra)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	7	28	18
13	Wavelength grid per temperature (NO2, Harwood-Jones spectra)	nm	fl	12236	48944	46
14	Cross-sections per temperature (NO2, Harwood-Jones spectra)	cm^2/mol	fl	12236	48944	48990

The spectral segment of the NO2 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 12236 entries (1748*7). Note that the wavelength grid is listed for each temperature though in this case it is independent of temperature.

Component: NO_2 Reference spectra (Vandaele) (GADS)

No of Records: 1
Record Size: 447914
Component Size: 447914 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (NO2, Vandaele spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures (NO2, Vandaele spectra)	-	us	1	2	13

Id	Comments	Unit	Type	#	Size	Offset
8	Number of spectral entries (NO2, Vandaele spectra)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	2	8	18
13	Wavelength grid per temperature (NO2, Vandaele spectra)	nm	fl	55986	223944	26
14	Cross-sections per temperature (NO2, Vandaele spectra)	cm^2/mol	fl	55986	223944	223970

The spectral segment of the NO2 Vandaele data covers a wavelength range from 238.08 nm up to 666.58 nm, a total of 27993 entries. The data is available for 2 different temperatures (220 K, 294 K). Each block contains a total of 27993 entries, the complete spectrum contains 55986 entries (27993*2). Note that the wavelength grid is listed for each temperature though in this case it is independent of temperature.

Component: H_2O Reference spectra (literature) (GADS)

No of Records: 1
Record Size: 312440
Component Size: 312440 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (H2O)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries (H2O)	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid (H2O)	nm	fl	39053	156212	16
14	Cross-sections (H2O)	cm^2/mol	fl	39053	156212	156228

The spectral segment of the H_2O 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_2O are available for each wavelength entry within the given spectral range, a total of 39053 entries.

Component: BrO Reference spectra (literature) (GADS)

No of Records: 1
Record Size: 15424
Component Size: 15424 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (BrO)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries (BrO)	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid for spectral segment (BrO)	nm	fl	1926	7704	16
14	Cross-sections for spectral segment (BrO)	cm^2/mol	fl	1926	7704	7720

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.

Component: BrO Reference spectra (Wilmouth) (GADS)

No of Records: 1
Record Size: 48768
Component Size: 48768 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (BrO Wilmouth)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries (BrO Wilmouth)	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid for spectral segment (BrO Wilmouth)	nm	fl	6094	24376	16
14	Cross-sections for spectral segment (BrO Wilmouth)	cm^2/mol	fl	6094	24376	24392

The spectral segment of the BrO spectrum covers the spectral range from 286.38 nm up to 383.05 nm, a total of 6094 entries. The cross sections of BrO are available for each wavelength entry within the given spectral range, a total of 6094 entries.

Component: SO_2 Reference spectra (literature) (GADS)

No of Records: 1
Record Size: 45016
Component Size: 45016 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (SO2)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries (SO2)	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid for spectral segment (SO_2)	nm	fl	5625	22500	16
14	Cross-sections for spectral segment (SO_2)	cm^2/mol	fl	5625	22500	22516

The spectral segment of the SO_2 spectrum covers the spectral range from 227.34 nm up to 339.82 nm, a total of 5625 entries. The cross sections of SO_2 are available for each wavelength entry within the given spectral range, a total of 5625 entries.

Component: HCHO Reference spectra (literature) (GADS)

No of Records: 1
Record Size: 40400
Component Size: 40400 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (HCHO)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries (HCHO)	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid for spectral segment (HCHO)	nm	fl	5048	20192	16
14	Cross-sections for spectral segment (HCHO)	cm^2/mol	fl	5048	20192	20208

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.

Component: HCHO Reference spectra (Cantrell) (GADS)

No of Records: 1
Record Size: 120160
Component Size: 120160 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (HCHO Cantrell)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries (HCHO Cantrell)	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid for spectral segment (HCHO Cantrell)	nm	fl	15018	60072	16
14	Cross-sections for spectral segment (HCHO Cantrell)	cm^2/mol	fl	15018	60072	60088

The spectral segment of the HCHO Cantrell spectrum covers the spectral range from 300.30 nm up to 385.79 nm, a total of 15018 entries. The cross sections of HCHO Cantrell are available for each wavelength entry within the given spectral range, a total of 15018 entries.

Component: OClO Reference spectra (literature) (GADS)

No of Records: 1
Record Size: 25696
Component Size: 25696 Bytes

Id	Comments	Unit	Type	#	Size	
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (OClO)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries (OClO)	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid for spectral segment (OClO)	nm	fl	3210	12840	16
14	Cross-sections for spectral segment (OClO)	cm^2/mol	fl	3210	12840	12856

The spectral segment of the OClO spectrum covers the spectral range from 242.59 nm up to 472.80 nm, a total of 3210entries. The cross sections of OClO are available for each wavelength entry within the given spectral range, a total of 3210 entries.

Component: OClO Reference spectra (Kromminga) (GADS)

No of Records: 1
Record Size: 1028878
Component Size: 1028878 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (OClO Kromminga)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures (OClO Kromminga)	-	us	1	2	13
8	Number of spectral entries (OClO Kromminga)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	5	20	18
13	Wavelength grid per temperature (OClO Kromminga)	nm	fl	128605	514420	38
14	Cross-sections per temperature (OClO Kromminga)	cm^2/mol	fl	128605	514420	514458

The spectral segment of the OClO Kromminga data covers a wavelength range from 312.5 nm up to 440.5 nm, a total of 25721 entries. The data is available for 5 different temperatures (213, 233, 253, 273, 293 K). Each block contains a total of 25721 entries, the complete spectrum contains 128605 entries (25721*5). Note that the wavelength grid is listed for each temperature though in this case it is independent of temperature.

Component: O_4 Reference spectra (literature) (GADS)

No of Records: 1
Record Size: 37394
Component Size: 37394 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (O_4)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries (O_4)	-	us	2	4	13
10	Type of wavelength information	-	uc	1	1	17
13	Wavelength grid per spectral segment (O_4)	nm	fl	4672	18688	17
14	Cross-sections for spectral segments (O_4)	cm^2/mol	fl	4672	18688	18706

The spectral segments of the O_4 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 entries. The cross sections of O_4 are available for each wavelength entry within the given spectral range, a total of 4672 entries.

Component: Ring Reference spectra (theoretically calculated) (GADS)

No of Records: 1
Record Size: 124842
Component Size: 124842 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Spectra type	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (channels)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries (per channel)	-	us	2	4	13
10	Type of wavelength information	-	uc	1	1	17
13	Wavelength information per channel	nm	fl	4	16	18
14	Ring spectrum values per channel	-	fl	31202	124808	34

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.

The type of wavelength information is 2 which means that field 13 contains λ_0 and λ_s of channel 2 and then λ_0 and λ_s of channel 3.

3.8.6 Flight-Model Reference Cross-Sections

After the pre-flight calibration and characterisation activity, a spectroscopic measurement phase was anticipated for the SCIAMACHY flight model. These measurements were conducted under the aegis of IFE Bremen, one of the SCIAMACHY instrument PIs.

The data base file consists of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	O_3 Reference Spectra (GOME-measured)	GADS
5	NO_2 Reference Spectra (GOME-measured)	GADS
6	Ring Reference Spectra (GOME-measured)	GADS
7	O_3 Reference Spectra (SCIA-measured)	GADS
8	NO_2 Reference Spectra (SCIA-measured)	GADS
9	BrO Reference Spectra (SCIA-measured)	GADS
10	SO_2 Reference Spectra (SCIA-measured)	GADS
11	HCHO Reference Spectra (SCIA-measured)	GADS
12	OClO Reference Spectra (SCIA-measured)	GADS
13	NO Reference Spectra (SCIA-measured)	GADS
14	O_2 Reference Spectra (SCIA-measured)	GADS
15	O_3D Reference Spectra (derived from GADS 7, temperatures 243K and 223K)	GADS

The following 16 components in this sub-section describe the GADS records for the file of FM measurement reference spectral data sets. For the header components of this product refer to section 3.5 above.

The first part of the data base contains GOME-measured absorption cross-sections of O_3 and NO_2, plus a Ring reference spectrum. The second part of the data base contains SCIAMACHY-measured absorption cross-sections of a number of molecules. The cross-sections are given as functions of wavelength and temperature. All spectra will be divided into a number of spectral segments.

The molecule names in the GADS records below are given in ASCII. Unused characters are left blank.

GOME FM data

Component: O_3 Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 155223
Component Size: 155223 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (O_3, GOME-FM-spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures per segment	-	us	2	4	13
7	Number of coefficients per segment	-	us	2	4	17
8	Number of spectral entries per segment (O_3, GOME-FM-spectra)	-	us	2	4	21
9	Type of formula for coefficients	-	uc	1	1	25
10	Type of wavelength information	-	uc	1	1	26
12	Temperature grid for first segment	K	fl	5	20	27
13	Wavelength grids for spectral segments (O_3, GOME-FM-spectra)	nm	fl	18046	72184	47
14	Cross-sections for first spectral segment per temperature (O_3, GOME-FM-spectra)	cm^2/mol	fl	16695	66780	72231
15	Cross-section coefficients for second spectral segment (O_3, GOME-FM-spectra, Hartley-Huggins bands)	-	fl	4053	16212	139011

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 generic refspec 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-section coefficients are stored in the data base. Three sets of coefficients (σ_0, σ_{lin}, σ_{quad}) 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 function of wavelength. The first entry corresponds to σ_0 and the first wavelength entry, running over coefficient and then over wavelength, a total of 4053 entries (1351*3).

The final ozone absorption cross-sections are calculated using :

$$\sigma(\lambda) = \sigma_0(\lambda) * (1 + \sigma_{lin}(\lambda)(T_{BP} - T_0) + \sigma_{quad}(\lambda)(T_{BP} - T_0)^2) * 10^{-20}$$

T_{BP} is the Bass-Paur temperature (T_0 = 273.15K). A formula type of “2” is given in field 9 in this case, 3 coefficients are indicated in field 7 for the second segment, 0 for the first one.

Component: NO_2 Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 109090
Component Size: 109090 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (NO_2, GOME-FM-spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries (NO_2, GOME-FM-spectra)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid (NO_2, GOME-FM-spectra)	K	fl	4	16	18
13	Wavelength grid per temperature (NO_2, GOME-FM-spectra)	nm	fl	13632	54528	34
14	Cross-sections per temperature (NO_2, GOME-FM- spectra)	cm^2/mol	fl	13632	54528	54562

The NO_2 spectra is specified in one segment and for 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.

Component: Ring Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 12834
Component Size: 12834 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Spectra type	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (channels)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries (per channel)	-	us	2	4	13
10	Type of wavelength information	-	uc	1	1	17
13	Wavelength grid per channel	nm	fl	1602	6408	18
14	Ring spectrum values per channel	-	fl	1602	6408	6426

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 seg-

ment 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.

SCIAMACHY FM data

Component: O_3 Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 169798
Component Size: 169798 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (O_3, SCIA-FM-spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries (O_3, SCIA-FM-spectra)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	5	20	18
13	Wavelength grid per temperature (O_3, SCIA-FM- spectra)	nm	fl	21220	84880	38
14	Cross-sections per temperature (O_3, SCIA-FM- spectra)	cm^2/mol	fl	21220	84880	84918

The O_3 spectrum is specified in one segment and for five different temperatures: 203, 223, 243, 273, 293 K. The wavelength grids cover the spectral range from about 230 nm up to about 1070 nm, a total of 4244 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.

Component: NO_2 Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 143038
Component Size: 143038 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (NO_2, SCIA-FM-spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13

Id	Comments	Unit	Type	#	Size	Offset
8	Number of spectral entries (NO_2, SCIA-FM-spectra)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	5	20	18
13	Wavelength grid per temperature (NO_2, SCIA-FM-spectra)	nm	fl	17875	71500	38
14	Cross-sections per temperature (NO_2, SCIA-FM- spectra)	cm^2/mol	fl	17875	71500	71538

The NO_2 spectrum is specified in one segment and for five different temperatures: 203, 223, 243, 273, 293 K. The wavelength grids cover the spectral range from about 233 nm up to about 890 nm, a total of 3575 entries. 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.

Component: BrO Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 177718
Component Size: 177718 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (BrO, SCIA-FM-spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries (BrO, SCIA-FM-spectra)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	5	20	18
13	Wavelength grid per temperature (BrO, SCIA-FM-spectra)	nm	fl	22210	88840	38
14	Cross-sections per temperature (BrO, SCIA-FM- spectra)	cm^2/mol	fl	22210	88840	88878

The BrO spectrum is specified in one segment and for five different temperatures: 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 five different temperatures. The number of cross-section entries is identical to the number of wavelength entries per block.

Component: SO_2 Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 56118
Component Size: 56118 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (SO_2, SCIA-FM-spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries (SO_2, SCIA-FM-spectra)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	5	20	18
13	Wavelength grid per temperature (SO_2, SCIA-FM-spectra)	nm	fl	7010	28040	38
14	Cross-sections per temperature (SO_2, SCIA-FM- spectra)	cm^2/mol	fl	7010	28040	28078

The SO_2 spectrum is specified in one segment and for five different temperatures: 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. 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.

Component: HCHO Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 11086
Component Size: 11086 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (HCHO, SCIA-FM-spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries (HCHO, SCIA-FM-spectra)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid per temperature (HCHO, SCIA-FM-spectra)	nm	fl	1383	5532	22
14	Cross-sections per temperature (HCHO, SCIA-FM-spectra)	cm^2/mol	fl	1383	5532	5554

The HCHO spectrum is specified in one segment and for one temperature (293 K). The wavelength grid covers 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.

Component: OClO Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 10046
Component Size: 10046 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (OClO, SCIA-FM-spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries (OClO, SCIA-FM-spectra)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid per temperature (OClO, SCIA-FM-spectra)	nm	fl	1253	5012	22
14	Cross-sections per temperature (OClO, SCIA-FM- spectra)	cm^2/mol	fl	1253	5012	5034

The OClO spectrum is specified in one segment and for one temperature (293 K). The wavelength grid covers 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.

Component: NO Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 3222
Component Size: 3222 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (NO, SCIA-FM-spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13

Id	Comments	Unit	Type	#	Size	Offset
8	Number of spectral entries (NO, SCIA-FM-spectra)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid per temperature (NO, SCIA-FM-spectra)	nm	fl	400	1600	22
14	Cross-sections per temperature (NO, SCIA-FM- spectra)	cm^2/mol	fl	400	1600	1622

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

Component: O_2 Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 98334
Component Size: 98334 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (O_2, SCIA-FM-spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries (O_2, SCIA-FM-spectra)	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	3	12	18
13	Wavelength grid per temperature (O_2, SCIA-FM- spectra)	nm	fl	12288	49152	30
14	Cross-sections per temperature (O_2, SCIA-FM- spectra)	cm^2/mol	fl	12288	49152	49182

The O_2 spectrum is specified in one segment and for three temperatures: 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.

Component: O_3D Reference spectra (measured) (GADS)

No of Records: 1
Record Size: 32560
Component Size: 32560 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (O_3 difference spectra)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries (O_3 difference spectra)	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid per temperature (O_3 diff. spectra)	nm	fl	4068	16272	16
14	Cross-sections per temperature (O_3 diff. spectra)	cm^2/mol	fl	4068	16272	16288

The O_3D is the difference spectrum derived from O_3 spectra at temperatures 243 K and 223 K and is specified in one segment. The wavelength grids cover the spectral range from about 230 nm up to about 1050 nm, a total of 4068 entries. Spectrum is based on a wavelength grid and therefore the type of wavelength information is 1.

3.8.7 Auxiliary Cross-Sections

The data base file consists of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	Hitran_H2O_BIRA Reference Spectrum	GADS
5	SCIA_FM_NO2_243K_BIRA Reference Spectrum	GADS
6	GREENBLATT_SHIFT_O4 Reference Spectrum	GADS
7	SOL_KITT_PEAK_CONV_CH2 Reference Spectrum	GADS
8	SOL_KITT_PEAK_CONV_CH3 Reference Spectrum	GADS
9	SCIA_FM_O3D_BIRA_S0020 Reference Spectrum	GADS
10	SCIA_FM_O3_243K_BIRA_S0025 Reference Spectrum	GADS
11	SCIA_FM_O3_243K_BIRA_S0020 Reference Spectrum	GADS
12	SCIA_RING_KPNO_ch2_BIRA Reference Spectrum	GADS
13	SCIA_RING_KPNO_ch3_BIRA Reference Spectrum	GADS
14	LIT_NO2_BOGUMIL_243K Reference Spectrum	GADS
15	RING1_BIRA_CH2 Reference Spectrum	GADS
16	RING2_BIRA_CH2 Reference Spectrum	GADS
17	RING_IFE_SO2 Reference Spectrum	GADS
18	LIT_BRO_FLEISCHMANN_223K Reference Spectrum	GADS
19	LIT_SO2_BIRA_VAC Reference Spectrum	GADS
20	USAMP_SO2_BREMEN Reference Spectrum	GADS
21	O3_BOGUMIL_243K_SO Reference Spectrum	GADS
22	O3_DIFF_SO2 Reference Spectrum	GADS
23	ETA_NADIR_BREMEN_2 Reference Spectrum	GADS
24	HERMANS_O4_BREMEN Reference Spectrum	GADS
25	KROMMINGA_OCLO_BREMEN Reference Spectrum	GADS
26	MAGIC_CORRECTION Reference Spectrum	GADS
27	RING_IFE_OCLO Reference Spectrum	GADS
28	USAMP_OCLO_BREMEN Reference Spectrum	GADS

During Algorithm Baseline Update from version 3.01 to version 4, all spectra needed for O3, NO2, BrO, and SO2 retrieval were assembled in Auxiliary Cross-Sections data base for reasons of convenience. In that way some spectra are duplicated: once they are in Literature Reference Cross-Sections data base as:

- Hitran_H2O_BIRA
- GREENBLATT_SHIFT_O4
- SCIA_RING_KPNO_ch2_BIRA
- SCIA_RING_KPNO_ch3_BIRA

or in Flight-Model Reference Cross-Sections data base as

- SCIA_FM_NO2_243K_BIRA
- SCIA_FM_O3D_BIRA_S0020

- SCIA_FM_O3_243K_BIRA_S0025
- SCIA_FM_O3_243K_BIRA_S0020,

and twice in Auxiliary Cross-Sections data base.

The following spectra:

- LIT_NO2_BOGUMIL_243K
- RING1_BIRA_CH2
- RING2_BIRA_CH2
- LIT_BRO_FLEISCHMANN_223K

were delivered by BIRA as a part of BrO retrieval settings.

IUP-UB provided for SO2 retrieval the following spectra:

- RING_IFE_SO2
- LIT_SO2_BIRA_VAC
- USAMP_SO2_BREMEN
- O3_BOGUMIL_243K_SO
- O3_DIFF_SO2
- ETA_NADIR_BREMEN_2

The type of wavelength information for all GADS in this section is 1 which means that field 13 contains the wavelength grid.

Component: Hitran_H2O_BIRA reference spectrum (GADS)

No of Records: 1
Record Size: 8214
Component Size: 8214 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1024	4096	22
14	Cross-sections	cm^2/mol	fl	1024	4096	4118

The spectral segment of Hitran_H2O_BIRA covers the spectral range from 383.56 nm up to 628.39 nm, a total of 1024 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1024 entries.

Component: SCIA_FM_NO2_243K_BIRA reference spectrum (GADS)

No of Records: 1
Record Size: 13198
Component Size: 13198 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1647	6588	22
14	Cross-sections	cm^2/mol	fl	1647	6588	6610

The spectral segment of SCIA_FM_NO2_243K_BIRA covers the spectral range from 300.10 nm up to 570.00 nm, a total of 1647 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1647 entries.

Component: GREENBLATT_SHIFT_O4 reference spectrum (GADS)

No of Records: 1
Record Size: 30182
Component Size: 30182 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	3770	15080	22
14	Cross-sections	cm^2/mol	fl	3770	15080	15102

The spectral segment of GREENBLATT_SHIFT_O4 covers the spectral range from 300.09 nm up to 677.09 nm, a total of 3770 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 3770 entries.

Component: SOL_KITT_PEAK_CONV_CH2 reference spectrum (GADS)

No of Records: 1
Record Size: 8134
Component Size: 8134 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1014	4056	22
14	Cross-sections	cm^2/mol	fl	1014	4056	4078

The spectral segment of SOL_KITT_PEAK_CONV_CH2 covers the spectral range from 301.78 nm up to 412.17 nm, a total of 1014 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1014 entries.

Component: SOL_KITT_PEAK_CONV_CH3 reference spectrum (GADS)

No of Records: 1
Record Size: 8214
Component Size: 8214 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1024	4096	22
14	Cross-sections	cm^2/mol	fl	1024	4096	4118

The spectral segment of SOL_KITT_PEAK_CONV_CH3 covers the spectral range from 383.52 nm up to 628.41 nm, a total of 1024 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1024 entries.

Component: SCIA_FM_O3D_BIRA_S0020 reference spectrum (GADS)

No of Records: 1
Record Size: 12934
Component Size: 12934 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1614	6456	22
14	Cross-sections	cm^2/mol	fl	1614	6456	6478

This absorption spectrum (as well as SCIA_FM_O3_243K_BIRA_S0025, SCIA_FM_O3_243K_BIRA_S0020, LIT_NO2_BOGUMIL_243K) was measured by Molecular Spectroscopy and Chemical Kinetics Group at IUP-UB. For more details see [S7].

In fact the spectral segment SCIA_FM_O3D_BIRA_S0020 represent a difference between O3 cross-sections for two temperatures 243 K (SCIA_FM_O3_243K_BIRA_S0020) and 223 K (not listed here). The spectral segment of SCIA_FM_O3D_BIRA_S0020 covers the spectral range from 300.01 nm up to 569.78 nm, a total of 1614 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1614 entries.

Component: SCIA_FM_O3_243K_BIRA_S0025 reference spectrum (GADS)

No of Records: 1
Record Size: 13006
Component Size: 13006 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1623	6492	22
14	Cross-sections	cm^2/mol	fl	1623	6492	6514

The spectral segment of SCIA_FM_O3_243K_BIRA_S0025 covers the spectral range from 300.02 nm up to 569.78 nm, a total of 1623 entries. The data from this spectral segment corresponds to a temperature of 243 K. The cross sections are available for each wavelength entry within the given spectral range, a total of 1623 entries.

Component: SCIA_FM_O3_243K_BIRA_S0020 reference spectrum (GADS)

No of Records: 1
Record Size: 12934
Component Size: 12934 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1614	6456	22
14	Cross-sections	cm^2/mol	fl	1614	6456	6478

The spectral segment of SCIA_FM_O3_243K_BIRA_S0020 covers the spectral range from 300.01 nm up to 569.78 nm, a total of 1614 entries. The data from this spectral segment corresponds to a temperature of 243 K. The cross sections are available for each wavelength entry within the given spectral range, a total of 1614 entries.

Component: SCIA_RING_KPNO_ch2_BIRA reference spectrum (GADS)

No of Records: 1
Record Size: 8134
Component Size: 8134 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1014	4056	22
14	Cross-sections	cm^2/mol	fl	1014	4056	4078

The spectral segment of SCIA_RING_KPNO_ch2_BIRA covers the spectral range from 301.78 nm up to 412.17 nm, a total of 1014 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1014 entries.

Component: SCIA_RING_KPNO_ch3_BIRA reference spectrum (GADS)

No of Records: 1
Record Size: 8214
Component Size: 8214 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1024	4096	22
14	Cross-sections	cm^2/mol	fl	1024	4096	4118

The spectral segment of SCIA_RING_KPNO_ch3_BIRA covers the spectral range from 383.52 nm up to 628.41 nm, a total of 1024 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1024 entries.

Component: LIT_NO2_BOGUMIL_243K reference spectrum (GADS)

No of Records: 1
Record Size: 28638
Component Size: 28638 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	3577	14308	22
14	Cross-sections	cm^2/mol	fl	3577	14308	14330

The spectral segment of LIT_NO2_BOGUMIL_243K covers the spectral range from 233.08 nm up to 890.08 nm, a total of 3577 entries. The data from this spectral segment corresponds to a temperature of 243 K. The cross sections are available for each wavelength entry within the given spectral range, a total of 3577 entries.

Component: RING1_BIRA_CH2 reference spectrum (GADS)

No of Records: 1
Record Size: 8134
Component Size: 8134 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1014	4056	22
14	Cross-sections	cm^2/mol	fl	1014	4056	4078

RING1_BIRA_CH2 and RING2_BIRA_CH2 are Ring spectra calculated using the SCIATRAN model. They are used for BrO retrieval following [S8].

The spectral segment of RING1_BIRA_CH2 covers the spectral range from 301.78 nm up to 412.17 nm, a total of 1014 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1014 entries.

Component: RING2_BIRA_CH2 reference spectrum (GADS)

No of Records: 1
Record Size: 8134
Component Size: 8134 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13

Id	Comments	Unit	Type	#	Size	Offset
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1014	4056	22
14	Cross-sections	cm^2/mol	fl	1014	4056	4078

The spectral segment of RING2_BIRA_CH2 covers the spectral range from 301.78 nm up to 412.17 nm, a total of 1014 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1014 entries.

Component: RING_IFE_SO2 reference spectrum (GADS)

No of Records: 1
Record Size: 5982
Component Size: 5982 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	745	2980	22
14	Cross-sections	cm^2/mol	fl	745	2980	3002

The spectral segment of RING_IFE_SO2 covers the spectral range from 300.11 nm up to 381.95 nm, a total of 745 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 745 entries.

Component: LIT_BRO_FLEISCHMANN_223K reference spectrum (GADS)

No of Records: 1
Record Size: 4454
Component Size: 4454 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11

Id	Comments	Unit	Type	#	Size	Offset
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	554	2216	22
14	Cross-sections	cm^2/mol	fl	554	2216	2238

The spectral segment of LIT_BRO_FLEISCHMANN_223K covers the spectral range from 320.17 nm up to 380.05 nm, a total of 554 entries. The shift of 0.17 nm was applied to this spectrum. The data from this spectral segment corresponds to a temperature of 223 K (average temperature of an stratospheric layer with the highest BrO concentration). The cross sections are available for each wavelength entry within the given spectral range, a total of 554 entries. For more details see [S9].

Component: LIT_SO2_BIRA_VAC reference spectrum (GADS)

No of Records: 1
Record Size: 10390
Component Size: 10390 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1296	5184	22
14	Cross-sections	cm^2/mol	fl	1296	5184	5206

This absorption spectrum was measured at Laboratoire de Chimie Physique Moléculaire, Université Libre de Bruxelles. The spectral segment of LIT_SO2_BIRA_VAC covers the spectral range from 250.03 nm up to 333.26 nm, a total of 1296 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1296 entries. For more details see [S10].

Component: USAMP_SO2_BREMEN reference spectrum (GADS)

No of Records: 1
Record Size: 1222
Component Size: 1222 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	150	600	22
14	Cross-sections	cm^2/mol	fl	150	600	622

The spectral segment of USAMP_SO2_BREMEN covers the spectral range from 313.03 nm up to 329.91 nm, a total of 150 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 150 entries.

Component: O3_BOGUMIL_243K_SO2 reference spectrum (GADS)

No of Records: 1
Record Size: 8478
Component Size: 8478 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1057	4228	22
14	Cross-sections	cm^2/mol	fl	1057	4228	4250

The spectral segment of O3_BOGUMIL_243K_SO2 covers the spectral range from 230.00 nm up to 351.11 nm, a total of 1057 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1057 entries.

Component: O3_DIFF_SO2 reference spectrum (GADS)

No of Records: 1
Record Size: 8478
Component Size: 8478 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1057	4228	22
14	Cross-sections	cm^2/mol	fl	1057	4228	4250

The spectral segment of O3_DIFF_SO2 covers the spectral range from 230.00 nm up to 351.11 nm, a total of 1057 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1057 entries.

Component: ETA_NADIR_BREMEN_2 reference spectrum (GADS)

No of Records: 1
Record Size: 8214
Component Size: 8214 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1024	4096	22
14	Cross-sections	cm^2/mol	fl	1024	4096	4118

The spectral segment of ETA_NADIR_BREMEN_2 covers the spectral range from 300.59 nm up to 412.18 nm, a total of 1024 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1024 entries.

Component: HERMANS_O4_BREMEN reference spectrum (GADS)

No of Records: 1
Record Size: 33198
Component Size: 33198 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	4147	16588	22
14	Cross-sections	cm^2/mol	fl	4147	16588	16610

The spectral segment of HERMANS_O4_BREMEN covers the spectral range from 327.98 nm up to 408.28 nm, a total of 4147 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 4147 entries.

Component: KROMMINGA_OCLO_BREMEN reference spectrum (GADS)

No of Records: 1
Record Size: 6750
Component Size: 6750 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	841	3364	22
14	Cross-sections	cm^2/mol	fl	841	3364	3386

The spectral segment of KROMMINGA_OCLO_BREMEN covers the spectral range from 330.10 nm up to 414.12 nm, a total of 841 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 841 entries.

Component: MAGIC_CORRECTION reference spectrum (GADS)

No of Records: 1
Record Size: 8214
Component Size: 8214 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	1024	4096	22
14	Cross-sections	cm^2/mol	fl	1024	4096	4118

The spectral segment of MAGIC_CORRECTION covers the spectral range from 300.59 nm up to 412.18 nm, a total of 1024 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 1024 entries.

Component: RING_IFE_OCLO reference spectrum (GADS)

No of Records: 1
Record Size: 5766
Component Size: 5766 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	718	2872	22
14	Cross-sections	cm^2/mol	fl	718	2872	2894

The spectral segment of RING_IFE_OCLO covers the spectral range from 319.98 nm up to 400.00 nm, a total of 718 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 718 entries.

Component: USAMP_OCLO_BREMEN reference spectrum (GADS)

No of Records: 1
Record Size: 1974
Component Size: 1974 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures	-	us	1	2	13
8	Number of spectral entries	-	us	1	2	15
10	Type of wavelength information	-	uc	1	1	17
12	Temperature grid	K	fl	1	4	18
13	Wavelength grid	cm^{-1}	fl	244	976	22
14	Cross-sections	cm^2/mol	fl	244	976	998

The spectral segment of USAMP_OCLO_BREMEN covers the spectral range from 364.10 nm up to 389.97 nm, a total of 244 entries. The cross sections are available for each wavelength entry within the given spectral range, a total of 244 entries.

3.8.8 Undersampling correction spectra

The data base file consists of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	Undersampling spectra channel 2	GADS
5	Undersampling spectra channel 3	GADS
6	Undersampling spectra channel 7	GADS
7	Undersampling spectra channel 8	GADS

The following component in this sub-section describes the GADS records for the file of undersampling spectra. For the header components of this product refer to section 3.5 above.

It has been recognised that there is a need to correct the DOAS and IAS fitting for instrumental effects (see [S2], [S3]). One such effect is the Doppler shift (in wavelength) between the recorded 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.

Component: Undersampling correction channel 2 (GADS)

No of Records: 1
Record Size: 8208
Component Size: 8208 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Spectra type	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (channel 2)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries in channel 2	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid channel 2	nm	fl	1024	4096	16
14	Cross-sections for channel 2	cm^2/mol	fl	1024	4096	4112

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

Component: Undersampling correction channel 3 (GADS)

No of Records: 1
Record Size: 8208
Component Size: 8208 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Spectra type	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (channel 3)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries in channel 3	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid channel 3	nm	fl	1024	4096	16
14	Cross-sections for channel 3	cm^2/mol	fl	1024	4096	4112

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

Component: Undersampling correction channel 7 (GADS)

No of Records: 1
Record Size: 8208
Component Size: 8208 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Spectra type	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (channel 7)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries in channel 7	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid channel 7	nm	fl	1024	4096	16
14	Cross-sections for channel 7	cm^2/mol	fl	1024	4096	4112

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

Component: Undersampling correction channel 8 (GADS)

No of Records: 1
Record Size: 8208
Component Size: 8208 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Spectra type	-	tx	5	5	0
2	Number of atmospheric levels	-	us	1	2	5
3	Number of spectral segments (channel 8)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
8	Number of spectral entries in channel 8	-	us	1	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid channel 8	nm	fl	1024	4096	16
14	Cross-sections for channel 8	cm^2/mol	fl	1024	4096	4112

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

3.8.9 ETA & ZETA key data

The data base file consists of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	ETA key data	GADS
5	ZETA key data	GADS

The following component in this sub-section describes the GADS records for the key data file. For the header components of this product refer to section 3.5 above. The SPH descriptor is set to “KEYDATA_FILE”.

Component: ETA key data (GADS)

No of Records: 1
Record Size: 58208
Component Size: 58208 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Key data type	-	tx	5 (“ETA“)	5	0
2	Number of atmospheric levels	-	us	1 (0)	2	5
3	Number of spectral segments	-	us	1 (1)	2	7
4	Maximum number of temperatures	-	us	1(0)	2	9
5	Maximum number of coefficients	-	us	1 (0)	2	11
8	Number of spectral entries	-	us	1 (7274)	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid channel 2	nm	fl	7274	29096	16
14	Key data	cm^2/mol	fl	7274	29096	29112

There is one spectral segment for ETA key data which covers the spectral range from 212.533 nm up to 2385.61 nm, a total of 7274 entries. The key data are available for each wavelength entry within the given spectral range, a total of 7274 entries.

Component: ZETA key data (GADS)

No of Records: 1
Record Size: 58208
Component Size: 58208 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Key data type	-	tx	5 (ZETA)	5	0
2	Number of atmospheric levels	-	us	1 (0)	2	5
3	Number of spectral segments	-	us	1 (1)	2	7
4	Maximum number of temperatures	-	us	1(0)	2	9
5	Maximum number of coefficients	-	us	1 (0)	2	11
8	Number of spectral entries	-	us	1 (7274)	2	13
10	Type of wavelength information	-	uc	1	1	15
13	Wavelength grid channel 2	nm	fl	7274	29096	16
14	Key data	cm^2/mol	fl	7274	29096	29112

There is one spectral segment for ZETA key data which covers the spectral range from 212.533 nm up to 2385.61 nm, a total of 7274 entries. The key data are available for each wavelength entry within the given spectral range, a total of 7274 entries.

3.8.10 ESFT HITRAN spectral data

Spectral data used as input for the SACURA cloud algorithm.

The data base file consists of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	O_2 spectral data	GADS

For the header components of this file refer to section 3.5 above. For the ESFT spectral GADS the common structure of Reference spectra (see section 3.8.5) is used with slight modifications:

Component: *mol* spectral data (GADS)

Field	Comments	Unit	Type	#	Size	
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric pressure levels (p)	-	us	1	2	5
3	Number of spectral segments (n)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures per segment (t_n)	-	us	n	2 * n	13
7	Number of coefficients per segment (c_n)	-	us	n	2 * n	
8	Number of spectral entries per segment (w_n)	-	us	n	2 * n	
9	Type of formula for coefficients	-	uc	1	1	
10	Type of wavelength information	-	uc	1	1	
11	Atmospheric levels pressure	hPa	do	p	8 * p	
12	Temperature grid per spectral segment	K	do	$t = \Sigma t_n$	8 * t	
13	Wavelength information per spectral segment	-	wl_inf	n	n * wl_{len}	
14	Weights per spectral segment	-	do	$m = \Sigma c_n$	8 * m	
15	Coefficients per spectral segment, wavelength, pressure, temperature	cm^2/mol	do	$c = \Sigma w_n * p * t_n * c_n$	8 * c	

Explanation (see also description of fields for Literature Reference spectra (section 3.8.5)):

- Field 9: Unused.
- Field 10: A type different from Literature Reference spectra is used, set to type=4.
- Field 13: Wavelength information is available as start and end wavelength boundaries. The wavelength currently assigned to the coefficients ist the center of each particular interval which can derived from the boundaries and the number of spectral entries for each segment.

  Type no. 4: Start and end wavelength

Field	Comments	Unit	Type	#	Size
1	Start wavelength (λ_0)	nm	do	1	8
2	End wavelength (λ_1)	nm	do	1	8

  Size of Component: $wl_{len} = 16$

The wavelength for spectral entry w in segment n is calculated by:

$$\lambda(w,n) = \lambda_0(n) + (w + 0.5) * (\lambda_1(n) - \lambda_0(n)) / w_n \text{ , with } w = 0 \ldots w_n\text{-}1$$

(*Note:* in the case getting ESFT spectral data for SACURA explicite wavelength calculation is not necessary.)

- Field 14: Is used (different from Literature Reference) to store the weight factors.
- Field 15: The cross-section coefficients are organised per segment, then per coefficient, then per temperature, then per pressure, then per wavelength.

Only spectra for molecule O_2 are contained currently. Other may be added in future (H_2O, CO_2, CH_4) if necessary in the same format.

The molecule names in the GADS records are given in ASCII. Unused characters are left blank.

Component: O_2 spectral data (GADS)

No of Records: 1
Record Size: 3456535
Component Size: 3456535 Bytes

Id	Comments	Unit	Type	#	Size	
1	Molecule name	-	tx	5	5	0
2	Number of atmospheric pressure levels (p)	-	us	1	2	5
3	Number of spectral segments (n)	-	us	1	2	7
4	Maximum number of temperatures	-	us	1	2	9
5	Maximum number of coefficients	-	us	1	2	11
6	Number of temperatures per segment (t_n)	-	us	4	8	13
7	Number of coefficients per segment (c_n)	-	us	4	8	21
8	Number of spectral entries per segment (w_n)	-	us	4	8	29
9	Type of formula for coefficients (unused)	-	uc	1	1	37
10	Type of wavelength information	-	uc	1	1	38
11	Atmospheric levels pressure	hPa	do	10	80	39
12	Temperature grid per spectral segment	K	do	24	192	119
13	Wavelength information per spectral segment	-	wl_inf	4	64	311
14	Weights per spectral segment	-	do	20	160	375
15	Coefficients per spectral segment, wavelength, pressure, temperature	cm^2/mol	do	432000	3456000	535

The O_2 spectral data are specified for 10 pressure levels in 4 segments as following:

Segment	λ_0 [nm]	λ_1 [nm]	w_n	t_n	c_n
1	625.00	640.00	300	6	5
2	685.00	702.00	340	6	5
3	755.00	775.00	400	6	5
4	1230.00	1310.00	400	6	5

The ESFT coefficients are stored as blocks for each segment. In each segment the first entry is the first coefficient for the first temperature, the first atmospheric level, and the first wavelength; the data runs first over wavelength as fastest index, then over atmospheric levels, then over temperatures and then over coefficients.

3.8.11 PMD minimum reflectance library

The PMD reflectance data base has been created from GOME PMD measurements. It contains minimum reflectance values as function of the geolocation. A more detailed description of the data base content and its derivation is given in [S6].

The GOME instrument has only three PMD's in the UV-VIS spectral range. Thus, the data base entries for the first three PMD's are based on real GOME measurements and the currently implemented algorithm makes use only of that data. Therefore the data base size depends on the entry in field 1. It is possible that the original GOME measurements will be replaced by SCIAMACHY measurements because the spectral coverage of GOME and SCIAMCHY UV-VIS PMD's is not the same. It is envisaged to allow for an easy update of the data base during or after the SCIAMACHY commissioning phase.

The data base consist of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	PMD minimum reflectance values	GADS

The following component in this sub-section describes the GADS records for the file of CCA threshold data. For the header components of this product refer to section 3.5 above.

Component: PMD minimum reflectance data base (GADS)

No of Records: 1
Record Size: 3000006
Component Size: 3000006 Bytes[1]

Id	Comments	Unit	Type	#	Size	Offset
1	Number of PMD-channels used in CCA (*n*)	-	us	1	2	0
2	Number of latitude entries	-	us	1	2	2
3	Number of longitude entries	-	us	1	2	4
4	Reflectance thresholds	-	ss	*n* * 500000	*n* * 1000000	6

The reflectance thresholds are given as function of the geolocation and the spectral 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 number of PMD-channels is n=3. 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 longitude and finally latitude, making a total of 1500000 entries (3*500*1000).

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 of 0.01 and then by a factor of 32768 (the maximum size of a signed short int).

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

3.9 Air Mass Factor Look-up Table

3.9.1 Identifier

SCI_MF2_AX

3.9.2 Type

Auxiliary

3.9.3 Description

The AMF look-up table file will include headers and a set of GADS records. The main product header (MPH) has already been described at the beginning of this chapter. The specific product header (SPH) will include the identification of the version of this AMF look-up table and the data set description records (DSD) for the following GADS records. There will be one GADS per molecule of this AMF look-up table, with a single DSR for each GADS, as described below.

3.9.4 Format

The detailed format description is divided into several tables representing the hierarchy of product content. The products consist of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	AMF Look-up Table for O_3	GADS
5	AMF Look-up Table for NO_2	GADS
6	AMC DOAS Look-up Table for H_2O	GADS

The following paragraphs describe the detailed definition of the common components listed above:

Main Product Header (MPH)

No of Records: 1
Record Size: 1247
Component Size: 1247 Bytes

Id	Name	Comments	Unit	Type	#	Size	Offset
1	MPH	The main product header is described in the ENVISAT product specification (volume 5)	-	tx	1247	1247	0

Specific Product Header of the AMF look-up table (SPH)

No of Records: 1
Record Size: 98
Component Size: 98 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	SPH_DESCRIPTOR=	keyword	tx	15	15	0
2	"AMF_LOOK_UP_FILE~~~~~~~~~~~~~~"	variable	tx	30	30	15
3	Newline character	terminator	tx	1	1	45
4	Spare	-	tx	51	51	46
5	Newline character	terminator	tx	1	1	97

Data Set Description (DSD)

No of Records: 2
Record Size: 280
Component Size: 560

Id	Name	Comments	Unit	Type	#	Size	Offset
1	DSD	The data set descriptor record is described in the ENVISAT product specification (volume 5)	-	tx	280	280	0

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 format of the two AMF look-up tables is identical. Therefore, only one format description is given here. The dataset identified by AMC_H2O is used by the AMC-DOAS algortithm, and has its own format.

Component: AMF Look-up Table for O_3 (GADS)

No of Records: 1
Record Size: 1747330
Component Size: 1747330 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of reference wavelengths	-	us	1	2	0
2	Number of reference heights	-	us	1	2	2
3	Number of reference 'scenarios' (see note)	-	us	1	2	4
4	Number of reference albedos	-	us	1	2	6
5	Number of reference aerosol types	-	us	1	2	8
6	Number of coefficients in solar zenith angle parameterisation	-	us	1	2	10
7	Number of coefficients in line-of-sight nadir angle parameterisation	-	us	1	2	12

Id	Comments	Unit	Type	#	Size	Offset
8	Number of azimuths	-	us	1	2	14
9	Number of reference days	-	us	1	2	16
10	Reference wavelengths	nm	fl	2	8	18
11	Reference heights	km	fl	7	28	26
12	Latitude grid of the reference scenarios	degree	fl	8	32	54
13	Reference albedos	%	fl	4	16	86
14	Reference azimuths	degree	fl	5	20	102
15	Reference days	-	us	4	8	122
16	Air Mass Factor coefficient O_3	-	do	218400	1747200	130

Component: AMF Look-up Table for NO_2 (GADS)

No of Records: 1
Record Size: 873726
Component Size: 873726 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of reference wavelengths	-	us	1	2	0
2	Number of reference heights	-	us	1	2	2
3	Number of reference 'scenarios' (see note)	-	us	1	2	4
4	Number of reference albedos	-	us	1	2	6
5	Number of reference aerosol types	-	us	1	2	8
6	Number of coefficients in solar zenith angle parameterisation	-	us	1	2	10
7	Number of coefficients in line-of-sight nadir angle parameterisation	-	us	1	2	12
8	Number of azimuths	-	us	1	2	14
9	Number of reference days	-	us	1	2	16
10	Reference wavelengths	nm	fl	1	4	18
11	Reference heights	km	fl	7	28	22
12	Latitude grid of the reference scenarios	degree	fl	8	32	50
13	Reference albedos	%	fl	4	16	82
14	Reference azimuths	degree	fl	5	20	98
15	Reference days	-	us	4	8	118
16	Air Mass Factor coefficient NO_2	-	do	109200	873600	126

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 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)

25 :latitude zone 10 degree the same for all seasons
26 :latitude zone -10 degree the same for all seasons
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)

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 data base, but they are parameterised using appropriate 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 2^{nd} 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_2 there is 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*26*5*7*4*2*15 = 218400) for O_3 and 109200 for NO_2.

Component: AMC Look-up Table for H_2O (GADS)

No of Records: 1
Record Size: 134476
Component Size: 134476 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of reference solar zenith angles	-	us	1	2	0
2	Number of reference wavelengths	-	us	1	2	2
3	Reference solar zenith angles	-	do	9	72	4
4	Reference wavelengths	-	do	600	4800	76
5	2D matrix of coefficients *b*	-	do	5400	43200	4876
6	2D matrix of coefficients *c*	-	do	5400	43200	48076
7	2D matrix of coefficients τ_{O2}	-	do	5400	43200	91276

The coefficients b, c and τ_{O2} are needed for the AMC-DOAS algorithm. They have been derived using the radiative transfer model SCITRAN [S11], for further details, see [S12]. Coefficients run first over SZAs, then over wavelengths. There is a total of 9*600=5400 entries for each coefficient.

3.9.5 Sizing

N/A

3.9.6 Volume

Approximately 2.6 MB for all gases.

3.9.7 Throughput

There is just one AMF look-up table file for the entire mission.

3.9.8 Remarks

N/A

3.10 AAIA Rayleigh Reflectance Look-up Table

3.10.1 Identifier

SCI_RC2_AX

3.10.2 Type

Auxiliary

3.10.3 Description

The AAIA Rayleigh reflectance look-up table includes headers and a set of GADS records. The main product header (MPH) has already been described at the beginning of this chapter. The specific product header (SPH) will include the identification of the version of this look-up table and the data set description records (DSD) for the following GADS records. There will be two GADS records, with two DSDs to match.

3.10.4 Format

The detailed format description is divided into several tables representing the hierarchy of product content. The products consist of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	AAIA Rayleigh Reflectance Look-up Table	GADS
5	AAIA KNMI Look-up Table	GADS

The following paragraphs describe the detailed definition of the common components listed above:

Main Product Header (MPH)

No of Records: 1
Record Size: 1247
Component Size: 1247 Bytes

Id	Name	Comments	Unit	Type	#	Size	Offset
1	MPH	The main product header is described in the ENVISAT product specification (volume 5)	-	tx	1247	1247	0

Specific Product Header of the AIRC look-up table (SPH)

No of Records: 1
Record Size: 98
Component Size: 98 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	SPH_DESCRIPTOR=	keyword	tx	15	15	0
2	"AIRC_LOOK_UP_FILE~~~~~~~~~~~~~~"	variable	tx	30	30	15
3	Newline character	terminator	tx	1	1	45
4	Spare	-	tx	51	51	46
5	Newline character	terminator	tx	1	1	97

Data Set Description (DSD)

No of Records: 1
Record Size: 280
Component Size: 280

Id	Name	Comments	Unit	Type	#	Size	Offset
1	DSD	The data set descriptor record is described in the ENVISAT product specification (volume 5)	-	tx	280	280	0

The DS_NAME field of the DSDs will be specified according to the content of the corresponding GADS; the fields are AAIA_REF_RC and AAIA_KNMI_REF_RC.

Component: AAIA Rayleigh Reflectance Look-up Table (GADS)

No of Records: 1
Record Size: 42336
Component Size: 42336 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of reference heights	-	us	1	2	0
2	Number of reference wavelengths	-	us	1	2	2
3	Number of reference albedos	-	us	1	2	4
4	Number of azimuth harmonics	-	us	1	2	6
5	Number of coefficients in solar zenith angle parameterisation	-	us	1	2	8
6	Number of coefficients in line-of-sight nadir angle parameterisation	-	us	1	2	10
7	Reference heights	km	fl	11	44	12
8	Reference wavelengths	nm	fl	2	8	56
9	Reference albedos	-	fl	8	32	64
10	Rayleigh reflectance coefficient, first harmonic	sr^{-1}	do	4224	33792	96
11	Rayleigh reflectance coefficient, second harmonic	sr^{-1}	do	528	4224	33888
12	Rayleigh reflectance coefficient, third harmonic	sr^{-1}	do	528	4224	38112

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, geometrical angles are not used directly in the data base, but they are parameterised using polynomial fits. The parameterisation scheme for this table has a 5th order polynomial (6 coefficients covering 14 calculated values) for the solar zenith cosine dependence and a 3rd order polynomial (4 coefficients covering 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. 24 zenith angle coefficients are specified for each harmonic giving in total 72 coefficients for the geometry. The fitting order for these coefficients is first the 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 albedo, 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*8*11*2=4224). The second and the 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 each (24*11*2=528) for harmonics 2 and 3.

Component: AAIA KNMI Look-up Table (GADS)

No of Records: 1
Record Size: 768670
Component Size: 768670 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	Number of wavelengths	-	us	1	2	0
2	Number of heights	-	us	1	2	2
3	Number of mu-points	-	us	1	2	4
4	Vector of wavelengths	nm	do	2	16	6
5	Vector of heights	km	do	9	72	22
6	Vector of mu-points	-	do	42	336	94
7	2D matrix of spherical albedos	-	do	18	144	430
8	3D matrix of transmission	-	do	756	6048	572
9	4D matrix of 0^{th} order Fourier coefficients	-	do	31752	254016	6622
10	4D matrix of 1^{st} order Fourier coefficients	-	do	31752	254016	260638
11	4D matrix of 2^{nd} order Fourier coefficients	-	do	31752	254016	514654

Wavelengths are 340 and 380 nm, heights range from 0 to 8 km. Spherical albedos run first over the wavelengths and then over the heights resulting in a 2-dimensional 2×9 matrix with 18 entries. Transmisson runs first over the wavelengths, then over the heights and finally over the gaussian mu-points resulting in a 3-dimensional 2×9×42 matrix with 756 entries. Fourier coefficients of order 0, 1 and 2 run first over the wavelengths, then over the heights and for sza and los over the gaussian mu-points resulting in three 4-dimensional 2×9×42×42 matrices with 31752 entries each.

3.10.5 Sizing

N/A

3.10.6 Volume

Approximately 0.8 MB.

3.10.7 Throughput

There is just one AAIA look-up table file for the entire mission.

3.10.8 Remarks

N/A

3.11 SO_2 Background Data Base

3.11.1 Identifier

SCI_SO2_AX

3.11.2 Type

Auxiliary

3.11.3 Description

The SO2 background data base will include headers and one GADS. The main product header (MPH) has already been described at the beginning of this chapter. The specific product header (SPH) will include the identification of the version of this data base and the data set description record (DSD) for the following GADS record. There will be one DSR, with one DSD to match.

3.11.4 Format

The detailed format description is divided into several tables representing the hierarchy of product content. The products consist of the following components:

Id	Product Components	Component Type
1	Main Product Header	MPH
2	Specific Product Header	SPH
3	Data Set Descriptor	DSD
4	SO_2 background data base	GADS

The following paragraphs describe the detailed definition of the common components listed above:

Main Product Header (MPH)

No of Records: 1
Record Size: 1247
Component Size: 1247 Bytes

Id	Name	Comments	Unit	Type	#	Size	Offset
1	MPH	The main product header is described in the ENVISAT product specification (volume 5)	-	tx	1247	1247	0

Specific Product Header of the SO2B look-up table (SPH)

No of Records: 1
Record Size: 98
Component Size: 98 Bytes

Id	Comments	Unit	Type	#	Size	Offset
1	SPH_DESCRIPTOR=	keyword	tx	15	15	0
2	"SO2B_LOOK_UP_FILE~~~~~~~~~~~~~~"	variable	tx	30	30	15
3	Newline character	terminator	tx	1	1	45
4	Spare	-	tx	51	51	46
5	Newline character	terminator	tx	1	1	97

Data Set Description (DSD)

No of Records: 1
Record Size: 280
Component Size: 280

Id	Name	Comments	Unit	Type	#	Size	Offset
1	DSD	The data set descriptor record is described in the ENVISAT product specification (volume 5)	-	tx	280	280	0

The DS_NAME field of the DSD will be specified according to the content of the corresponding GADS; this field is named SO2_BACKGROUND.

Component: SO_2 background look-up table (GADS)

No of Records: 1
Record Size: variable (2142)
Component Size: variable (2142 Bytes)

Id	Comments	Unit	Type	#	Size	Offset
1	SO_2 background records	-	SO2B	n (9)	(2142)	0

The DSR is split into SO2B records of size 238. Each of these records refers to 1 day. For the specification of the SO2B record see section 4.2. Sizes given in brackets are examples for a data base with 9 SO2B records.

3.11.5 Sizing

N/A

3.11.6 Volume

variable

3.11.7 Throughput

The SO_2 background data base is continuously filled during the mission.

3.11.8 Remarks

An empty SO_2 data base DSR must contain exactly one byte with value x‘00’, i.e. the DSR size is 1.

An entry is added or modified whenever SO_2 data is retrieved and the following

conditions are satisfied:

- the ground pixel is in the "reference sector" i.e. the center longitude is between 180° and 220° (over Pacific Ocean);
- the ground pixel is in the descending node of the orbit i.e. the flight direction was north to south;
- the RMS of the retrieval is lower than 0.007;
- the fractional cloud cover is smaller than 0.5;
- at least 1 latitude bin with data quality > 0 was found;
- the orbit was not used earlier to add data to the DB (duplicate entering would distort the entries).

4 Generic Data Representations

4.1 Data Types

The data types used for the definition of the file formats in the present document may be divided into basic and compound data types. If the basic data types are the atoms of each file, then compound data types are important molecules which are used to simplify the definition of the file format. The compound data types are commonly used data structures which are again build on the basis of the basic data types. The detailed definition of these compound data types is given in the following section.

The byte ordering of integer values is as such that the least significant byte is on the lower address.

The IEEE 754-1985 is the chosen standard for storing real numbers which is in line with [A2].

- The following basic data types are used:

Notation	Description	Bytes
b	binary field (e.g. for flags, detailed description in the remarks column)	1
do	double (8-byte floating point number): 1.79e+308 maximum absolute value to 2.22e-308 minimum absolute value	8
fl	float (4-byte floating point number): 3.40282347e+38 maximum absolute value to 1.17549435e-38 minimum absolute value	4
sc	signed character (1-byte integer): -128 to 127	1
sl	signed long (4-byte integer): -2.147.483.648 to 2.147.483.647	4
ss	signed short (2-byte integer): -32768 to 32767	2
tx	text field	1
uc	unsigned character (1-byte integer): 0 to 255	1
ul	unsigned long (4-byte integer): 0 to 4.294.967.295	4
us	unsigned short (2-byte integer): 0 to 65535	2

- The following compound data types are used:

Notation	Description	Bytes
Coord	Geographical Coordinate (ISO 6709)	8
LayerRec	Limb Profile Layer Record	16
MeasGrid	Measurement grid record	33
MJD	Modified Julian Date	12
StateVec	State vector record	12
SO2B	SO2 background record	238
SO2BD	SO2 background data entry	5

4.2 Compound Data Types

In the present section the detailed format of the compound data types is given (order by compound data type notation), as listed in the section before.

Geographical Coordinate (ISO 6709) (Coord)

Compound Size: 8 Bytes

No	Name	Comments	Unit	Type	#	Size	Offset
1	LAT	Latitude (-90 to 90, -90 is the south pole, 90 the north pole and 0 the equator)	degree	sl	1	4	0
2	LONG	Longitude (-180 to 180, 0 is the meridian and moving east in the positive direction)	degree	sl	1	4	4

Limb Profile Layer Record (LayerRec)

Compound Size: 16 Bytes

No	Name	Comments	Unit	Type	#	Size	Offset
1	TANGVMR	Tangent layer volume mixing ratio	ppV	fl	1	4	0
2	ERRTANGVMR	Error on the tangent layer volume mixing ratio	%	fl	1	4	4
3	VERTCOL	Vertical column density above lower layer boundary	molecule/cm^2	fl	1	4	8
4	ERRVERTCOL	Error on the vertical column density above lower layer boundary	%	fl	1	4	12

The limb profile layer record is used twice in the limb fitting window application data set record.

Measurement grid record (MeasGrid)

Compound Size: 33 Bytes

No	Name	Comments	Unit	Type	#	Size	Offset
1	STARTTIME	Start time of the measurement at that specific layer	-	MJD	1	12	0
2	TANGH	Mean tangent height of measurement	km	fl	1	4	12
3	TANGP	Pressure at tangent height	hPa	fl	1	4	16
4	TANGT	Temperature at tangent height	K	fl	1	4	20
5	NUM_WIN	Number of fitting windows	-	uc	1	1	24
6	WINMIN	Minimum wavelength over all fitting windows	nm	fl	1	4	25
7	WINMAX	Maximum wavelength over all fitting windows	nm	fl	1	4	29

The measurement grid record is used in the limb fitting window application data set record.

Modified Julian Date (MJD)

Compound Size: 12 Bytes

No	Name	Comments	Unit	Type	#	Size	Offset
1	DAYS	Number of days elapsed since the date of 1.1.2000 00:00 hour	day	sl	1	4	0
2	SECONDS	Seconds elapsed since the beginning of the day	s	ul	1	4	4
3	USECS	Microseconds elapsed since the beginning of the last second	us	ul	1	4	8

State vector record (StateVec)

Compound Size: 12 Bytes

No	Name	Comments	Unit	Type	#	Size	Offset
1	VALUE	Value of the State vector entry	-	fl	1	4	0
2	ERROR	Error of the value of the state vector entry	%	fl	1	4	4
3	TYPE	Type of the value of the state vector entry (Annotation)	-	b	4	4	8

The state vector record is used in the limb fitting window application data set record.

SO_2 background record (SO2B)

Compound Size: 238 Bytes

No	Name	Comments	Unit	Type	#	Size	Offset
1	DAY	Number of days elapsed since the date of 1.1.2000 00:00 hour; this field serves as key in the SO_2 background data base	-	us	1	2	0
2	SO2B_DATA	SO_2 background data entries; each entry corresponds to a latitude bin of 5°; bins are sorted from north to south, starting with index 0 at (+90,+85), and ending with index 35 at (-85,-90).	-	SO2BD	36	180	2
3	SO2B_HIST	SO_2 background history; keeps the orbit numbers that were used to fill the SO_2 background data; at most 14 orbit numbers are possible	-	ui	14	56	182

The SO_2 background record is used in the SO_2 background data base.

SO_2 background data entry (SO2BD)

Compound Size: 5 Bytes

No	Name	Comments	Unit	Type	#	Size	Offset
1	SCV	SO_2 slant column value	-	fl	1	4	0
2	QUALITY	SO_2 background data quality; 0 means that no data is available for this latitude bin; 1 means lowest quality, 255 is best quality	-	uc	1	1	4

The SO_2 background data entry is used in the SO_2 background record.

Appendix A Reference Timeline and Mode Examples for SCIAMACHY

To size of a typical level 1b product, one can consider a reference time line representing one typical measurement scenario. The time line described in the following table is a nominal “No Moon / Sun Diffuser / Sub-solar Calibration“ orbit mission scenario. Its characteristics are as follows:

- start with limb measurements prior to sun diffuser observations
- perform sun diffuser measurement
- append optimised limb/nadir sequence after the sun diffuser state until the start of the sub-solar window
- perform sub-solar measurement
- append optimised limb/nadir sequence until start of eclipse phase
- perform nadir eclipse, dark current or other calibration measurements for the rest of the orbit

This reference orbit, as described in detail in [R3], is listed in the following table. Duration figures are given in seconds. Each state has a set-up and cleanup phase taking a certain amount of time. Therefore, the addition of execution times of the measurement phases does not correspond exactly with the absolute time in orbit.

Index	StateID	Description	Duration	End Time in Orbit
1	28	Limb, ESM & ASM scanning, swath width 960 km, 1.5 sec integration time	59	T_1+59.95
2	28	see above	59	
3	28	see above	59	
4	28	see above	59	
5	52	Sun Diffuser Calibration, ND filter out	30	
6	28	see above	59	
7	29	Limb, ESM & ASM scanning, swath width 960 km, 1.5 sec integration time (different co-adding scheme)	59	
8	29	see above	59	
9	30	Limb, ESM & ASM scanning, swath width 960 km, 1.5 (channel 1a) and 0.375 sec integration time	59	
10	1	Nadir, ESM scanning, swath width 960 km, 80 and 1 (channel 7, 8) sec integration time	80	
11	30	see above	59	
12	2	Nadir, ESM scanning, swath width 960 km, 80 (channel 1), 40 and 1 (channel 7, 8) sec integration time	80	
13	30	see above	59	
14	3	Nadir, ESM scanning, swath width 960 km, 20 (channel 1a), 5 (channel 1b, 2a) and 1 sec integration time	80	
15	31	Limb, ESM & ASM scanning, swath width 960 km, 1.5 (channel 1a) and 0.375 sec integration time (different co-adding scheme)	59	
16	4	Nadir, ESM scanning, swath width 960 km, 1 sec integration time	65	
17	32	Limb, ESM & ASM scanning, swath width 960 km, 1.5 (channel 1a) and 0.375 sec integration time (different co-adding scheme)	59	
18	4	see above	65	

19	32	see above	59	
20	5	Nadir, ESM scanning, swath width 960 km, 1 sec integration time (different co-adding scheme)	65	
21	32	see above	59	
22	6	Nadir, ESM scanning, swath width 960 km, 1 sec integration time (different co-adding scheme)	65	
23	32	see above	59	
24	6	see above	65	
25	32	see above	59	
26	6	see above	65	
27	32	see above	59	
28	7	Nadir, ESM scanning, swath width 960 km, 1 sec integration time (different co-adding scheme)	65	
29	32	see above	59	
30	7	see above	65	
31	32	see above	59	
32	7	see above	65	
33	32	see above	59	
34	58 or 60	Sub-solar Calibration	22	
35	8	Nadir, ESM scanning, swath width 960 km, 1 sec integration time (different co-adding scheme)	65	
36	32	see above	59	
37	7	see above	65	
38	32	see above	59	
39	7	see above	65	
40	32	see above	59	
41	7	see above	65	
42	32	see above	59	
43	6	see above	65	
44	33	Limb, ESM & ASM scanning, swath width 960 km, 1.5 sec integration time	59	
45	6	see above	65	
46	34	Limb, ESM & ASM scanning, swath width 960 km, 1.5 (channel 1a) and 0.375 sec integration time (different co-adding scheme)	59	
47	6	see above	65	
48	34	see above	59	
49	5	see above	65	
50	35	Limb, ESM & ASM scanning, swath width 120 km, 1.5 (channel 1a) and 0.375 sec integration time (different co-adding scheme)	59	
51	4	see above	65	
52	36	Limb, ESM & ASM scanning, swath width 120 km, 1.5 (channel 1a) and 0.375 sec integration time (different co-adding scheme)	59	
53	4	see above	65	
54	3	see above	80	
55	3	see above	80	

56	2	see above	80	
57	2	see above	80	
58	1	see above	80	T_1+3905.6
59 ff.	26			
	63			T_1+6036.0

Appendix B Example of an Initialization File

The following listing is an example for the proposed XML content of the initialization file[1]:

```
<scia_configuration>

<operation>

 <file_version>$Revision: 1.8 $</file_version>

 <output_control
  debug_write="true"
  scenario_write="true"
  results_write="true"
  breakpoints_write="false"
  keep_log="true"
  severity_level="info"
  debug_level="3">
 </output_control>

 <sza_cutoff>
  89.0
 </sza_cutoff>

 <extended_field_of_view calculate="true">
  Parabolic
 </extended_field_of_view>

 <optical_thickness>
  20.0
 </optical_thickness>

</operation>

<doas>
 <doas_control
  error_weighting_of_fitting="false"
  unweighted_sigma="0.001"
  filter_cross_sections="false"
  use_ratioed_measurement_data="false"
  exclusion_of_solar_spectrum="true"
  atmosphere_height="100.0">
 </doas_control>

 <atmospheric_profiles>
  <haloe_profile_set>SunSet</haloe_profile_set>
  <hydrostatic_profile>IFE_BL</hydrostatic_profile>
  <overwrite_T_profile>-</overwrite_T_profile>
  <overwrite_P_profile>-</overwrite_P_profile>
  <overwrite_Z_profile>-</overwrite_Z_profile>
  <use_TOMS_doubling>false</use_TOMS_doubling>
  <load_TOMS_profile_from_prev_pixel>false</load_TOMS_profile_from_prev_pixel>
  <initial_TOMS_column>250.0</initial_TOMS_column>
  <concentrations num_of_molecules="7">
```

1. Please note: This is a shortened version of the file used for SCIA_12OL version 5.00 All parameters are still subject to change.

```
    <molecule name="BRO" source="MPI"> </molecule>
    <molecule name="NO2" source="HALOE"> </molecule>
    <molecule name="H2O" source="USA"> </molecule>
    <molecule name="SO2" source="USA"> </molecule>
    <molecule name="HCHO" source="USA"> </molecule>
    <molecule name="O3" source="KNMI"> </molecule>
    <molecule name="OCLO" source="MPI"> </molecule>
  </concentrations>
</atmospheric_profiles>

<aerosol_climatology>
  <aerosol_scheme>LOWTRAN</aerosol_scheme>
  <phase_moments_function>HG</phase_moments_function>
  <legendre_members>40</legendre_members>
  <profile>
    <st_regime>Bkgd</st_regime>
    <ms_regime>Normal</ms_regime>
  </profile>
  <lowtran_parameters>
    <bl_ext_regime_land>Rural</bl_ext_regime_land>
    <bl_ext_regime_sea>Maritim</bl_ext_regime_sea>
    <tr_ext_regime>Normal</tr_ext_regime>
    <st_ext_regime>Bkgd</st_ext_regime>
    <ms_ext_regime>Meteoric</ms_ext_regime>
  </lowtran_parameters>
  <wmo_parameters number_of_layers="2">
    <layer name="Maritime polluted" boundary_height="1.5"
     humidity="80.0" number_of_mix_aerosols="4" >
     <mix_aerosol aerosol_id="1" weight="0.422">
     </mix_aerosol>
     <mix_aerosol aerosol_id="2" weight="0.002">
     </mix_aerosol>
     <mix_aerosol aerosol_id="3" weight="0.356E-6">
     </mix_aerosol>
     <mix_aerosol aerosol_id="6" weight="0.576">
     </mix_aerosol>
    </layer>
    <layer name="troposphere volcanic" boundary_height="5.0"
     humidity="50.0" number_of_mix_aerosols="3" >
     <mix_aerosol aerosol_id="1" weight="0.1">
     </mix_aerosol>
     <mix_aerosol aerosol_id="5" weight="0.1">
     </mix_aerosol>
     <mix_aerosol aerosol_id="11" weight="0.8">
     </mix_aerosol>
    </layer>
  </wmo_parameters>
</aerosol_climatology>

<surface
  do_tesselation="true"
  type="LERTOMSAdjusted"
  pressure_source="USA_fix">
</surface>

<lidort
  co2_ppmv_mixing_ratio="360.0"
```

```
 lidort_option="3"
 discrete_ordinates="4"
 do_aerosol="false"
 use_internal_aerosol="true">
</lidort>

<spectra
 use_always_wavelength_grid_of_sun_spectrum="true"
 use_doppler_shift="false"
 doppler_shift="0.0"
 fit_solar_spectrum="true"
 xcorr_convergence="0.0010">
</spectra>

<slit_function
 wing_extension="5.0">
</slit_function>

<window_parameters overlay_size="0" number_of_windows="4">

 <window number_of_species="5" vcd_algorithm="Iterative"
  initial_O3_column="250.0"
  initial_vcd_from_previous_pixel="false"
  mds_name="NAD_UV0_O3" amf_ref_wavelength = "325.5">
  <!-- vcd_algorithm = “Standard” for all other gases -->

  <calibration>
   <radiometric> true </radiometric>
   <ppg> true </ppg>
   <polarisation> true </polarisation>
   <memory_effect> true </memory_effect>
   <leakage>  true </leakage>
   <straylight> true </straylight>
   <radiometric_pmd> true </radiometric_pmd>
   <calculate_errors> true </calculate_errors>
   <etalon> false </etalon>
   <m_factors> true </m_factors>
  </calibration>

  <gases>
   <doas_gases number="1">
    <doas_gas name="O3"
     amf="Lidort"
     ds_name="SCIA_FM_O3_243K_BIRA_S0020"
     path="/home/aristo01/scia/psm/reference_data/SCI_UX2_AX.inp"
     iteration="5"
     convergence="0.001"
     profile_source="KNMI">
    </doas_gas>
   </doas_gases>
 </gases>

 <doas_wavelength_boundaries number = "1">
  <window_boundary start="325.0" end="335.0">
  </window_boundary>
 </doas_wavelength_boundaries>
```

```
  <fitting
   number_of_fitted_spectra="5"
   degree_of_additive_polynomial="4"
   degree_of_multiplicative_polynomial="0"
   do_iterated_slant_columns="false"
   max_number_of_iterations="10"
   convergence="0.001">
   DOAS_40
   <scaling> 1.0 </scaling>
  </fitting>

  <smoothing enable="false" index="2">
   2.50
  </smoothing>

  <species ds_name="SOL"
   x_corr_ref="SOL_KITT_PEAK_CONV_CH2"
   path="/home/aristo01/scia/psm/reference_data//SCI_UX2_AX.inp"
   molecule="SOL">
   <temperatures number="1"> 0.0 </temperatures>
   <smoothing enable="false" index="2"> 2.50 </smoothing>
   <convolution flag="false" to_measurement="false"> </convolution>
   <scaling> 1.00e+00 </scaling>
   <shift  max="0.110" min="-0.110" fixed="0.0"> false </shift>
   <squeeze max="1.0" min="1.0" fixed="1.000"> false </squeeze>
  </species>

  <!-- data for 4 more species left out in order to save space -->

 </window>

 <!-- data for 3 more windows left out in this example -->

</window_parameters>

</doas>

<cloud
 cloud_fraction_source="OCRA"
 cloudtop_pressure_source="CloudTopHeight"
 cloudtop_height_source="Sacura"
 cloudtop_albedo_source="Sacura" >
 <ocra_pmd_offsets number="3">
  25.0 25.0 25.0
 </ocra_pmd_offsets>
 <ocra_pmd_scaling number="3">
  0.001 0.00066 0.00067
 </ocra_pmd_scaling>
 <sacura number_of_species="3">
  <window_boundary start="758.20" end="772.60">
  </window_boundary>
  <species ds_name="FM_SCIA_CS_O3"
   path="/home/aristo01/scia/psm/reference_data/SCI_FM2_AX.inp"
   molecule="O3">
  </species>
  <species ds_name="FM_SCIA_CS_NO2"
   path="/home/aristo01/scia/psm/reference_data/SCI_FM2_AX.inp"
```

```
    molecule="NO2">
   </species>
   <species ds_name="ESFT_O2"
    path="/home/aristo01/scia/psm/reference_data/SCI_ES2_AX.inp"
    molecule="O2">
   </species>
   <control iteration="10"
    convergence="0.005"
    lower_reflectance="0.2"
    cloudtop_height_convergence="0.2">
    <geometrical_thickness min="0.8" max="10.0">
    </geometrical_thickness>
    <cloudtop_height_constrains min="1.1" max="17.0">
    </cloudtop_height_constrains>
   </control>
  </sacura>
</cloud>

<aaia>
 <reference_wavelength band_pass="1.0">
  340.0
 </reference_wavelength>
 <ratio_wavelengths number_of_values="1">
  <ratio_wl band_pass="1.0">380.0</ratio_wl>
 </ratio_wavelengths>
 <smoothing enable="false" index="2">
  2.0
 </smoothing>
</aaia>

<bias>

 <application_parameters number="1">

  <bias_application mds_name="NAD_IR3_CO">

   <fit_control>
    <separable> false </separable>
    <error_weight> false </error_weight>
    <max_iter> 10 </max_iter>
    <x_convergence> 1.0e-02 </x_convergence>
    <y_convergence> 1.0e-02 </y_convergence>
    <wing_pixel_ext> 2.0 </wing_pixel_ext>
    <max_function_calls> 200 </max_function_calls>
   </fit_control>

   <window_boundary start="2324.4" end="2335.0">
   </window_boundary>

   <trace_gas_cols number="3">
    <trace_gas_col  line_file="/home/aristo01/scia/psm/reference_data/IR/hitran/lines.NIR" init="1.0">
     co
    </trace_gas_col>
    <trace_gas_col  line_file="/home/aristo01/scia/psm/reference_data/IR/hitran/lines.NIR" init="1.0">
     ch4
    </trace_gas_col>
    <trace_gas_col  line_file="/home/aristo01/scia/psm/reference_data/IR/hitran/01_hit06.par" init="1.0">
```

```
        h2o
      </trace_gas_col>
    </trace_gas_cols>
<!--
                possible additional fit parameters (polynomial) are:
                - reflection (albedo), max. degree 3
                - baseline, max. degree 3
                - Gauss, Hyperbolic, Lorentz (i.e. type of HWHM), only degree 1
                as many init values should be supplied as the degree requires,
                though missing values are set to 0 and excess values are ignored
-->
    <fit_pars number="2">
      <fit_par degree="1" init="0.1 0 0"> reflection </fit_par>
      <fit_par degree="1" init="0.2"> Gauss </fit_par>
    </fit_pars>
<!--
                defines the profiles to be read from file, possible:
                - pressure
                - temperature
                - density
                will be completed with trace gases automatically
                the required profiles must be available in the file
-->
    <atmosphere number="2" file="/home/aristo01/scia/psm/reference_data/IR/bias.nml">
      <id> pressure </id>
      <id> temperature </id>
    </atmosphere>
<!--
                additional data bases needed;
                an empty path string is equivalent to a missing entry
-->
    <data_bases number="3">
      <db id="molecules" path="/home/aristo01/scia/psm/reference_data/IR/molecules"> </db>
      <db id="continuum" path="/home/aristo01/scia/psm/reference_data/IR/ckd"> </db>
      <db id="surface_spectrum" path=""> </db>
    </data_bases>

   </bias_application>

  </application_parameters>

</bias>

<limb num_of_limb_applications="2">

<limb_application mds_name="LIM_UV0_O3">

  <high_level_control
    do_VMR_retrieval="true"
    do_PT_retrieval="false"
    do_convolution="false"
    do_infra_red_apps="false"
    do_scia_fm_x_sections="true"
    use_prev_l2_values="false"
    use_prev_pth="false"
    use_scan_ratio="true"
    max_num_of_limb_cols="4">
```

```
</high_level_control>

<debug_control
 do_scenario_debug="false"
 do_buffering_debug="false"
 do_geometry_debug="false"
 do_forward_model_debug="false"
 do_retrieval_l1_debug="false"
 do_retrieval_l2_debug="false"
 do_history_residual_debug="false"
 do_history_iterates_debug="false"
 do_history_lambda_debug= "false"
 do_initial_spectra_debug="false"
 do_spectra_debug="false">
</debug_control>

<retrieval_control
 fitting_method="4"
 max_num_of_iterations="20"
 num_of_height_regimes="1">
 <height_regime
  lower_height="0.000"
  upper_height="100.000"
  num_of_windows="1">
  520.000 590.000
 </height_regime>
 <retrieval_fine_control
  do_albedo_retrieval="false"
  use_multiple_albedo="false"
  do_ring_retrieval="false"
  do_pols_retrieval="false"
  do_amplification_retrieval="true"
  do_lin_amplif_retrieval="false"
  do_spectral_offset_retrieval="false"
  do_pointing_retrieval="false">
 </retrieval_fine_control>
</retrieval_control>

<least_squares
 Alamda_start_value="0.0"
 finite_difference_factor="0"
 finite_differencing="0"
 slatec_ftol_value="0.0"
 slatec_gtol_value="0.0"
 slatec_mode_value="0"
 slatec_print_value="0"
 slatec_xtol_value="0.0">
</least_squares>

<optimal_estimation_control
 do_cost_function="true"
 do_param_convergence="true">
 <apriori_fudge_factor>0.000001</apriori_fudge_factor>
 <cost_criterion>     0.001   </cost_criterion>
 <param_criterion>    0.0001  </param_criterion>
</optimal_estimation_control>
```

```
 <state_vector_control
  num_of_aux_gases ="1"
  num_of_main_gases="2">
  <names_of_main_gases> O3 NO2 </names_of_main_gases>
  <include_zero_order> false </include_zero_order>
  <include_first_order> false </include_first_order>
  <include_pol_sens> false </include_pol_sens>
  <pol_sens_scale_factor> 5.0000000000000003E-02 </pol_sens_scale_factor>
  <max_pol_sens_scale_factor> 0.2 </max_pol_sens_scale_factor>
  <include_ring> false </include_ring>
  <ring_scale_factor> 0.1 </ring_scale_factor>
  <max_ring_scale_factor> 0.3 </max_ring_scale_factor>
  <albedo_error> 1.0 </albedo_error>
  <auxiliary_levels> 1.0 </auxiliary_levels>
  <auxiliary_scale_factors> 1.0 </auxiliary_scale_factors>
  <effective_albedo> 0.3000000000000000 </effective_albedo>
  <first_order_error> 0.1000000000000000 </first_order_error>
  <first_order_value> 1.0000000000000000E-03 </first_order_value>
  <main_diagonal_levels> 1.0 0.2 </main_diagonal_levels>
  <main_off_diagonal_levels> 0.25 0.25 3.2E-02 2.0E-03 </main_off_diagonal_levels>
  <pol_sens_error> 1.00 </pol_sens_error>
  <pol_sens_value> 1.00 </pol_sens_value>
  <ring_error> 1.00 </ring_error>
  <ring_value> 1.00 </ring_value>
  <zero_order_error> 0.10 </zero_order_error>
  <zero_order_value> 1.00 </zero_order_value>
  <pointing_error> 1.00 </pointing_error>
  <maingas_apriori_error_diag> 1.0 0.2 </maingas_apriori_error_diag>
  <closure_amplification> 1.0 </closure_amplification>
  <closure_offset> 0.01 </closure_offset>
  <tangent_height> 0.005 </tangent_height>
  <delta_height> 0.05 </delta_height>
  <scale_state_vector> true </scale_state_vector>
  <use_x_apriori> true </use_x_apriori>
  <do_effective_troposhere> false </do_effective_troposhere>
 </state_vector_control>

 <forward_model_control
  aerosol_ref_wavelength="330.0"
  num_of_limb_los="0"
  num_of_solar_pos="0"
  use_henyey_greenstein="true"
  use_doa_approach="true"
  ndegree="5"
  include_polarisation="false"
  include_ring="false"
  include_amplification="true"
  include_linear_amplif="false"
  include_spectral_offset="false">

  <disort_control
   compute_correction_factors="true"
   mrank_value="12"
   num_mrank_iterations="7"
   n_do="8"
   n_theta="91"
   do_convergence_test="false"
```

```
    convergence_epsilon="1.0E-03"
    do_fine_grid="true"
    number_theta_groups="4"
    number_wavelength_intervals="1">
    <number_points_per_interval> 36 </number_points_per_interval>
    <lower_bound_wavelength_interval> 5.20E+02  </lower_bound_wavelength_interval>
    <upper_bound_wavelength_interval> 5.90E+02  </upper_bound_wavelength_interval>
  </disort_control>

</forward_model_control>

<layering_control
  use_height_grid="false"
  num_of_grid_levels="33">
  <finelayer_divisions>
    <--! 33 entries left out in order to save space -->
  </finelayer_divisions>
  <height_grid_levels>
    <--! 33 entries left out in order to save space -->
  </height_grid_levels>
  <pressure_grid_levels>
    <--! 33 entries left out in order to save space -->
  </pressure_grid_levels>
</layering_control>

<IRGN_control
  irgn_ftol_rel="0.01"
  irgn_ftol_abs="0.01"
  irgn_ztol_value="0.0005"
  irgn_gtol_value="1.e-5">
  <bounds_control>
    <bounds_maingas_profile>
      <--! 32 lines with 4 entries each left out in order to save space -->
    </bounds_maingas_profile>
    <bounds_maingas_column>
      -0.1  0.1
    </bounds_maingas_column>
    <bounds_auxgas_scale>
      -0.3  0.3
    </bounds_auxgas_scale>
    <bounds_pointing>
      -3.00    3.00
    </bounds_pointing>
  </bounds_control>

  <diagnostic_control
    compute_picard="false"
    compute_L_curve="false"
    compute_GCV_curve="false"
    compute_error_curve="false"
    compute_upre_curve="false"
    do_nonlinear_L_curve="false"
    do_statistics="true">
  </diagnostic_control>

  <init_guess_control
    do_init_guess_improvement="false"
```

```
    init_guess_source="0">
    <bounds_init_guess_discrete_search> 0.3 </bounds_init_guess_discrete_search>
    <max_niter_discrete_search> 9 </max_niter_discrete_search>
    <max_niter_evolution> 10 </max_niter_evolution>
  </init_guess_control>

  <param_weight_control
    do_automatic_pointing_weights="false" >
    <weight_maingas> 1.0 0.99 </weight_maingas>
    <weight_auxgas> 0.3 </weight_auxgas>
    <weight_pressure> 0.0 </weight_pressure>
    <weight_albedo> 1.0000000000000000E-04 </weight_albedo>
    <weight_ring> 1.0000000000000000E-04 </weight_ring>
    <weight_pols> 1.0000000000000000E-04 </weight_pols>
    <weight_closure> 2.0000000000000000E-02 </weight_closure>
    <weight_pointing> 1.E-8 </weight_pointing>
  </param_weight_control>

  <regularization_control>
    <regularization_method>TRIRGN</regularization_method>
    <lambda_LVMR> 10.0 </lambda_LVMR>
    <lambda_selection_criterion>OEM</lambda_selection_criterion>
    <noise_level> 0.2 </noise_level>
    <relative_radius> 5.0000000000000003E-02 </relative_radius>
    <VMR_regularization_type> COVMATEXP COVMATEXP </VMR_regularization_type>
    <VMR_correlation_length> 3.3 3.3 </VMR_correlation_length>
    <use_apriori_noisevariance> true </use_apriori_noisevariance>
    <noise_variance> 1.0000000000000000E-02 </noise_variance>
    <do_scale_regularization_matrices> false </do_scale_regularization_matrices>
  </regularization_control>
</IRGN_control>

<scan_control>
  <highest_tang_height> 46.0 </highest_tang_height>
  <lowest_tang_height> 13.5 </lowest_tang_height>
  <ratio_height> 46.0 </ratio_height>
</scan_control>

<buffering_control
  do_lbl_schreier="true"
  do_pixelwise_division="true"
  do_pt_derivatives="false"
  slit_function_tail="5.0"
  wavelength_overlap="1.0"
  wavelength_spacing="0.01"
  wavenumber_spacing="0.01">
</buffering_control>

<vmr_auxiliary_input_control>
  <surface_pressure> 1012.0 </surface_pressure>
  <surface_topo_height> 0.0000 </surface_topo_height>
  <surface_mask> false </surface_mask>
    <prev_retr_mains num_of_prev_retr_mains="2">
      f f
    </prev_retr_mains>
    <prev_retr_prof_elems num_of_prev_retr_prof_elems="2">
      0.0
```

```
      0.0
    </prev_retr_prof_elems>
  </vmr_auxiliary_input_control>

</limb_application>

<!-- second limb aplication left out in order to save space -->

</limb>

<limb_clouds
  num_of_cols="3"
  num_of_geoloc_heights="13"
  num_of_types="4">

  <limb_cloud_type
    type_name="WCL"
    lower_bound_cir="1.4"
    upper_bound_cir="2.2"
    min_th="0"
    max_th="30"
    warn_th="18"
    num_of_wlw="2">
    <wl_window start="750" end="751"></wl_window>
    <wl_window start="1088" end="1092"></wl_window>
  </limb_cloud_type>

  <limb_cloud_type
    type_name="ICL"
    lower_bound_cir="1.25"
    min_th="0"
    max_th="30"
    warn_th="18"
    num_of_wlw="2">
    <wl_window start="1550" end="1553.2"></wl_window>
    <wl_window start="1630" end="1634"></wl_window>
  </limb_cloud_type>

  <limb_cloud_type
    type_name="PSC"
    lower_bound_cir="1.3"
    min_abs_lat="50"
    min_th="15"
    max_th="30"
    num_of_wlw="2">
    <wl_window start="750" end="751"></wl_window>
    <wl_window start="1088" end="1092"></wl_window>
  </limb_cloud_type>

</limb_clouds>

<data_bases number="8">
  <db id="profile"
     path="/home/aristo01/scia/psm/reference_data/SCI_PR2_AX.inp">
  </db>

  <db id="cloud"
```

```
    path="/home/aristo01/scia/psm/reference_data/SCI_CL2_AX.inp">
  </db>

  <db id="CCA"
    path="/home/aristo01/scia/psm/reference_data/SCI_CC2_AX.inp">
  </db>

  <db id="surface"
    path="/home/aristo01/scia/psm/reference_data/SCI_SF2_AX.inp">
  </db>

  <db id="Rayleigh"
    path="/home/aristo01/scia/psm/reference_data/SCI_RC2_AX.inp">
  </db>

  <db id="AMF"
    path="/home/aristo01/scia/psm/reference_data/SCI_MF2_AX.inp">
  </db>

  <db id="TOPO"
    path="/home/aristo01/scia/ax_files/GTOP_data">
  </db>

  <db id="SO2_BACKGROUND"
    path="/home/aristo01/scia/psm/reference_data/SCI_SO2_AX.dat">
  </db>

</data_bases>

</scia_configuration>
```