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01	01	21/02/2013	Started “Acronyms and abbreviations” section; Added new definitions in Section 2; Table 2.1 updated; Added clarification that certain data types are not to be delivered (Level 3 and Merged Level 3 data sections)	New revision for KO+12 Workshop
01	02	04/03/2013	“Acronyms and abbreviations” section completed; Removed “Historical” sub-sections in	

			Level 2 data section; Added NetCDF specification tables for temperature climatologies in Level 3 data section	
01	03	19/03/2013	Level 2 data section for OSIRIS aerosol updated (e.g. text converted to tables)	Revisions from UA team (addressing reviewer requests)
01	04	19/03/2013	Correction to Table 2.1	Revisions from CT team
01	05	20/03/2013	Added Executive Summary	
01	06	20/03/2013	Level 2 data section for GOMOS ozone updated (complete rewrite and addition of format tables)	Revisions from FMI team (addressing reviewer requests)
01	07	20/03/2013	Level 2 and Level 3 data sections for SCIAMACHY aerosol and water vapour updated; Level 2 data descriptions moved to subsections for products that require more effort to mature	Revisions from UB team
01	08	21/03/2013	Level 2 and Level 3 data sections for SCIAMACHY aerosol and water vapour updated (text converted to tables)	Revisions from UB team (addressing reviewer requests)
01	09	25/03/2013		Delivered to ESA for KO+12 delayed deadline
02	01	5/03/2014	All sections updated	Final version for ESA review

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Executive summary

This document is the Product Specification Document (Version 1), which is a deliverable of the ESA project SPIN. SPIN delivers matured level 2 data, new level 3 climatologies and merged level 3 datasets from a mixture of satellites over a range of quantities. This document provides detailed specifications of these various datasets. Datasets have been produced from the following ESA and ESA-TPM instruments: ACE-FTS, GOMOS, MIPAS, OSIRIS, SCIAMACHY and SMR. The datasets include the following quantities: ozone, aerosol, water vapour, short-lived species and temperature.

Applicable and reference documents

- [AD-1] Statement of Work (SoW), ESA SPARC Initiative, Support To Science Element, EOEP-STSE-EOPS-SW-011-0003, Final Issue, March 2011.
- [AD-2] SPIN User Requirements Document (URD) for the Essential Climate Variables (ECVs) Temperature and Water Vapour Issue 01, Revision 02, Final Issue, 22 October 2012.

Acronyms and abbreviations

ACE	Atmospheric Chemistry Experiment
ASCII	American Standard Code for Information Interchange
CHAMP	CHALLENGING Minisatellite Payload
ECMWF	European Centre for Medium-Range Weather Forecasts
EOS	Earth Observing System
ERA	ECMWF Re-Analysis
ESA	European Space Agency
ESA-TPM	ESA Third Party Mission
FTS	Fourier Transform Spectrometer
GOMOS	Global Ozone Monitoring by Occultation of Stars
GRACE	Gravity Recovery and Climate Experiment
HDF	Hierarchical Data Format
IUP	Institut für Umweltphysik
LST	Local Solar Time
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MSIS	Mass Spectrometer Incoherent Scatter
NetCDF	Network Common Data Form
OSIRIS	Optical Spectrograph and Infra-Red Imager System
ppV	part per Volume (unit for volume mixing ratio, that is the ratio of the number of molecules of a substance in a given volume to the number of molecules of all constituents of air in that volume)
PSC	Polar Stratospheric Cloud
PSD	Product Specification Document
SCIAMACHY	SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY
SMR	Sub-Millimetre Radiometer
SPARC	Stratospheric Processes and their Role in Climate
SPARC-DI	SPARC Data Initiative
SPIN	SPARC INitiative
SSU	Stratospheric Sounding Unit
TAI	International Atomic Time
TSX	TerraSAR-X
URD	User Requirement Document
UTC	Universal Time Coordinated

1. Introduction

This is the Product Specification Document (PSD) for the ESA SPIN project. The PSD incorporates the user requirements as described in the SPIN User Requirements Document (URD) (AD-2).

2. SPIN data products

This section presents an overview of the different data products that have been generated in the project. Detailed specifications are given in the next section. SPIN delivers level 2 and level 3 data from multiple ESA and ESA-TPM instruments, including ACE-FTS, GOMOS, MIPAS, OSIRIS, SCIAMACHY and SMR. *Level 2* data include geolocated profiles along the platform orbit, *Level 3* data include regridded data products (e.g. on a regular latitude-longitude grid) and usually involves averaging of profiles, and *merged Level 3* data is the same as Level 3 data, but involves a combination of two or several datasets from different sensors. Table 2.1 gives an overview of the species and instruments considered in SPIN, and their different data types.

Table 2.1 Data types delivered in SPIN.

Measured quantity	Instrument	Level 2	Level 3 (monthly means)	Merged Level 3 (monthly means)
Ozone	GOMOS	Yes ⁶⁾	Yes ²⁾	Yes ^{3,2)} (GOMOS, SAGE-II)
Aerosol	OSIRIS	Yes ⁷⁾	No	No
	SCIAMACHY	Yes ³⁾	Yes ³⁾	No
Water vapour	SCIAMACHY	Yes ³⁾	Yes ³⁾	No
Short-lived species ⁵⁾	SMR	No	Yes ²⁾	No
	OSIRIS	No	Yes ²⁾	No
Temperature	ACE-FTS	No	Yes ²⁾	No
	GOMOS	No	Yes ^{2,4)}	No
	MIPAS	No	Yes ²⁾	Yes ¹⁾ (merged with SSU)
	SMR	No	Yes ²⁾	No

1) Format not yet specified

2) SPARC-DI NetCDF format

3) NetCDF format

- 4) As of March 2013 this dataset has not yet been produced
- 5) Short-lived species climatologies created for SPARC-DI are not included in this list
- 6) HDF-5 format
- 7) HDF-EOS5 format

Following the ESA Statement of Work, the SPIN project concentrates on the maturation of relevant ESA and ESA-TPM data products to make them of “climate quality”. The use of these matured data to generate new CDRs for stratospheric temperature and ozone (which are the most mature data sets), and laying the groundwork for the generation of new CDRs for stratospheric water vapour and aerosol (which are less mature and emerging global data sets).

3. Specifications of the SPIN data products

This section provides details on the various data products provided in the project.

3.1. Level 2 data product specifications

3.1.1. Ozone

Ozone products are provided from GOMOS.

3.1.1.1. Mature ESA products

3.1.1.1.1. GOMOS

This section covers the GOMOS bright limb (GBL) level 2 data files. The processing of the GOMOS bright limb ozone data was done within work package WP17. A detailed explanation of the retrieval method and the product quality can be found elsewhere (see ATBD, data analysis report and product validation report).

The GOMOS bright limb profiles are provided as HDF5-files (one file for each scan). The file includes retrieved profiles and error estimates, geolocation information, a-priori information, residuals of the fit and some auxiliary information. The GOMOS bright limb dataset consists of about 323000 files and the size of a single file is about 60-70 kB. Thus, the size of the whole dataset is about 20 GB. The current version of the GBL data is 1.1.

The GOMOS bright limb level 2 filename convention is following the GOMOS level 1 naming. The GBL filenames are of form:

GOM_GBL_<file_identifier>.h5

where <file_identifier> is directly taken from the corresponding level 1 file.

The structure of the GBL file is shown in figure 3.1.1.1.1 and more detailed description of the fields is provided in tables 3.1.1.1.1-5. The dimension N is the number of measurements (tangent heights) in each scan.

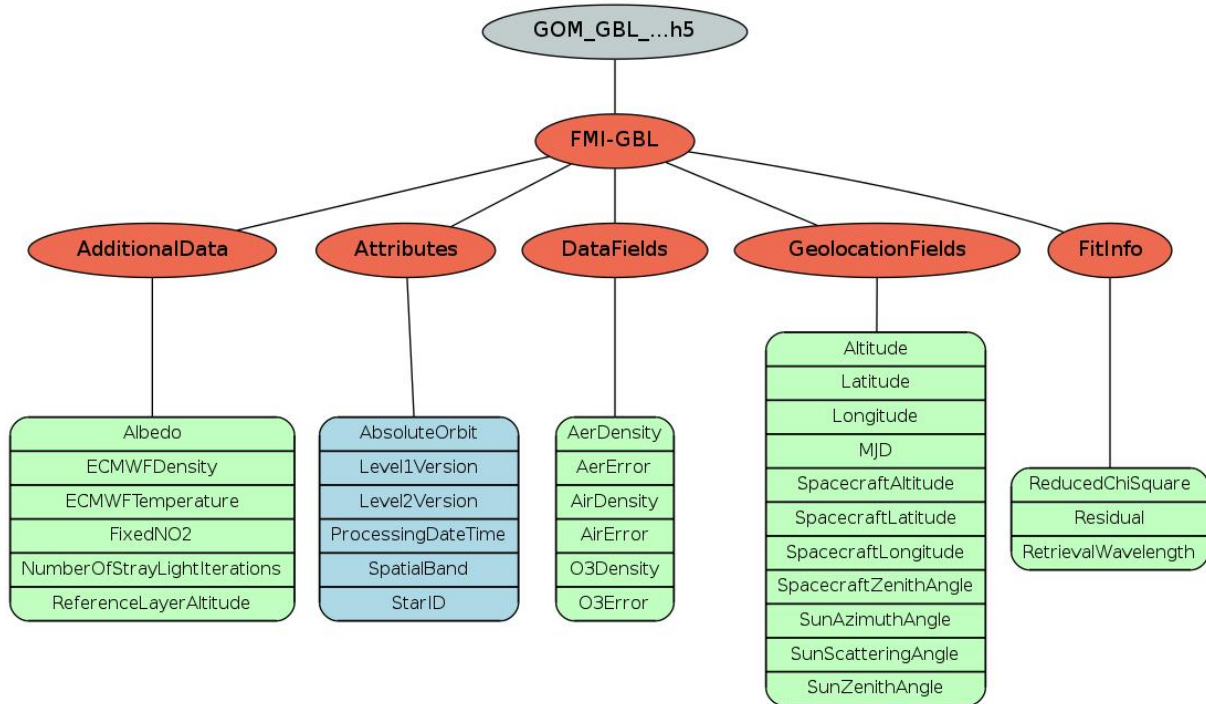


Figure 3.1.1.1.1: Structure of the GBL product file. Colours indicate groups (red), attributes (blue) and data fields (green).

Table 3.1.1.1.1.1: GOMOS GBL "AdditionalData" group.

Name	Type	Dimension	Notes
Albedo	H5T_IEEE_F64LE	1	From a climatology
ECMWFDensity	H5T_IEEE_F64LE	N	
ECMWFTemperature	H5T_IEEE_F64LE	N	
FixedNO2	H5T_IEEE_F64LE	N	From a climatology
NumberOfStrayLightIterations	H5T_STD_I32LE	1	
ReferenceLayerAltitude	H5T_IEEE_F64LE	1	

Table 3.1.1.1.1.2: GOMOS GBL "Attributes" group.

Name	Type	Dimension	Notes
AbsoluteOrbit	H5T_STD_I32LE	1	
Level1Version	H5T_STRING	1	"GOMOS/6.01" or so
Level2Version	H5T_STRING	1	"FMI-GBL/1.1" or so
ProcessingDateTime	H5T_STRING	1	"yyyymmddhhmm"
SpatialBand	H5T_STRING	1	"upper" or "lower"
StarID	H5T_STD_I32LE	1	

Table 3.1.1.1.1.3: GOMOS GBL "DataFields" group.

Name	Type	Dimension	Notes
AerDensity	H5T_IEEE_F64LE	N	
AerError	H5T_IEEE_F64LE	N	
AirDensity	H5T_IEEE_F64LE	N	
AirError	H5T_IEEE_F64LE	N	
O3Density	H5T_IEEE_F64LE	N	
O3Error	H5T_IEEE_F64LE	N	

Table 3.1.1.1.1.4: GOMOS GBL “FitInfo” group.

Name	Type	Dimension	Notes
ReducedChiSquare	H5T_IEEE_F64LE	N	
Residual	H5T_IEEE_F32LE	326 * N	
RetrievalWavelength	H5T_IEEE_F64LE	326	

Table 3.1.1.1.1.5: GOMOS GBL “GeolocationFields” group.

Name	Type	Dimension	Notes
Altitude	H5T_IEEE_F64LE	N	20..60 km
Latitude	H5T_IEEE_F64LE	N	
Longitude	H5T_IEEE_F64LE	N	0..360
MJD	H5T_IEEE_F64LE	N	Modified Julian Date
SpacecraftAltitude	H5T_IEEE_F64LE	N	
SpacecraftLatitude	H5T_IEEE_F64LE	N	
SpacecraftLongitude	H5T_IEEE_F64LE	N	
SpacecraftZenithAngle	H5T_IEEE_F64LE	N	
SunAzimuthAngle	H5T_IEEE_F64LE	N	
SunScatteringAngle	H5T_IEEE_F64LE	N	
SunZenithAngle	H5T_IEEE_F64LE	N	0..90

3.1.1.2. ESA products that require more effort to mature

There are no Level 2 ozone datasets that require more effort to mature.

3.1.2. Aerosol

Aerosol products are provided from OSIRIS and SCIAMACHY.

3.1.2.1. Mature ESA products including those from third party missions

3.1.2.1.1. OSIRIS

The maturation of the OSIRIS aerosol product is contained within Work Package 12 and broadly entails the creation of an improved aerosol extinction retrieval algorithm that incorporates a retrieval of particle size information. The current aerosol product is Version 5.07; this work results in the creation of Version 6.00 of the entire OSIRIS aerosol data product. The product will be released in the existing HDF-EOS5 format, which is currently used for release of Version 5.07 through the ESA Third Party mission distribution system. Full documentation of these formats can be found in <http://odin-osiris.usask.ca>; however, relevant information and any required modifications are detailed below.

Retrieved height profiles have a one-to-one correspondence with the satellite radiance scan measurements. Not all scans can be processed by the algorithm, for example most will reject scans where the solar zenith angle is greater than 90°. The height profiles that are successfully generated are calculated on fixed height scales suitable for storage in an HDF-EOS5 swath format. A single time and geographic location is assigned to each profile that refers to the instant when the spacecraft was staring at the 20 km reference altitude during the scan. Timing within OSIRIS data products are based upon UTC (Coordinated Universal Time), rather than TAI. This does not affect the geographic location of the measurement.

All of the height profiles for aerosol extinction, which are specified on an identical altitude grid, are grouped together according to their date of observation and written to a single HDF-EOS5, daily, data product file. OSIRIS aeronomy observations occasionally stop shortly after midnight (UTC) and results in a daily data product with only one or two height profiles for that day. Conceptually, each daily data product file contains a two-dimensional array stored as a HDF-EOS5 swath where the X axis is scan number, or time, and the Y axis is altitude. Missing values are inserted into the array elements where inversion values are not available. We also store the atmospheric state and radiative transfer inputs used in the inversion so users can replicate the conditions used in the inversion algorithm.

The OSIRIS Level 2, Daily, Data Products are distributed using HDF-EOS5. This is a file format that has been commonly adopted by the Earth sciences community, is available on most operating systems and has considerable resources on the web for the end user. Details and downloads of HDF-EOS5 can be found at <http://hdfeos.net>.

Table 3.1.2.1.1.1. Details of the file format.

Swath Name	OSIRIS-Odin Aerosol MART
Instrument ID	OSIRIS-Odin
Data Type	L2-Aerosol-Limb-MART
Version	6.00

Along with all relevant geolocation and satellite parameters, the aerosol product is specified with the following parameters in the HDF-EOS swaths:

Table 3.1.2.1.1.2. Details of Aerosol Swath Geolocation Fields.

Aerosol Swath Fields	Description
AerosolExtinction	Height profiles of Aerosol extinction coefficient per kilometer at 750 nm on the given Altitude grid. The profiles are bounded at upper and lower altitudes by "Missing Value". Units of extinction per kilometer.
AerosolAngstrom	The height profile of the retrieved Angstrom exponent on the given Altitude grid. The profiles are bounded at upper and lower altitudes by "Missing Value". Dimensionless quantity.
RTMAlbedo	The ground albedo value used in the radiative transfer code. The ground albedo is assumed to have no wavelength dependence. No units.
RTModel AirDensity	The atmospheric air density profile used in the radiative transfer model. The RTModel AirDensity is derived from interpolation of an ECMWF T106 data product. The ECMWF analysis has been extended to the (virtual) ground when required using logarithmic extrapolation. The upper end of the profile, typically above approx. 60 km, has been extended using a simple MSIS model which is scaled to join the ECWMF model at its highest pressure level. Units of Molecules/cm ³ .
RTModel Temperature	The atmospheric temperature profile used in the radiative transfer model in the inversion algorithms. The profile is derived from linear interpolation of an ECMWF T106 data product. The ECMWF analysis has been extended to the (virtual) ground when required

	using linear extrapolation and extended above the top of ECMWF using MSIS.
RTModel AerosolInitialGuess	The initial guess aerosol model, expressed as extinction per kilometer at 750 nm. Note that the field is not an a-priori in the sense used by statistical matrix inversion schemes (e.g. optimal estimation).
RTModel AerosolExtinction	The aerosol profile expressed as extinction per kilometer at 750 nm used in the last iteration of the radiative transfer model. This is identical to the primary data product, AerosolExtinction, except it is not bounded at lower and upper altitudes by "Missing Value" according to the vertical extent of the retrieval, i.e. it extends from 0.5 km to 99.5 km.

3.1.2.2. ESA products that require more effort to mature

3.1.2.2.1. SCIAMACHY

This section describes the format of data files containing vertical profiles of aerosol extinction coefficient retrieved from SCIAMACHY limb measurements at the Institute of Environmental Physics, University of Bremen (IUP Bremen).

The results are given as vertical profiles of the aerosol extinction coefficient at 470 nm and 750 nm at altitude levels from 9 to 40 km with 1 km spacing. Values below 13 km and above 32 km are outside the sensitivity region. Retrievals are done azimuthally resolved, i.e., depending on the illumination of the atmosphere 2 - 4 profiles for different azimuthal angles are retrieved for each limb measurement sequence (also referenced as limb state). The retrieval is based on the Level 1 data version 7.04 (consolidation W). A detailed description of the retrieval process is given by Ernst et al. (2012).

For every month NetCDF (version 3) files containing all profiles retrieved from single SCIAMACHY limb measurements are provided. The names of the data files are

SCIA_Limb_AER__<version_number>_<YYYYMM>.nc

where <version_number> is "V1.1" and <YYYYMM> denotes the year and the month, e.g. "200301" for January 2003. The format of the NetCDF files is described in Table 3.1.2.2.1.1.

Table 3.1.2.2.1.1. NetCDF format for SCIAMACHY aerosol level 2 data.

Data field	Dimension	Units	Description
longitude	Number of profiles	degrees	Average longitude of the tangent point
latitude	Number of profiles	degrees	Average latitude of the tangent point
solz	Number of profiles	degrees	Average solar zenith angle at the tangent point
date_time	Number of profiles		Date and time of the begin of the limb measurement as

			YYYYMMDDhhmmss
orbit	Number of profiles		Orbit number according to SCIAMACHY Level 1 data set
state	Number of profiles		Sequential number of the limb measurement within the SCIAMACHY orbit file
azimuth	Number of profiles		Number of the measurement within the horizontal scan (starting from 0)
heights	Number of altitudes	km	Altitude grid of the retrieved profiles (same for all profiles)
aer\470nm\	Number of profiles times number of altitudes	km ⁻¹	Retrieved aerosol extinction coefficients at 470 nm
aer\750nm\	Number of profiles times number of altitudes	km ⁻¹	Retrieved aerosol extinction coefficients at 750 nm

The global attributes list provides the following information: the title ("SCIAMACHY Limb AER"), institute and its ID, the experiment name "SCIAMACHY", the experiment description, the data source ("ENVISAT"), the data version ("V1.1"), the level 1 versions used ("7.04W"), the name of the person who has created the data file, the contact email, the year and month of the data contained in the dataset (as YYYYMM) and the dummy value ("-999.000").

The time of each profile is the measurement start time (at the lowest altitude). It takes about 1 minute to measure all four profiles in one state. The measurement time varies more between the lowest and the highest altitude of the state than between the four different azimuth profiles. The position (longitude and latitude) is the average position of all nominal tangent heights. The dummy value for all level 2 fields is -999.0.

3.1.3. Water Vapour

Water vapour products are provided from SCIAMACHY.

3.1.3.1. Mature ESA products including those from third party missions

There are no mature Level 2 water vapour datasets.

3.1.3.2. ESA products that require more effort to mature

3.1.3.2.1. SCIAMACHY

This section describes the format of data files containing vertical profiles of water vapour retrieved from SCIAMACHY limb measurements at the Institute of Environmental Physics, University of Bremen (IUP Bremen).

The results are given as concentrations in molecules/cm³ and as volume mixing ratios in ppmV at altitude levels from 9 to 40 km with 1 km spacing. Values below 11 km and above 25 km are outside the sensitivity region and should be used only if a convolution with averaging kernels is needed. Please note, that the number densities are the primary retrieval product whereas volume mixing ratios are calculated from the retrieved number densities using the pressure and temperature information from the ECMWF database. Here, the ERA-Interim reanalysis of ECMWF with a spatial resolution of 5°x5° and a temporal resolution of 6 hours is used. Retrievals are done azimuthally resolved, i.e., depending on the illumination of the atmosphere 2-4 profiles for different azimuthal angles are retrieved for each limb measurement sequence (also referenced as limb state). Additionally, the product contains a priori profiles of water vapour used in the retrieval as well as error estimations in both number density and volume mixing ratio representations. The product also contains the vertical resolution of the retrieved profiles, which is usually between 3 and 10 km. The retrieval is based on the Level 1 data version 7.03 (before 17.06.2010) and 7.04 thereafter, both consolidation U and W of version 7.04 were used. The Level 1 version has no large effect on the resulting water vapour (the mean values differ generally by less than 0.1 between Level 1 data version 7.03 and 7.04 consolidation W for three days in February 2005, see Data Analysis Report). A detailed description of the retrieval process is given by Rozanov et al. (2011).

For every month NetCDF (version 3) files containing all profiles retrieved from single SCIAMACHY limb measurements are provided. The names of the data files are

SCIA_Limb_H2O_<version_number>_<YYYYMM>.nc

where <version_number> can be “V3.01” or “V3.02” and <YYYYMM> denotes the year and the month, e.g. “200301” for January 2003. The format of the NetCDF files is described in Table 3.1.3.2.1.1.

Table 3.1.3.2.1.1. NetCDF format for SCIAMACHY water vapour level 2 data.

Data field	Dimension	Units	Description
longitude	Number of profiles	degrees	Average longitude of the tangent point
latitude	Number of profiles	degrees	Average latitude of the tangent point
solar_zenith_angle	Number of profiles	degrees	Average solar zenith angle at the tangent point
date_time	Number of profiles		Date and time of the begin of the limb measurement as YYYYMMDDhhmmss
orbit	Number of profiles		Orbit number according to SCIAMACHY Level 1 data set
state	Number of profiles		Sequential number of the limb measurement within the SCIAMACHY orbit file
azimuth	Number of profiles		Number of the measurement within the horizontal scan (starting from 0)

heights	Number of altitudes	km	Altitude grid of the retrieved profiles (same for all profiles)
h2o_vmr	Number of profiles times number of altitudes	ppmV	Retrieved water vapour mixing ratio
h2o_vmr_ap	Number of profiles times number of altitudes	ppmV	Apriori profile for used in the retrieval
h2o_vmr_err	Number of profiles times number of altitudes	ppmV	Estimated retrieval error
h2o_nd	Number of profiles times number of altitudes	molecules/cm ³	Retrieved water vapour number density
h2o_nd_ap	Number of profiles times number of altitudes	molecules/cm ³	Apriori profile for used in the retrieval
h2o_nd_er	Number of profiles times number of altitudes	molecules/cm ³	Estimated retrieval error
h2o_res	Number of profiles times number of altitudes	km	Vertical resolution of the retrieval
h2o_msc	Number of profiles times number of altitudes		Measurement response
avk	Number of profiles times number of altitudes times number of altitudes		Averaging kernels

The global attributes list provides the following information: the title ("SCIAMACHY Limb H2O"), institute and its ID, the experiment name ("SCIAMACHY"), the experiment description, the data source ("ENVISAT"), the data version ("3.01" or "3.02"), the version of the cloud detection algorithm ("SCODA V1.9"), the level 1 versions used ("7.03U/7.04U and/or 7.04W"), the name of the person who has created the data file, the contact email, the creation time of the file, the year and month of the data contained in the dataset (as YYYYMM) and the dummy value ("-999.000").

The time of each profile is the measurement start time (at the lowest altitude). It takes about 1 minute to measure all four profiles in one state up to 90km height. The water vapour profile uses measurements from the 6th to the 10th tangent height, about 10 to 17s after the start time. The measurement time varies more between the lowest and the highest altitude of the state than between the four different azimuth profiles. The position (longitude and latitude) is the average position of all nominal tangent heights. The dummy value for all level 2 fields is -999.0. Only profiles, where no clouds are present above 10km (according to the cloud detection algorithm SCODA V1.9) are included in the retrieval, therefore no cloud information is provided with the data. Data are provided for both data version V3.01 and V3.02. Since the only difference between these versions is a stricter filter, which is applied to

V3.02, individual profiles are identical for both data versions, but V3.01 contains more profiles.

3.1.4. Short-lived Species

It is not planned within the SPIN project to improve or deliver level 2 data for short-lived species. Please see section 3.2 concerning level 3 data products.

3.1.5. Temperature

It is not planned within the SPIN project to improve or deliver level 2 data for temperature. Please see section 3.2 concerning level 3 data products.

3.2. Level 3 data product specification

Some level 3 data (short-lived species, Section 3.2.4, and temperature, Section 3.2.5) are delivered as climatologies in a format following the specifications of the SPARC Data Initiative. This section provides a brief description of the SPARC-DI format (for further details, see the SPIN ATBD and the SPARC-DI report). Other level 3 data (Ozone, section 3.2.1, Aerosol, Section 3.2.2, and Water vapour, Section 3.2.3) are provided in different formats, described separately, in Sections 3.2.1-3.

Zonal and monthly mean climatologies have been calculated for temperature and several trace gases (listed in Table 3.2.4.1) on the SPARC-DI grid using 5° latitude bins (with mid-points at -87.5°, -82.5°, -77.5°, ..., 87.5°) and 28 pressure levels (300, 250, 200, 170, 150, 130, 115, 100, 90, 80, 70, 50, 30, 20, 15, 10, 7, 5, 3, 2, 1.5, 1, 0.7, 0.5, 0.3, 0.2, 0.15, and 0.1 hPa). Note that some temperature climatologies are provided on a slightly extended vertical grid, as discussed in Section 3.2.5. Time is specified as days since 1 January 1950, with the 15th of each month chosen for each monthly mean value. Temperature is reported as degrees (Kelvin), and trace gas species as volume mixing ratios (ppV). The monthly zonal mean value and the 1 σ standard deviation along with the number of averaged data values are given for each month, latitude bin and pressure level. The mean, minimum, and maximum local solar time (LST), average day of the month, and average latitude of the data within each bin for one selected pressure level are also provided. Note, these latter data are not provided for the temperature climatologies based on radio occultation measurements (Section 3.2.5).

For species with large diurnal variations SPARC-DI climatologies have been calculated separately for am and pm, sunset and sunrise, or day and night, depending on the various satellite sensors' observational characteristics (sun-synchronous orbit with fixed equator crossing times, solar occultation observations, or orbits drifting with respect to local solar time). This separation has been based on the LST of the measurements (see detailed discussion in Section 3.1.1 of the SPARC-DI report). Additional climatologies have been built using a photochemical box model to scale the measurements to a common LST in order to enable direct comparison between products from different instruments with different sampling patterns.

The data is delivered in the SPARC-DI NetCDF format. See SPARC-DI report (to be repeated here once SPARC-DI report available). Each year of data is stored in a separate data file, each named with the following convention:

SPARC_DI_T2Mz_[species]_[year]_[instrument]_[original_dataset_version]_[zonal_mean_dataset_version].

3.2.1. Ozone

The GOMOS bright limb Level 3 dataset is provided in NetCDF format. The file contains zonally and monthly averaged GBL values. The altitude is gridded between 19 and 59 km with 1 km step. The file format is described in Table 3.2.2.0. The GBL climatology can be downloaded from <ftp.fmi.fi> (user: gomosGBL, pass: kOs20mos!).

Table 3.2.2.0. NetCDF format for GOMOS bright limb ozone climatology.

Data field	Dimension	Units	Description
latitude	Number of latitudes	degrees	Latitude grid
altitude	Number of altitudes	km	Altitude grid
time	Number of months	months	Time grid
gbL3	Time x latitude x altitude	cm ⁻³	Monthly and zonally averaged ozone profiles

3.2.2. Aerosol

The SCIAMACHY stratospheric aerosol extinction coefficient climatology is provided in NetCDF format. The file contains monthly averaged and spatially binned (5 by 5 deg) aerosol extinction coefficients at 470 nm and 750 nm (unit: 1/km) on an equidistant altitude grid with 1 km spacing. The names of the data files are

SCIA_Limb_AER_GMM_<version_number>_<YYYYMM>.nc

where <version_number> is “V1.1” and <YYYYMM> denotes the year and the month, e.g. “200301” for January 2003. The format of the NetCDF files is described in Table 3.2.2.1.

Table 3.2.2.1. NetCDF format for SCIAMACHY aerosol climatology.

Data field	Dimension	Units	Description
longitude	Number of longitudes	degrees	Longitude grid
latitude	Number of latitudes	degrees	Latitude grid
heights	Number of altitudes	km	Altitude grid
nuber_of_profiles	Number of longitudes times number of latitudes times number of altitudes		Number of averaged profiles for each latitude-longitude bin and each altitude level.
aer\470nm\	Number of longitudes times	km ⁻¹	Monthly averaged and spatially binned aerosol extinction

	number of latitudes times number of altitudes		coefficients at 470 nm
aer(750nm)	Number of longitudes times number of latitudes times number of altitudes	km ⁻¹	Monthly averaged and spatially binned aerosol extinction coefficients at 750 nm

The global attributes list provides the following information: the title ("SCIAMACHY Limb AER gridded data, 5x5 degrees"), institute and its ID, the experiment name ("SCIAMACHY"), the experiment description, the data source ("ENVISAT"), the data version ("V1.1"), the level 1 versions used ("7.04W"), the name of the person who has created the data file, the contact email, the creation time of the file, the year and month of the data contained in the dataset (as YYYYMM) and the dummy value ("-999.000").

The dummy value for most of the level 3 fields is -999.0. For the standard deviation of aerosol extinction -999.0 is also given if there is only one measurement in a grid cell. The number of measurements is 0 if no profiles are found in one grid cell.

3.2.3. Water Vapour

The SCIAMACHY stratospheric water vapour climatology is provided in NetCDF format. The files contain monthly averaged and spatially binned (5 by 5 deg) vertical profiles of water vapour number densities (ND) (unit: molecules/cm³) on an equidistant altitude grid with 1 km spacing. The names of the data files are

SCIA_Limb_H2O_GMM_<version_number>_<YYYYMM>.nc

where <version_number> can be "V3.01" or "V3.02" and <YYYYMM> denotes the year and the month, e.g. "200301" for January 2003. The format of the NetCDF files is described in Table 3.2.3.1.

Table 3.2.3.1. NetCDF format for SCIAMACHY water vapour climatology.

Data field	Dimension	Units	Description
longitude	Number of longitudes	degrees	Longitude grid
latitude	Number of latitudes	degrees	Latitude grid
heights	Number of altitudes	km	Altitude grid
nuber_of_profiles	Number of longitudes times number of latitudes times number of altitudes		Number of averaged profiles for each latitude-longitude bin and each altitude level.
h2o_vmr	Number of longitudes times number of latitudes	ppmV	Monthly averaged and spatially binned water vapour mixing ratio profiles

	times number of altitudes		
h2o_vmr_ap	Number of longitudes times number of latitudes times number of altitudes	ppmV	Monthly averaged and spatially binned apriori profiles
h2o_vmr_err	Number of longitudes times number of latitudes times number of altitudes	ppmV	Standard deviations for the monthly averaged and spatially binned water vapour profiles
h2o_nd	Number of longitudes times number of latitudes times number of altitudes	molecules/cm ³	Monthly averaged and spatially binned water vapour number density profiles
h2o_nd_ap	Number of longitudes times number of latitudes times number of altitudes	molecules/cm ³	Monthly averaged and spatially binned apriori profiles
h2o_nd_er	Number of longitudes times number of latitudes times number of altitudes	molecules/cm ³	Standard deviations for the monthly averaged and spatially binned water vapour profiles
h2o_res	Number of longitudes times number of latitudes times number of altitudes	km	Monthly averaged and spatially binned values for the vertical resolution of the retrieval

The global attributes list provides the following information: the title ("SCIAMACHY Limb H2O gridded data, 5x5 degrees"), institute and its ID, the experiment name ("SCIAMACHY"), the experiment description, the data source ("ENVISAT"), the data version ("3.01" or "3.02"), the version of the cloud detection algorithm ("SCODA V1.9"), the level 1 versions used ("7.03U/7.04U and/or 7.04W"), the name of the person who has created the data file, the contact email, the creation time of the file, the year and month of the data contained in the dataset (as YYYYMM) and the dummy value ("-999.000").

The dummy value for most of the level 3 fields is -999.0. For the standard deviation of water vapour -999.0 is also given if there is only one measurement in a grid cell. The number of measurements is 0 if no profiles are found in one grid cell.

3.2.4. Short-lived Species

Short-lived species climatologies prepared within the SPARC data initiative and all updates prepared within SPIN are provided in the SPARC-DI NetCDF format. Files follow the same naming convention as defined by SPARC-DI. See Section 3.2 for the detailed definition.

Table 3.2.4.1 presents a list of short lived species climatologies produced by SPARC-DI which are relevant for SPIN (i.e. focus on ESA and ESA third party missions):

Table 3.2.4.1. List of short lived species climatologies produced by SPARC-DI which are relevant for SPIN.

Species	SPARC-DI climatologies
NO	Odin/SMR am+pm , Odin/SMR scaled 10am+10pm, MIPAS 10am+10pm, ACE sr+ss
NO2	Odin/OSIRIS am+pm, Odin/OSIRIS scaled, MIPAS 10am+10pm, ACE sr+ss, SCIAMACHY am+pm, GOMOS (tbd)
CIO	Odin/SMR am+pm, Odin/SMR scaled 1:30am+1:30pm, Aura/MLS am+pm
HO2	Odin/SMR am+pm, Odin/SMR scaled 1:30am+1:30pm, Aura/MLS am+pm

Note that SPARC-DI climatologies and scaled products are currently under evaluation (as of September 2012). The selection and production of matured products of the scaled climatologies envisaged in SPIN depends on the results of this evaluation.

3.2.5. Temperature

Temperature is considered in WP18, which delivers temperature climatologies from ESA and ESA-TPM instruments, and in WP25, which explores how ESA and ESA-TPM measurements can be used to improve the detection of cold point tropopause temperatures (especially in the tropics).

In WP18 monthly and zonal mean multi-year climatologies from ESA and ESA-TPM instruments, including ACE-FTS, MIPAS, and SMR, and from radio occultations (RO) instruments, including CHAMP, GRACE and TSX have been produced. Each climatology is provided on the standard SPARC-DI latitude-pressure grid (see section 3.2), except as noted below.

The climatology from ACE-FTS is provided on a vertically extended grid using the following pressure levels in addition to the SPARC-DI levels: 0.07, 0.05, 0.03, 0.02, 0.015, 0.01, 0.007, 0.005, 0.003, 0.002, 0.0015, and 0.001 hPa.

For SMR, two climatologies have been produced, one for each retrieval channel, at 544.6 GHz and 556.9 GHz, respectively. The former provides data primarily in the stratosphere, while the latter provides data primarily in the mesosphere. For the SMR channel 556.9 GHz climatology, the following pressure levels are used in addition to the SPARC-DI levels: 0.07, 0.05, 0.03, 0.02, 0.015, 0.01, 0.007, 0.005, 0.003, 0.002, 0.0015, 0.001, 0.0007, 0.0005, 0.0003, 0.0002, 0.00015, 0.0001, 0.00007, 0.00005, 0.00003, 0.00002, 0.000015, and 0.00001 hPa.

The RO climatologies are provided on a vertical extended grid that includes the following extra levels: 1000, 850, 700, 500, and 400 hPa.

Table 3.2.5.1 specifies the data versions and temporal and approximate vertical coverage of the climatologies. Table 3.2.5.2-5 provides a specification of the NetCDF data files provided. Table 3.2.5.2, 3, 4, and 5, lists the dimensions, coordinate variables, variables and global attributes, respectively, of the NetCDF files.

Table 3.2.5.1. Temporal and approximate vertical coverage of SPIN temperature climatologies.

Instrument	Version	Temporal Coverage	Vertical Coverage	Comment
ACE-FTS	3.0	Feb 2004 - Mar 2011	100 - 0.001 hPa	
GOMOS	H RTP 6.0	-	-	Not produced yet
MIPAS	V3O_T_8 and V5R_T_220	Jun 2002 - Apr 2011	300 - 0.1 hPa	High spectral resolution data V3O_T_8 is used for Jun 2002 - Mar 2004 and reduced spectral resolution data V5R_T_220 is used for Jan 2005 - Apr 2010.
SMR-strat	2.0	Aug 2001 - Apr 2012	200 - 0.1 hPa	544.6 GHz retrieval band
SMR-mes	2.1	Aug 2001 - Apr 2012	2 - 0.001 hPa	556.9 GHz retrieval band
CHAMP	2.0	May 2001 - Oct 2008	300 - 1 hPa	Radio occultation data
GRACE	POCS version 6.0	Jan 2006 - Dec 2011	300 - 1 hPa	Radio occultation data
TSX	POCS version 6.0	Jul 2008 - Mar 2012	300 - 1 hPa	Radio occultation data

Table 3.2.5.2. Specification of NetCDF files for temperature climatologies: Dimensions.

Name	Size	Comment
time	12	Twelve months per file
plev	28	Number of vertical levels (note there are some exceptions: SMR-mes has 56 levels; ACE-FTS has 45 levels; CHAMP, GRACE and TSX have 33 levels)
lat	36	Number of latitudes

Table 3.2.5.3. Specification of NetCDF files for temperature climatologies: Coordinate variables.

Name	Dimensions	Data type	Standard name	Long name	Axis	Units	Other
time	1-D array (size of time dimension)	Int	N/A	time	T	days since 1950-01-01 00:00:00	calendar = "standard"
plev	1-D array (size of plev dimension)	float / double	air_pressure	pressure	Z	hPa	positive = "down"
lat	1-D array (size of lat dimension)	float / double	Latitude	latitude	Y	degrees_north	

Table 3.2.5.4. Specification of NetCDF files for temperature climatologies: Variables.

Name	Data type	Dimensions	Long name	Units	Fill value
T	float/double	3-D array (size of time, size of plev, size of lat)	Temperature	K	-999
T_STD	float/double	3-D array (size of time, size of plev, size of lat)	temperature standard deviation	K	-999

T_NR	float/double	3-D array (size of time, size of plev, size of lat)	number of values	N/A	-999
LST_MEAN	float/double	2-D array (size of time, size of lat)	Mean of local solar time	hours	-999
LST_MIN	float/double	2-D array (size of time, size of lat)	Minimum of local solar time	hours	-999
LST_MAX	float/double	2-D array (size of time, size of lat)	Maximum of local solar time	hours	-999
AVE_DOM	float/double	2-D array (size of time, size of lat)	Average day of month	days	-999
AVE_LAT	float/double	2-D array (size of time, size of lat)	Average latitude	degrees north	-999

Table 3.2.5.5. Specification of NetCDF files for temperature climatologies: Global attributes.

Name	Example	Comment
experiment	"MIPAS"	
data_version	"V3O_T_10"	
organisation	"IMK"	
type_of_data	"MEASUREMENTS"	
platform	"SATELLITE"	
name_of_platform	"ENVISAT"	
pi_name	"Thomas von Clarmann, Gabriele P. Stiller, and Bernd Funke"	
file_creation_time	"31-05-2012 at 11:23:37.5"	
file_modification_time	"31-05-2012 at 11:23:37.5"	
fields	"T2Mz: Monthly-mean zonal mean 2-d atmosphere"	
climatology_version	"i02"	
author	"Thomas von Clarmann and Bernd Funke"	
institute	"KIT-IMK/IAA-CSIC"	
address	"P.O.B. 3640, 76021 Karlsruhe, Germany / Apartado Postal 3004, E-18080 Granada, Spain"	
email	"thomas.clarmann@kit.edu / bernd@iaa.es"	
project_id	"SPARC_Data_Initiative"	
comment	""	
distribution_statement	"Please follow data policy instructions for the use of this data to be found on the data distribution site!"	
calculation_of_zonal_mean	"interpolation to center latitude"	
scaling_of_data	"no scaling applied"	
LST_level	"2 hPa"	Level used for calculation of LST_MEAN
ave_dom_level	"2 hPa"	Level used for calculation of AVE_DOM
ave_lat_level	"all levels"	Level used for calculation of AVE_LAT

The ESA and ESA-TPM based climatologies are used in WP23 to extend the historical stratospheric temperature record from SSU (see section 3.3.5).

In WP25, ESA(TPM) temperature measurements were referenced to the tropopause height obtained from NCEP (National Centers for Environmental Prediction) CFSR (Climate Forecast System Reanalysis) reanalyses. Zonal mean monthly mean temperatures with respect to the local instantaneous tropopause height were calculated for the following four instruments: MIPAS, ACE-FTS, SMR (544.6 GHz channel only) and GOMOS-HRTP. The temperature data sets are provided in NetCDF files named

`<instr>_ZonalMeanTempTP.nc`

All four data sets extend to 2010 since this only go to 2010¹. The files contain zonal mean monthly mean temperatures in 5° latitude bins (with mid-points at 87.5°, 82.5°, 77.5°, ..., -87.5°) on altitude levels from -15 km to 30 km with respect to the tropopause height. The format of the NetCDF files is described in Table 3.2.5.6.

Table 3.2.5.6. NetCDF format for the temperature data sets referenced to the tropopause height.

Data field	Dimension	Units	Description
time	size of time	days since January 1950	Mid-point of month
latitude	36	degrees	Mid-point of 5° latitude zone
altitude	46	km	Altitude w.r.t. tropopause height
temperature	size of time, size of latitude, size of altitude	K	Zonal mean monthly mean temperature
counts	size of time, size of latitude, size of altitude		Number of temperature measurements averaged

The dummy value of the temperature is -999. This value is saved as attribute `fillvalue` of the temperature data field in the NetCDF file. The global attributes are listed in Table 3.2.5.7.

Table 3.2.5.7. Global attributes for temperature data set NetCDF files.

Name	Example
title	“MIPAS Temperature Data Set referenced to Tropopause”
description	“Monthly mean zonal mean temperature w.r.t. tropopause height”
version	“1.0”
organization	“Bodeker Scientific, Alexandra, New Zealand”
instrument	“MIPAS”
author	“Andreas Penckwitt”
email	“andreas@bodekerscientific.com”
created	“2013-12-30 11:51:00”
modified	“2014-02-04 02:05:56”

A similar file is also provided for temperatures extracted from the NCEPCFSR reanalyses. All data fields are as described above with two exceptions: The NetCDF file has no field `counts`

¹ NCEPCFSR is used for a mean representativeness correction, but we only had the data available until 2010.

as the zonal mean monthly means are not calculated from individual profiles, but from reanalyses data on a regular grid, and the field instrument is replaced by source.

3.3. Merged Level 3 data product specification

3.3.1. Ozone

3.3.1.1. Bokeker Scientific product

The Bodeker Scientific merged SAGE II – GOMOS ozone profile data set is provided in a single NetCDF file

MergedSAGE2AndGOMOS.nc

The data set combines measurements from SAGE II v7.00 and GOMOS Level 2 processor version GOMOS/6.01. The merged data set covers October 1984 to April 2012.

The file contains zonal mean monthly mean ozone number densities in 5° latitude bins (with mid-points at 87.5°, 82.5°, 77.5°, ..., -87.5°) on an equidistant altitude grid from 10 km to 69 km with 1 km spacing. The format of the NetCDF file is described in Table 3.3.1.1.

Table 3.3.1.1. NetCDF format for the Bodeker Scientific merged SAGE II – GOMOS ozone data set.

Data field	Dimension	Units	Description
time	348	days since 1 January 1950	Mid-point of month from January 1984 to December 2012
latitude	36	degrees	Mid-point of 5° latitude zone
altitude	60	km	Altitude grid
counts	size of time, size of latitude, size of altitude		Number of ozone measurements averaged
o3	size of time, size of latitude, size of altitude	10 ¹⁸ molec./m ³	Zonal mean monthly mean ozone number density
o3_error	size of time, size of latitude, size of altitude	10 ¹⁸ molec./m ³	1σ uncertainty of zonal mean monthly mean ozone number density

The dummy value of the ozone number density is -999. This value is saved as attribute fillvalue of the o3 data field in the NetCDF file. The global attributes are listed in Table 3.3.1.2.

Table 3.3.1.2. Global attributes for the Bodeker Scientific merged SAGE II – GOMOS ozone data set NetCDF file.

Name	Value
title	“Merged SAGE II and GOMOS Climate Data Record of Stratospheric Ozone”
description	“Zonal mean monthly mean ozone number densities on equidistant altitude levels from 10 to 69 km with 1 km spacing calculated from SAGE Version 7.0 and GOMOS IPF 6.01”
version	“1.0”
organization	“Bodeker Scientific, Alexandra, New Zealand”

author	“Andreas Penckwitt”
email	“andreas@bodekerscientific.com”
created	“2013-12-23 12:28:17”
modified	“2014-01-29 03:53:23”

3.3.1.2. FMI product

The FMI’s merged SAGE II - GOMOS ozone profile data set is provided in a NetCDF file

SAGE2GOMOSTimeseriesO3.nc

The file can be downloaded from <http://igaco-o3.fmi.fi/VDO/data.html>.

This data set combines ozone measurements from SAGE II v7 and GOMOS Level 2 processor version IPF 6.01. The merged data set covers from October 1984 to December 2011. The file contains zonal monthly median ozone number densities in 10° latitude bins on an equidistant altitude grid from 10 km to 70 km with 1 km spacing. The format of the NetCDF file is described in Tables 3.3.1.3-3.3.1.4. More details can be found from the publication: Kyrola et al. Combined SAGE II-GOMOS ozone profile data set 1984-2011 and trend analysis of the vertical distribution of ozone. Atmospheric Chemistry & Physics,13, 10645-10658, 2013.

Table 3.3.1.3 NetCDF format for the FMI merged SAGE II – GOMOS ozone data set.

Data field	Dimension	Units	Description
days_since2003	327	days since 1 January 2003	Mid-point of month from January 1984 to December 2011
calendar	327x12	yy mm dd ... hh mm ss	Calendar dates of the time grid cells (start and end)
latitude_centers	12	degrees	-55,-45,..., 55 deg.
altitudes	61	km	Merged data altitude grid 10-70 km
altitudes_sage	140	km	SAGE II altitude grid 0.5-70 km
altitudes_gomos	111	km	GOMOS altitude grid 10-120 km
number_measurements	327x61x12	unitless	Number of measurements. Note in 2002-2005 GOMOS +SAGE II.
number_density	327x61x12	molec./cm ³	Zonal monthly median ozone number density. During the joint measurement time in 2002-2005 weighted mean of of the individual instrument medians.

number_density_error	327x61x12	molec./cm ³	Uncertainty of the number density
number_density_sage	327x140x12	molec./cm ³	Zonal monthly median ozone number density
number_density_error_sage	327x140x12	molec./cm ³	Uncertainty of number density
number_density_gomos	327x111x12	molec./cm ³	Zonal monthly median ozone number density
number_density_error_gomos	327x111x12	molec./cm ³	Uncertainty of number density
Asymmetries_gomos	327x2	unitless	Scaled deviations of mean measurement time and mean latitude from the center of the lat-time grid cells.
Asymmetries_sage	327x2	unitless	Same as above.

Table 3.3.1.4. Global attributes for the FMI merged SAGE II-GOMOS data set NetCDF file.

Name	Value
title	SAGE II-GOMOS combined O3 time series 1984-2011
version	1.0
file_modification_time	04-Nov-2013
reference	Kyrola et al. Combined SAGE II-GOMOS ozone profile data set 1984-2011 and trend analysis of the vertical distribution of ozone. Atmospheric Chemistry & Physics,13, 10645-10658, 2013
database author	Erkki Kyrölä
institute	Finnish Meteorological Institute (FMI)
address	P. O. Box 503, 00101 Helsinki, Finland
email	erkki.kyrola@fmi.fi
project_funding_ids	MIDAT (Finnish Academy and ESA SPIN)
project_other_ids	SI2N
distribution_statement	Open, but contact the author for updates
type_of_data	Combined time series
platform	Satellite
name_of_platforms	ERBS (SAGE II) and ENVISAT (GOMOS)
experiments	SAGE II and GOMOS
measurement_methods	Extinction in solar (SAGE II) and stellar (GOMOS) occultation
SAGEII_data:	NASA Langley
GOMOS_data:	ESA
GOMOS_data_vertical_gridded_product:	FMI
general_data_selection_1	Minimum number of measurements = 5
general_data_selection_2	Outlier screening (see reference above)
SAGEII_data_filter	Langley pre-filtered data as 24-Sep-2013. See reference.
GOMOS_data_selection	Solar zenith angle > 105 deg. at tangent point
GOMOS_data_filter	Weak-cold stars and unphysical profiles

	eliminated. See the reference
calculation_instrumental_averages	Median over latitude bins
unit_of_data	number density in ccm
data_grid	10 deg. in latitude from 60S to 60N and one month in time from Oct 1984 to Dec. 2011
data_characterisation_1	Numtable-variable giving number of SAGE II + GOMOS accepted measurements.
data_characterisation_2	GOMOS and SAGE II asymmetry variables ([lat_as time_as]. For definitions, see the reference.
SAGEII_GOMOS_bias	SAGE II sunrise and sunset profiles corrected using bias estimates from collocated comparisons. See reference
SAGEII_GOMOS_fusing_2002-2005	Using weighted mean from instrument medians. See reference
GOMOS_data_version	IPF v6.0
SAGEII_data_version	v7.0
GOMOS_algorithm_reference	E. Kyrola et al., Retrieval of atmospheric parameters from GOMOS data, Atmospheric Chemistry & Physics, 10, 11881-11903, 2010.
SAGEII_algorithm_reference	Damadeo, et al., SAGE version 7.0 algorithm: application to SAGE II, Atmos. Meas. Tech., 6, 3539-3561, 3539-2013, 2013
database_created	15-Oct-2013
database_specific_id	acpfinalprefil

3.3.2. Aerosol

SPIN will not deliver any merged level 3 data for OSIRIS or SCIAMACHY aerosol.

3.3.3. Water Vapour

The merged water vapour product generated in WP27 is provided as a NetCDF file. The data and their associated errors are calculated as monthly mean zonal means in 5° latitude zones bins at altitude levels of 1 to 70 km with 1 km spacing. The merged data set covers Oct 1984 to April 2012. A description of the variables in this NetCDF files are shown in Table 3.3.3.1. Two versions of this database were created (as described in the ATBD), one where SAGE II was used as the initial data set, with all other data sets being homogenized and merged with SAGE II, and one where HALOE was used as the initial data set. The names of the two files generated are:

BS_MergedH2O<Instrument>.nc

where <Instrument> is “HALOE” or “SAGEII” and donates the starting instrument for the generation of the merged water vapour data set.

The time stamp for each value represents the number of decimal days since the 1st January 1950 and is the centre of the monthly mean. All data products have a fill value of -999 which is stored as the fill value for each variable. All negative values were filled with the fill value.

Table 3.3.3.1. Specification of water vapour NetCDF file: Variables

Data Field	Dimension Size	Units	Description
altitude	70	km	Altitude of value
instrument	5		Names of instruments
latitude	36	degrees	Centre of latitude bin
time	348	days since 1950-01-01	Mid-point of the month
order	instrument x latitude x altitude		Order of inclusion of instrument (zero based)
h2o	time x latitude x altitude	ppm	Monthly mean zonal mean water vapour mixing ratio
h2o_error	time x latitude x altitude	ppm	Error on monthly mean zonal mean water vapour mixing ratio value

SPIN will not deliver any merged level 3 data for SCIAMACHY water vapour.

3.3.4. Short-lived Species

SPIN will not deliver any merged level 3 data for short-lived species.

3.3.5. Temperature

3.3.5.1. U of T product

Temperature is considered in WP23, which delivers a merged SSU/ESA/ESA-TPM stratospheric near global temperature dataset, and in WP24, which delivers zonal mean monthly mean temperature records from MIPAS, ACE-FTS and SMR merged with those from radio occultation measurements from CHAMP, GRACE and TSX.

Table 3.3.5.1-4 provide a specification of the NetCDF data file provided. Table 3.3.5.1, 2, 3, and 4, list the dimensions, coordinate variables, variables and global attributes, respectively, of the NetCDF file.

The name of the NetCDF data file containing the merged SSU and SSU-weighted MIPAS near-global mean temperatures is

`merged_SSU_MIPAS_T0M_ta_1978-2011.nc_`

Table 3.3.5.1. Specification of NetCDF file for merged SSU/ESA temperatures: Dimensions.

Name	Size	Comment
time	408	Twelve months times 34 years per file

Table 3.3.5.2. Specification of NetCDF file for merged SSU/ESA temperatures: Coordinate variables.

Name	Dimensions	Data type	Standard name	Long name	Axis	Units	Other
time	1-D array (size of time dimension)	Int	N/A	time	T	days since 1950-01-01 00:00:00	calendar = "standard"

Table 3.3.5.3. Specification of NetCDF file for merged SSU/ESA temperatures: Variables.

Name	Data type	Dimensions	Long name	Units	Fill
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					value
T1	float	1-D array (size of time)	Temperature (Channel 1)	K	-999
T2	float	1-D array (size of time)	Temperature (Channel 2)	K	-999
T3	float	1-D array (size of time)	Temperature (Channel 3)	K	-999

Table 3.3.5.4. Specification of NetCDF file for merged SSU/ESA temperatures: Global attributes.

Name	Example	Comment
experiment	"SSU/MIPAS"	
platform	"SATELLITE"	
pi_name	"Theodore G. Shepherd"	
file_creation_time	"Tue Mar 18 13:49:16 2014"	
fields	"TOM: monthly mean 0-d atmosphere"	
author	"Charles McLandress"	
institute	"University of Toronto"	
address	"60 St. George St; Toronto, Ontario, Canada M5S 1A7"	
email	charles@atmosph.physics.utoronto.ca	
comment	"Merged near-global mean (70S-70N) SSU and *offset* SSU-weighted MIPAS data: SSU from January 1978 to December 2005 & MIPAS from January 2006 to December 2011; MIPAS data in overlap period (January 2002 to December 2005) are used to compute the constant offsets"	
scaling_of_data	"no scaling applied"	

3.3.5.2. Bodeker Scientific product

Bodeker Scientific created a merged zonal mean monthly mean temperature record from the ESA(TPM) instruments MIPAS, ACE-FTS and SMR (544.6 GHz channel only) with those from radio occultation measurements from CHAMP, GRACE and TSX. These six source data sets were created in WP 18 and are described in Section 3.2.5.

The merged temperature data set is provided in a single NetCDF file

BSUTLS_MergedTemp.nc

which covers May 2001 to April 2012.

The file contains zonal mean monthly mean temperatures in 5° latitude zones (with mid-points at 87.5°, 82.5°, 77.5°, ..., -87.5°) on the following pressure levels: 300, 250, 200, 170, 150, 130, 115, 100, 90, 80, 70, 50, 30, 20, 15, 10 and 7 hPa. The format of the NetCDF file is described in Table 3.3.5.5.

Table 3.3.5.5. NetCDF format for the Bodeker Scientific merged temperature data set.

Data field	Dimension	Units	Description
time	144	months since January 1950	From January 2001 to December 2012 (January 1950 is month 0)
latitude	36	degrees	Mid-point of 5° latitude zone

pressurelevel	17	hPa	Pressure levels
temperature	size of time, size of latitude, size of pressure level	K	Zonal mean monthly mean temperature
temperature_error	size of time, size of latitude, size of pressure level	K	1 σ uncertainty of zonal mean monthly mean temperature

The dummy value of the temperature and temperature error is -999. This value is saved as attribute fillvalue of the temperature and temperature_error data fields in the NetCDF file. The global attributes are listed in Table 3.3.5.6.

Table 3.3.5.6. Global attributes for the Bodeker Scientific merged temperature data set NetCDF file.

Name	Value
Title	“Bodeker Scientific UTLS Merged Temperature Data Set”
description	“Zonal mean monthly mean temperatures on 17 pressure levels. Starting with the CHAMP temperature climate data record, MIPAS, GRACE, TSX, ACE-FTS and SMR (544.6 GHz) data sets are first bias corrected and then merged with CHAMP”
Version	“1.0”
Organization	“Bodeker Scientific, Alexandra, New Zealand”
Program	“clim7_netcdf.py”
Author	“Patrick Stoll”
Email	“patrick@bodekerscientific.com”
created	“2013-09-04 01:35:43”
modified	“2014-02-04 00:52:02”

This data set was then vertically integrated, using the MSU channel 4 vertical weighting function and the AMSU channel 9 off-nadir weighting function (described further in the ATBD), to calculate weighted means for comparison with MSU4 + AMSU9. This time series is provided in the NetCDF file

WeightedMergedTemps_BodekerScientificFinal.nc

The file contains zonal mean monthly mean temperatures integrated using the MSU channel 4 and AMSU channel 9 off-nadir weighting functions over all pressure levels. Latitudinal zones are 5° (with mid-points at 87.5°, 82.5°, 77.5°, ..., -87.5°). The format of the NetCDF file is described in Table 3.3.5.7.

Table 3.3.5.7. NetCDF format for the Bodeker Scientific vertically weighted temperature data set.

Data field	Dimension	Units	Description
time	144	months since January 1950	From January 2001 to December 2012 (January 1950 is month 0)
latitude	36	degrees	Mid-point of latitude zone
temperature	size of latitude, size of time	K	Zonal mean monthly mean temperature
temperature_uncertainties	size of latitude, size of time	K	1 σ uncertainty of zonal mean monthly mean temperature
nan_count	size of latitude,		Number of missing values in

	size of time		BSUTLS merged temperature data set
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If nan_count > 0 no vertically weighted temperature is calculated and both the temperature and temperature_uncertainties are set to 0. The global attributes are listed in Table 3.3.5.8.

Table 3.3.5.8. Global attributes of the Bodeker Scientific weighted temperature NetCDF file.

Name	Value
title	“Bodeker Scientific Vertically Weighted Mean Temperature”
description	“Zonal mean monthly mean temperature time series. Temperature profiles from BSUTLS merged temperature data set are averaged vertically to obtain time series for comparison with MSU4 + AMSU9”
version	“1.0”
organization	“Bodeker Scientific, Alexandra, New Zealand”
program	“BS_calculateWeightedTemp_intpress_netcdf.py”
author	“Patrick Stoll”
email	“patrick@bodekerscientific.com”
created	“2013-12-09 10:24:00”
modified	“2014-02-04 00:51:35”

4. References

- Ernst, F., C. von Savigny, A. Rozanov, V. Rozanov, K.-U. Eichmann, L. A. Brinkhoff, H. Bovensmann, and J. P. Burrows (2012), Global stratospheric aerosol extinction profile retrievals from SCIAMACHY limb-scatter observations, *Atmos. Meas. Tech. Discuss.*, 5, 5993-6035.
- Rozanov, A., Weigel, K., Bovensmann, H., Dhomse, S., Eichmann, K.-U., Kivi, R., Rozanov, V., Vömel, H., Weber, M., and Burrows, J. P.: Retrieval of water vapor vertical distributions in the upper troposphere and the lower stratosphere from SCIAMACHY limb measurements, *Atmos. Meas. Tech.*, 4, 933-954, doi:10.5194/amt-4-933-2011, 2011.