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ODIN/SMR

# Verification Dataset: Technical Note

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# Chapter 1 | Introduction

## 1.1 Aim and scope of this document

Odin/SMR performs passive limb measurements of the atmosphere, mainly at wavelengths and frequencies around 0.6 mm and 500 GHz, respectively. From these measurements, profiles of O<sub>3</sub>, ClO, N<sub>2</sub>O, HNO<sub>3</sub>, H<sub>2</sub>O, CO, and isotopologues of H<sub>2</sub>O, and O<sub>3</sub>, that are species that are of interest for studying stratospheric and mesospheric chemistry and dynamics, can be derived. Odin/SMR has been in operation for approximately 14 years, and thus, the Level2 dataset can potentially be applied for scientifically interesting trend analysis.

A new Odin/SMR Level2 product dataset will be generated, and this dataset will be based on updated/revised processing algorithms and input data. A verification dataset (VDS) will be used as a tool to verify the new processing system/Level2 products.

The aim of this document is to describe this VDS, and the API used for accessing the data. This VDS is a representative subset of the Odin/SMR Level1B dataset and collocated correlative measurements from similar instruments, i.e. Level2 data from Odin/OSIRIS, Aura/MLS, ENVISAT/MIPAS, ISS/JEM/SMILES, and Meteor3M/SAGEIII. Ground based measurements, i.e. ozone sonde and lidar observations, from a number of different stations, will also be used to verify the new Odin/SMR Level2 products. For convenience, the Odin/SMR Level2 data product produced with the older 2.0/2.1 versions of the processing chain is also accessible for the data in the VDS through the same API.

## 1.2 Document structure

This document is organized as follows: Chapter 2 describes the Odin/SMR Level2 data products. Chapter 3 describes the verification/correlative datasets included in the VDS, and how the VDS was constructed. Chapter 4 describes an API to the VDS.

# Chapter 2 | Odin/SMR Level2 data products

## 2.1 The Odin mission

The Odin satellite was launched on the 20th of February 2001, into a sun-synchronous 18:00 hour ascending node orbit, carrying two co-aligned limb sounding instruments: OSIRIS (Optical spectrograph and infrared imaging system) and SMR (Sub-millimetre radiometer) (Murtagh et al., 2002). Originally, Odin was used for both atmospheric and astronomical observations, but since 2007 only its aeronomy mission is active. Odin is a Swedish-led project, in cooperation with Canada, France and Finland. Both of Odin’s instruments are still functional, and the present operation of the satellite is partly performed as an ESA third party mission.

## 2.2 The SMR instrument

The Odin/SMR package is highly flexible (Frisk et al., 2003). In short, the four main receiver chains can be tuned to cover frequencies in the ranges 486–504 GHz and 541–581 GHz, but the maximum total instantaneous bandwidth is only 1.6 GHz. This bandwidth is determined by the two auto-correlation spectrometers (ACs) used for atmospheric observations. The two ACs can be coupled to any of the four front-ends, but only two or three front-ends are used simultaneously. The ACs cover 400 or 800 MHz per front-end, depending on configuration. In the configuration applied for atmospheric sounding, the channels of the ACs have a spacing of 1 MHz, while the frequency resolution is only 2 MHz. To cover all molecular transitions of interest (see Table 2.1 and Table 2.2 for an overview), a number of “observation modes” have been defined. Each observation mode makes use of two or three frequency bands. Single sideband operation is obtained by tunable Martin–Pupplet interferometers. The nominal sideband suppression is better than 19 dB across the image band.

Odin/SMR also has a receiver chain around the 118 GHz oxygen transition that was heavily used during Odin’s astronomy mission. For the atmospheric mission, this front-end was planned to be used for retrieving temperature profiles, but a technical problem (drifting LO frequency) and the fact that the analysis requires treatment of Zeeman splitting have given these data low priority.

The main reflector of Odin/SMR has a diameter of 1.1 m, giving a vertical resolution at the tangent point of about 2 km. The vertical scanning of the two instruments’ line-of-sight is achieved by a rotation of the satellite platform, with a rate matching a vertical speed of the tangent altitude of 750 m/s. Measurements are performed during both upward and downward scanning. The lower end of the scan is typically at about 7 km, the upper end

Table 2.1: Characteristics of Odin/SMR Level2 main data products.

Product	Frequency [GHz]	Vertical coverage	Vertical resolution	Precision	Reference
O <sub>3</sub>	501.5	~19–50 km	~2 km	0.5–2 ppmv	(Urban et al., 2005)
ClO	501.3	~19–67 km	1.5–2 km	0.15–0.2 ppbv	(Urban et al., 2005)
N <sub>2</sub> O	502.3	~15–70 km	~1.5 km	15–35 ppbv	(Urban et al., 2005)
O <sub>3</sub>	544.9	~18–70 km	~1.5 km	0.2–0.4 ppmv	(Urban et al., 2005)
HNO <sub>3</sub>	544.4	~21–67 km	1.5–2 km	1 ppbv	(Urban et al., 2005)

Table 2.2: Characteristics of Odin/SMR Level2 science data products.

Product	Frequency [GHz]	Vertical coverage	Vertical resolution	Precision	Reference
CO	578.6	~17–110 km	3–4 km	25 ppbv–2 ppmv	(Dupuy et al., 2004)
H <sub>2</sub> <sup>16</sup> O	556.9	~40–100 km	~3 km	0.5–1 ppmv	(Urban et al., 2007)
H <sub>2</sub> <sup>16</sup> O	488.5	~20–70 km	~3 km	0.5–1 ppmv	(Urban et al., 2007)
HDO	490.6	~20–70 km	3–4 km	0.5 ppbv	(Urban et al., 2007)
H <sub>2</sub> <sup>18</sup> O	489.1	~20–65 km	3–4 km	20–30 ppbv	(Urban et al., 2007)
H <sub>2</sub> <sup>17</sup> O	552.0	~20–70 km	~3 km	0.4 ppbv	(Urban et al., 2007)
NO	551.7	~40–100 km	~7 km	40 %	(Sheese et al., 2013)
<sup>16</sup> O <sup>18</sup> O <sup>16</sup> O	490.4	~27–41 km	4–6 km	25 %	(Urban et al., 2013)
<sup>16</sup> O <sup>16</sup> O <sup>18</sup> O	490.0	~25–45 km	3–4 km	25 %	(Urban et al., 2013)
<sup>16</sup> O <sup>16</sup> O <sup>17</sup> O	490.6	~31–39 km	5–6 km	25 %	(Urban et al., 2013)

varies between 70 and 110 km, depending on observation mode. In correspondence, the horizontal sampling ranges from 1 scan per 600 km to 1 scan per 1000 km. Measurements are in general performed along the orbit plane, providing a latitude coverage between 82.5°S and 82.5°N. Since the end of 2004 Odin is also pointing off-track during certain periods, e.g. during the austral summer season, allowing the latitudinal coverage to be extended towards the poles.

## 2.3 Odin/SMR Level2 data products

Odin/SMR data are categorized into main and science Level2 products, and Table 2.1 and Table 2.2 describe the characteristics of these products, respectively. The main products are retrieved from the so called “stratospheric” observation mode of Odin/SMR, and this mode cover approximately 50 % of the Odin/SMR observation time. In this mode spectra in frequency bands around 501 and 544 GHz are collected. The science data products are derived from less frequently applied observation modes (typically applied a few days per month).

### 2.3.1 Main data products

Ozone, ClO, N<sub>2</sub>O, and HNO<sub>3</sub> profiles are the main Odin/SMR Level2 products. ClO and N<sub>2</sub>O profiles are retrieved from spectra covering transitions around 501 GHz, and HNO<sub>3</sub> from spectra around 544 GHz. Ozone can be retrieved from both the 501 and the 544 GHz band. Table 2.1 describes characteristics of these Level2 products that have been derived from earlier Odin/SMR Level2 data studies. The characteristics can not be expected to be changed/improved dramatically for a new Level2 data product, because

these characteristics depend on the physics of the measurement and the sensor.

Possibly more important than the characteristics described in Table 2.1 are the accuracy and stability of the profiles, since the latter enable trend studies. The overall aim of the new Level2 data processing also reflects this aspect, and the objective is therefore that the accuracy and stability outperforms that from earlier Odin/SMR Level2 data products.

### 2.3.2 Science data products

Profiles of H<sub>2</sub>O, CO, NO and isotopologues of H<sub>2</sub>O, and O<sub>3</sub> are considered as science data products for Odin/SMR, and characteristics of these products are described in Table 2.2. Observations covering the science data products are performed on a less frequent basis than the main data products. The aim of the Level2 processing of the science data products is in principle identical to that for the main data products, although the main data products will be given a higher priority.

# Chapter 3 | Verification Dataset

## 3.1 Overview

The verification dataset (VDS) consists of a representative subset of the Odin/SMR complete dataset, and correlative datasets. In short, the VDS is a dataset of Odin/SMR measurements and collocated measurements from a number of correlative limb-sounding instruments, i.e. Aura/MLS, ENVISAT/MIPAS, ISS/JEM/SMILES, Meteor3M/SAGEIII, and Odin/OSIRIS. Table 3.1 gives an overview of the correlative datasets included in the VDS, and these datasets are described in more detail in Sect. 3.2. Collocated ground based measurements, i.e. ozone sonde and lidar observations, from a number of stations is also included in the VDS, and these are described in Sect. 3.3. Sect. 3.4 describes the collocation criteria applied and how the VDS was selected.

## 3.2 Correlative limb measurements

### 3.2.1 Aura/MLS

The Aura satellite was launched on 2004-07-15 into a sun-synchronous orbit at 705 km altitude, with an ascending equator crossing local time of 13:45. Its orbit is near-polar with a  $98^\circ$  inclination, and the daily Microwave Limb Sounder (MLS) measurements cover the latitudinal range from about  $82^\circ$  S to  $82^\circ$  N. MLS measures temperature and trace gas profiles using thermal emission data from the upper troposphere to the mesosphere. MLS performs each limb scan and related calibration in 25 s, and obtains  $\sim 3500$  vertical profiles a day (Waters et al., 2006). The MLS data processing algorithms are based on the optimal estimation method (OEM), as explained by Livesey et al. (2015). MLS uses spectral bands centered near 118, 190, 240, 640 GHz, and 2.3 THz.

The Aura/MLS Level2 products, and characteristics, included in the VDS are found in Table 3.2.

### 3.2.2 ENVISAT/MIPAS

The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) is a mid-infrared emission spectrometer mounted on the European ENVironmental SATellite (ENVISAT), which was launched in 2002-03-01 (Fischer et al., 2008), and was in operation until 2012-04-08. ENVISAT has a sun-synchronous orbit at an altitude of 800 km and with a  $98.55^\circ$  inclination and descending equator crossing local time of 10:00.

The failure of a MIPAS mirror slide in 2004 led to the division of the 10 years of MIPAS data into two operational periods: 2002–2004 when the instrument measured with high spectral resolution and 2005–2012 when the instrument measured with lower spectral but better vertical resolution.



Table 3.1: Odin/SMR VDS content for the various frequency modes of Odin/SMR:

Odin/SMR Frequency mode	Odin/SMR Frequency range [GHz]	Instrument	Species	Number of measurements
01	501.180–501.580, 501.980–502.380	SMILES	O <sub>3</sub> , ClO	2398,1384
		MLS	O <sub>3</sub> , ClO, N <sub>2</sub> O	11050
		MIPAS	O <sub>3</sub> , N <sub>2</sub> O	7228
		SAGEIII	O <sub>3</sub>	3115
		OSIRIS	O <sub>3</sub>	7168
02	544.102–544.902	SMILES	O <sub>3</sub> , HNO <sub>3</sub>	2367,1353
		MLS	O <sub>3</sub> , HNO <sub>3</sub>	10824
		MIPAS	O <sub>3</sub> , HNO <sub>3</sub>	7176
		SAGEIII	O <sub>3</sub>	3063
		OSIRIS	O <sub>3</sub>	7079
08	488.950–489.350, 488.350–488.750	SMILES	O <sub>3</sub>	618
		MLS	O <sub>3</sub> , H <sub>2</sub> O	10759
		MIPAS	O <sub>3</sub> , H <sub>2</sub> O	6249
		SAGEIII	O <sub>3</sub> , H <sub>2</sub> O	284
		OSIRIS	O <sub>3</sub>	2749
13	556.598–557.398	SMILES	O <sub>3</sub>	364
		MLS	O <sub>3</sub> , H <sub>2</sub> O	9352
		MIPAS	O <sub>3</sub> , H <sub>2</sub> O	5001
		SAGEIII	O <sub>3</sub> , H <sub>2</sub> O	170
		OSIRIS	O <sub>3</sub>	1870
14	576.062–576.862	SMILES	O <sub>3</sub>	409
		MLS	O <sub>3</sub> , CO	9547
		MIPAS	O <sub>3</sub> , CO	5005
		SAGEIII	O <sub>3</sub>	170
		OSIRIS	O <sub>3</sub>	1913
17	489.950–490.750	SMILES	O <sub>3</sub>	527
		MLS	O <sub>3</sub> , H <sub>2</sub> O	10566
		MIPAS	O <sub>3</sub> , H <sub>2</sub> O	6126
		SAGEIII	O <sub>3</sub> , H <sub>2</sub> O	263
		OSIRIS	O <sub>3</sub>	2638
19	556.550–557.350	SMILES	O <sub>3</sub>	604
		MLS	O <sub>3</sub> , H <sub>2</sub> O	10190
		MIPAS	O <sub>3</sub> , H <sub>2</sub> O	6127
		SAGEIII	O <sub>3</sub> , H <sub>2</sub> O	444
		OSIRIS	O <sub>3</sub>	2578
21	551.152–551.552, 551.752–552.152	SMILES	O <sub>3</sub>	583
		MLS	O <sub>3</sub> , H <sub>2</sub> O	9573
		MIPAS	O <sub>3</sub> , H <sub>2</sub> O, NO	4819
		SAGEIII	O <sub>3</sub> , H <sub>2</sub> O	80
		OSIRIS	O <sub>3</sub>	2508

Table 3.2: Characteristics of Aura/MLS, ENVISAT/MIPAS, ISS/JEM/SMILES, Meteor3M/SAGEIII, and Odin/OSIRIS Level2 data products included in the VDS.

Aura/MLS					
Product	Vertical coverage	Vertical resolution	Precision	Version	Reference
O <sub>3</sub>	261–0.02 hPa	3.5–5.5 km	0.03–1.2 ppmv	v04-20	(Livesey et al., 2015)
ClO	147–1.0 hPa	3–4.5 km	0.1–0.3 ppbv	v04-20	(Livesey et al., 2015)
N <sub>2</sub> O	68–0.46 hPa	5.4–11 km	~15 ppbv	v04-20	(Livesey et al., 2015)
HNO <sub>3</sub>	215–1.5 hPa	4–4.5 km	1–0.5 ppbv	v04-20	(Livesey et al., 2015)
H <sub>2</sub> O	316–0.002 hPa	1.3–10 km	4–152 %	v04-20	(Livesey et al., 2015)
CO	215–0.0046 hPa	3.8–6.2 km	9 ppbv–11 ppmv	v04-20	(Livesey et al., 2015)
ENVISAT/MIPAS					
Product	Vertical coverage	Vertical resolution	Precision	Version	Reference
O <sub>3</sub>	~10–60 km	3.5 – 8 km	0.1–0.2 ppmv	V5H-O3-21	(Steck et al., 2007)
	~10–70 km	2 – 6 km	0.03–0.09 ppmv	2002-07 – 2004-03 V5R-O3-22(4/5) 2005-01 – 2012-04	(Laeng et al., 2014)
N <sub>2</sub> O	~15–60 km	3–6 km	10–20 %	V5H-N2O-21	(Plieninger et al., 2015)
	~15–60 km	2.5–6 km	10–20 %	2002-07 – 2004-03 V5R-N2O-22(4/5) 2005-01 – 2012-04	(Plieninger et al., 2015)
HNO <sub>3</sub>	~20–50 km	3–8 km	2–6 %	V5H-HNO3-22 2002-07 – 2004-03 V5R-HNO3-22(4/5) 2005-01 – 2012-04	(Wang et al., 2007)
H <sub>2</sub> O	~15–50 km	3.5–4.5 km	5–10 %	V5H-H2O-20	(Milz et al., 2009)
	~20–50 km	2.3–6.9 km	0.2 – 0.9 ppmv	2002-07 – 2004-03 V5R-H2O-22(0/1) 2005-01 – 2012-04	(Stiller et al., 2012)
CO	~10–70 km	6–12 km	10–70 %	V5H-CO-20 2002-07 – 2004-03 V5R-H2O-22(0/1) 2005-01 – 2012-04	(Funke et al., 2007)
NO	~20–60 km	3.5–12 km	0.2–0.3 ppbv	V5H-NO-20 2002-07 – 2004-03 V5R-NO-22(0/1) 2005-01 – 2012-04	(Funke et al., 2005)
ISS/JEM/SMILES					
Product	Vertical coverage	Vertical resolution	Precision	Version	Reference
O <sub>3</sub>	16–73 km	2.3–3 km	2–5 %	JAXA v2.4 (008-11-0502)	(Imai et al., 2013)
ClO	20–60 km	3.5–10 km	20–50 %	JAXA v2.4 (008-11-0502)	(JAXA, 2013)
HNO <sub>3</sub>	18–40 km	~10 km	20–50 %	JAXA v2.4 (008-11-0502)	(JAXA, 2013)
Meteor3M/SAGEIII					
Product	Vertical coverage	Vertical resolution	Precision	Version	Reference
O <sub>3</sub>	6–85 km	~1 km	10 %	NASA v04	(NASA, 2004)
H <sub>2</sub> O	0–50 km	~1 km	5–15 %	NASA v04	(NASA, 2004)
Odin/OSIRIS					
Product	Vertical coverage	Vertical resolution	Precision	Version	Reference
O <sub>3</sub>	10–60 km	~2–3 km	3–4 %	SaskMART v5.07	(Adams et al., 2014)

MIPAS observed five mid-infrared spectral bands within the frequency range of 685 to 2410  $\text{cm}^{-1}$  (14.6 to 4.15  $\mu\text{m}$ ), with a resolution of 0.0625  $\text{cm}^{-1}$ . Until 2004-03-26 MIPAS scanned 17 tangent altitudes from 6 to 68 km with 3–8 km resolution. From January 2005 MIPAS started operating in a new mode at a reduced spectral resolution but at a finer altitude grid. The latitudinal coverage was from 87° S to 89° N. In the latter mode, MIPAS had about 95 scans per orbit, and about 1360 vertical profiles were recorded in a day.

Operational Level2 data from MIPAS is generated by ESA, but we here consider the MIPAS scientific data product generated by the Institut für Meteorologie und Klimatforschung (IMK) at Karlsruhe Institute of Technology (KIT).

The ENVISAT/MIPAS Level2 products and characteristics included in the VDS are found in Table 3.2.

### 3.2.3 ISS/JEM/SMILES

The Superconducting Submillimeter-Wave Limb-Emission Sounder (SMILES), attached to the Exposed Facility of the Japanese Experiment Module (JEM), on the International Space Station (ISS), is a joint project of the National Institute of Information and Communications Technology (NICT) and the Japan Aerospace Exploration Agency (JAXA). The ISS has a non-sun-synchronous circular orbit at altitudes of 340–360 km with an inclination angle of 51.6° to the equator.

SMILES observed a number of trace gases, e.g.:  $\text{O}_3$ ,  $\text{H}^{35}\text{Cl}$ ,  $\text{H}^{37}\text{Cl}$ ,  $\text{ClO}$ ,  $\text{HOCl}$ ,  $\text{HO}_2$ ,  $\text{BrO}$ , and  $\text{HNO}_3$ , from the upper troposphere up to the lower thermosphere, with a nominal latitudinal coverage from 38° S to 65° N, between 2009-10-12 and 2010-04-21. Trace gas profiles are derived from observed thermal emission in two frequency bands around 625 GHz and one around 650 GHz; 624.32–625.52 GHz (Band-A), 625.12–626.32 GHz (Band-B), and 649.12–650.32 GHz (Band-C), with a frequency resolution and channel separation of about 1 MHz and 0.8 MHz, respectively. During each measurement, two out of the three SMILES frequency bands were observed simultaneously, by two acousto-optical spectrometers, and with a receiver noise temperature of 310–350 K.

SMILES performed 1630 scans per day, where the limb was scanned from about -20 km to 120 km (geometric altitude), with a sampling interval of about 2 km, and with an angle of about 45° from the orbital plane. The size of the antenna beam, at the tangent point, was about 3 and 6 km in the vertical and horizontal direction, respectively.

An interesting feature of SMILES observation is related to the fact that ISS has a non-sunsynchronous orbit, which gives that SMILES observations cover different local times and thereby provides insight of the diurnal variation of atmospheric short-lived species (e.g.  $\text{ClO}$ ,  $\text{BrO}$ ,  $\text{HO}_2$ , and  $\text{HOCl}$ ). A two month period is required to accumulate measurements covering 24 h in local time for a given "position". However, such a dataset can also contain variation due to dynamical, seasonal, and latitudinal effects. A second characteristic of SMILES observation is that measured spectra and retrieved profiles have high precision due to its 4 K mechanically cooled superconducting receiver system.

The SMILES Level2 products and characteristics included in the VDS are found in Table 3.2.

### 3.2.4 Meteor3M/SAGE III

SAGE III on Meteor-3M (SAGEIII) was a third generation, satellite-borne instrument and an element in NASA's Earth Observing System (EOS) (NASA, 2004). The instrument was launched on the Russian Meteor-3M spacecraft on 2001-12-10 into a Sun-synchronous

orbit at an altitude of 1020 km and with an approximate 9:00 a.m. equatorial crossing time. The instrument was active from 2002-02-27 to 2005-11-12.

The SAGEIII instrument measures the attenuation of solar radiation resulting from the scattering and absorption by atmospheric constituents in the Earth's atmosphere as the spacecraft observes a sunrise or sunset event. Due to the orbital parameters, solar occultation measurement opportunities are limited to mostly high latitudes in the Northern Hemisphere (between 50° and 80° N) and mid-latitudes in the Southern Hemisphere (between 30° and 50° S). Level2 products from these measurements include profiles of ozone (O<sub>3</sub>), water vapour (H<sub>2</sub>O) and nitrogen dioxide (NO<sub>2</sub>). Of these O<sub>3</sub> and H<sub>2</sub>O have been included in the VDS. The ozone profiles are reported as reliable within 10% for the altitude range 6–85 km, whereas the water vapour profiles are reported reliable to have an uncertainty of less than 5% for altitudes of 0–33 km and in the interval 5–15% for altitudes 33–50 km. The SAGEIII Level2 products and characteristics included in the VDS are found in Table 3.2.

Similar measurements were made during the lunar moonrise and moonset. These measurements were made only during the second and third quarter phases of the Moon and when the atmosphere along the line-of-sight was not directly illuminated by the Sun. Level2 products from these measurements include profiles of ozone (O<sub>3</sub>), nitrogen dioxide (NO<sub>2</sub>), nitrogen trioxide (NO<sub>3</sub>) and chlorine dioxide (ClO). Due to poor data coverage, none of these products have been included in the VDS, but are listed here for completeness.

### 3.2.5 Odin/OSIRIS

Odin has two optically co-aligned instruments: the SMR and the Optical Spectrograph and InfraRed Imager System (OSIRIS) (Llewellyn et al., 2004). OSIRIS measures limb-scattered sunlight within the wavelength range of 280 - 800 nm with a spectral resolution of approximately 1 nm, OSIRIS is capable of measuring vertical profiles of stratospheric O<sub>3</sub>, NO<sub>2</sub>, and aerosols. Ozone measurements are only taken in the summer hemisphere, with coverage in both hemispheres in the spring and autumn. Nominally OSIRIS generates approximately 30 O<sub>3</sub> profiles per orbit over the sunlit hemisphere. Characteristics of OSIRIS Level2 O<sub>3</sub> product are found in Table 3.2.

## 3.3 Ground based measurements

### 3.3.1 NDACC, SHADOZ, and WOUDC networks

The vertical distribution of ozone can be measured by ground-based stratospheric ozone lidars and by balloon-borne electrochemical ozonesondes. Such ground-based instruments are often operated in networks, and one of the principal goals of these networks are to provide independent calibrations and validations of space-based sensors of the atmosphere and to make complementary measurements.

The international Network for the Detection of Atmospheric Composition Change (NDACC) (<http://www.ndsc.ncep.noaa.gov/>). is composed of more than 70 high-quality, research stations for observing and understanding the physical and chemical state of the upper troposphere, stratosphere and mesosphere, and for assessing the impact of changes in the stratosphere on the underlying troposphere and on global climate. Ozone and key ozone-related chemical compounds and parameters are targeted for measurements. NDACC is a major component of the international upper atmosphere research effort.

Southern Hemisphere ADditional OZonesondes (SHADOZ) (<http://croc.gsfc.nasa.gov/shadoz/>) is a collection ozonesonde stations that are operating in the tropics and

Table 3.3: Sonde and lidar stations included in the VDS. Nr of profiles = number of collocations to Odin/SMR frequency mode 1 ozone measurements.

Network	Station	Coordinates	Technique	Nr of profiles
NDACC	ANDOYA	69.3°N 16.0°E	Lidar	148
NDACC	DUMONT D'URV	66.7°S 140.0°E	Lidar	162
NDACC	EUREKA	80.0°N 86.3°W	Lidar	53
NDACC	HOHENPEISSEN	47.8°N 11.06°E	Lidar	380
NDACC	LAUDER	45.0°S 169.7°E	Lidar/Sonde	339/185
NDACC	MAUNA LOA	19.5°N 155.2°W	Lidar	486
NDACC	NY-ALESUND	78.6°N 12.0°E	Lidar/Sonde	249/252
NDACC	OHP	43.9°N 5.7°E	Lidar	530
NDACC	RIO GALLEGOS	51.6°S 69.3°W	Lidar	74
NDACC	REUNION.ST	20.9°S 55.480°E	Lidar	14
NDACC	TABLE MTN	34.4°N 117.7°W	Lidar	412
NDACC	TSUKUBA	36.0°N 140.1°E	Lidar	71
NDACC	ALERT	82.5°N 62.3°E	Sonde	261
NDACC	SOUTH POLE	89.6°S 24.5°W	Sonde	302
NDACC	BOULDER	39.7°N 105.0°W	Sonde	148
NDACC	DE BILT	52.1°N 5.18°E	Sonde	344
NDACC	TORONTO	43.8°N 79.5°W	Sonde	147
NDACC	EUREKA	80.0°N 86.3°W	Sonde	319
NDACC	HILO	19.7°N 155.1°W	Sonde	124
NDACC	HOHENPEISSEN	47.8°N 11.02°E	Sonde	694
NDACC	HUNTSVILLE	34.72°N 86.65°W	Sonde	95
NDACC	IZANA	28.3°N 16.5°W	Sonde	163
NDACC	PRAHA	50.01°N 14.45°E	Sonde	363
NDACC	MACQUARIE	54.5°S 158.94°E	Sonde	198
NDACC	SCOTT BASE	77.85°S 166.78°E	Sonde	137
NDACC	NATAL	6.1°S 35.3°W	Sonde	123
NDACC	PAYERNE	46.82°N 6.95°E	Sonde	1073
NDACC	PARAMARIBO	5.75°N 55.2°W	Sonde	155
NDACC	REUNION.ST	20.9°S 55.48°E	Sonde	141
NDACC	RESOLUTE	74.2°N 95.0°W	Sonde	160
NDACC	IZANA	28.3°N 16.5°W	Sonde	36
NDACC	SCORESBYSUND	71.0°N 22.0°W	Sonde	393
NDACC	SODANKYLA	67.0°N 27.0°E	Sonde	277
NDACC	SUMMIT	72.34°N 38.29°W	Sonde	143
NDACC	SYOWA BASE	69.0°S 39.6°E	Sonde	387
NDACC	THULE	77.3°N 69.3°W	Sonde	68
NDACC	TABLE MTN	34.4°N 117.7°W	Sonde	7
NDACC	SAMOA	14.23°S 170.56°W	Sonde	75
NDACC	UCCLE	50.8°N 4.35°E	Sonde	990
NDACC	VALENTIA	51.93°N 10.25°W	Sonde	174
NDACC	GSFC	38.9°N 76.7°W	Sonde	5
NDACC	ALTZOMONI	19.12°N 98.66°W	Sonde	7
NDACC	ASCENSION IS.	8.0°S 14.4°W	Sonde	151
SHADOZ	FIJI IS.	18.1°S 178.4°W	Sonde	54
SHADOZ	NAIROBI	1.3°S 36.8°W	Sonde	167
SHADOZ	MALININDI	3.0°S 40.2°W	Sonde	20
SHADOZ	SAN CRISTOBAL	0.9°S 89.60°E	Sonde	87
SHADOZ	IRENE	25.9°S 28.2°W	Sonde	57
SHADOZ	WATUKOSEL	7.5°S 112.6°E	Sonde	72
WOUDC	REGINA	50.21°N 104.71°W	Sonde	143
WOUDC	EDMONTON	53.55°N 114.1°W	Sonde	274
WOUDC	GOOSE BAY	53.31°N 60.363°W	Sonde	234
WOUDC	KELOWNA	49.92°N 119.4°W	Sonde	160
WOUDC	YARMOUTH	43.87°N 66.11°W	Sonde	174
-	MADRID	40.45°N 3.71°W	Sonde	238
-	TRINIDAD HEAD	40.80°N 124.15°W	Sonde	23
-	PELLSTON	45.56°N 84.68 °W	Sonde	2
-	HOUSTON	29.72°N 95.4°W	Sonde	16
-	MARAMBIO	64.23°S 56.6°W	Sonde	318
-	NEUMAYER	70.688°S 8.26°W	Sonde	536
-	BROADMEADOW	37.78°S 144.95°E	Sonde	190
-	COTONUO	6.21°N 2.23°E	Sonde	40
-	DAVIS	68.588°S 77.97°E	Sonde	160
-	VANSCOY	52.02°N 107.03°W	Sonde	7
-	BARBADOS	13.16°N 59.43°W	Sonde	4
-		32.48°N 51.42°E	Sonde	46

subtropics.

The World Ozone and Ultraviolet Radiation Data Centre (WOUDC) is a data center operated by the Meteorological Service of Canada. There are over 500 registered stations, and O<sub>3</sub> data-sets include vertical profile data from lidar measurements and ozonesonde flights.

Data from 12 (lidar: all from NDACC) and 57 (sonde: from NDACC, SHADOZ, and WOUDC) stations is included in the VDS. The station names and coordinates are given in Table 3.3. An overview of the geographical positions of the stations and collocations to Odin/SMR is displayed in Fig. 3.1.

## 3.4 Verification Dataset: collocation criteria and data selection

### 3.4.1 Limb observation

The VDS should ideally include Odin/SMR measurements and correlative collocated data from the complete mission and for all geographical regions. In this section we describe how the VDS was constructed in order to fulfill this criteria.

Two measurements are considered to be collocated if they are close in time and space. The applied collocations criteria are adjusted for the various sensors, in order to result in a useful comparison dataset, as described below:

Odin/SMR and SMILES measurements are considered to be collocated if the differences in distance and observation time between the two profiles are less than 300 km and 1 h, respectively. All measurements that fulfill this criteria are included in the VDS. This subset of the VDS covers 60° N–40° S for the SMILES active observation period, as can be seen in Fig. 3.2.

Odin/SMR and SAGEIII measurements are considered to be collocated if the difference in distance and observation time between the two profiles are less than 300 km and 3 h, respectively. This subset of the VDS covers approximately 80° N–50° N and 40° S–60° S for the SAGEIII active observation period, as can be seen in Fig. 3.2

A problem with a “strict” time difference criteria between Odin/SMR and both ENVISAT/MIPAS and Aura/MLS is that collocations are only found for high latitudes (around 80° N and around 80° S), due to the fact each of these platform follows a sun-synchronous orbit with quite different ascending equator crossing local times (18:00 hour for Odin/SMR 10:00 hour for ENVISAT/MIPAS, 13:45 hour for Aura/MLS). Thus, for low latitudes the time difference criteria is relaxed to 6 hour for ENVISAT/MIPAS and Aura/MLS. This gives effectively that collocated ENVISAT/MIPAS and Aura/MLS measurements can be found for almost all Odin/SMR measurements, and a strategy to reduce the size of the VDS must be applied.

The set of collocated measurements for ENVISAT/MIPAS and Aura/MLS is reduced in size in the following way: For each Odin/SMR observation mode and month, five collocated scans each for ENVISAT/MIPAS and Aura/MLS are selected, within each 10° latitude bin (85° N–75° N, 75° N–65° N, . . . , 75° S–85° S), to be included in the VDS. For the two outer latitude bins the time difference criteria is 1 h, while for the other bins it is set to 6 h. Figure 3.2 shows a graphical view of the position in time and space for the measurements included in the VDS for frequency mode 1 of Odin/SMR.

The Odin/SMR and Odin/OSIRIS instruments are optically co-alignend and thus the measurements can always be seen as highly collocated. The selection of which OSIRIS measurements to include in the VDS is based on which measurements that are included

for MIPAS, MLS, SAGEIII, and SMILES, in order to not construct a too large VDS. That is, OSIRIS measurements are included in the VDS for all selected collocations between Odin/SMR and the other sensors, given that OSIRIS measurements are available.

The total number of limb measurement collocations included in the VDS, for the various Odin/SMR frequency modes, is displayed in Table 3.1. This gives that a few percent of the total Odin/SMR dataset is included in the VDS. Included measurements cover approximately all geographical positions and the complete observation period of Odin/SMR.

#### 3.4.2 Ground based observation

The VDS also contains collocations between Odin/SMR and ground based observations (lidar and sonde measurements). This collocation dataset was compiled by Daan Hubert using data that was used within the Ozone CCI project (<http://www.esa-ozone-cci.org/>). Collocations criterias for this dataset is that the distance and observation time between the two Ozone profiles are less than 1000 km and 12 h, respectively. The locations of the included stations and an overview of the collocations are given in Figure 3.1. The total size of this dataset is 14000 samples (11482 sonde- and 2918 lidar-profiles).



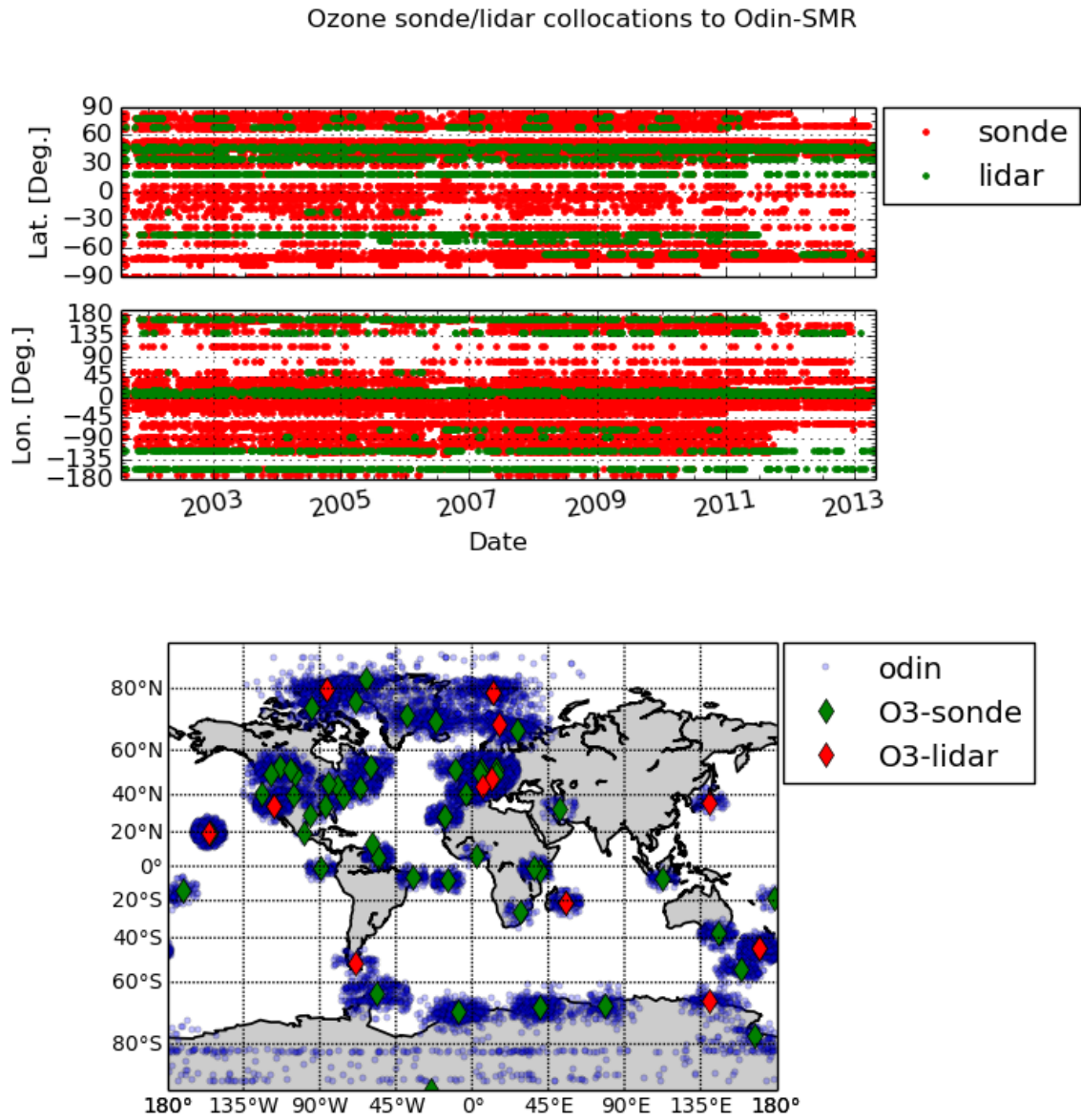


Figure 3.1: Positions of ground based ozone sonde and lidar stations included in the VDS. The figure also displays collocations between ground based and Odin/SMR measurements that is included in the VDS.



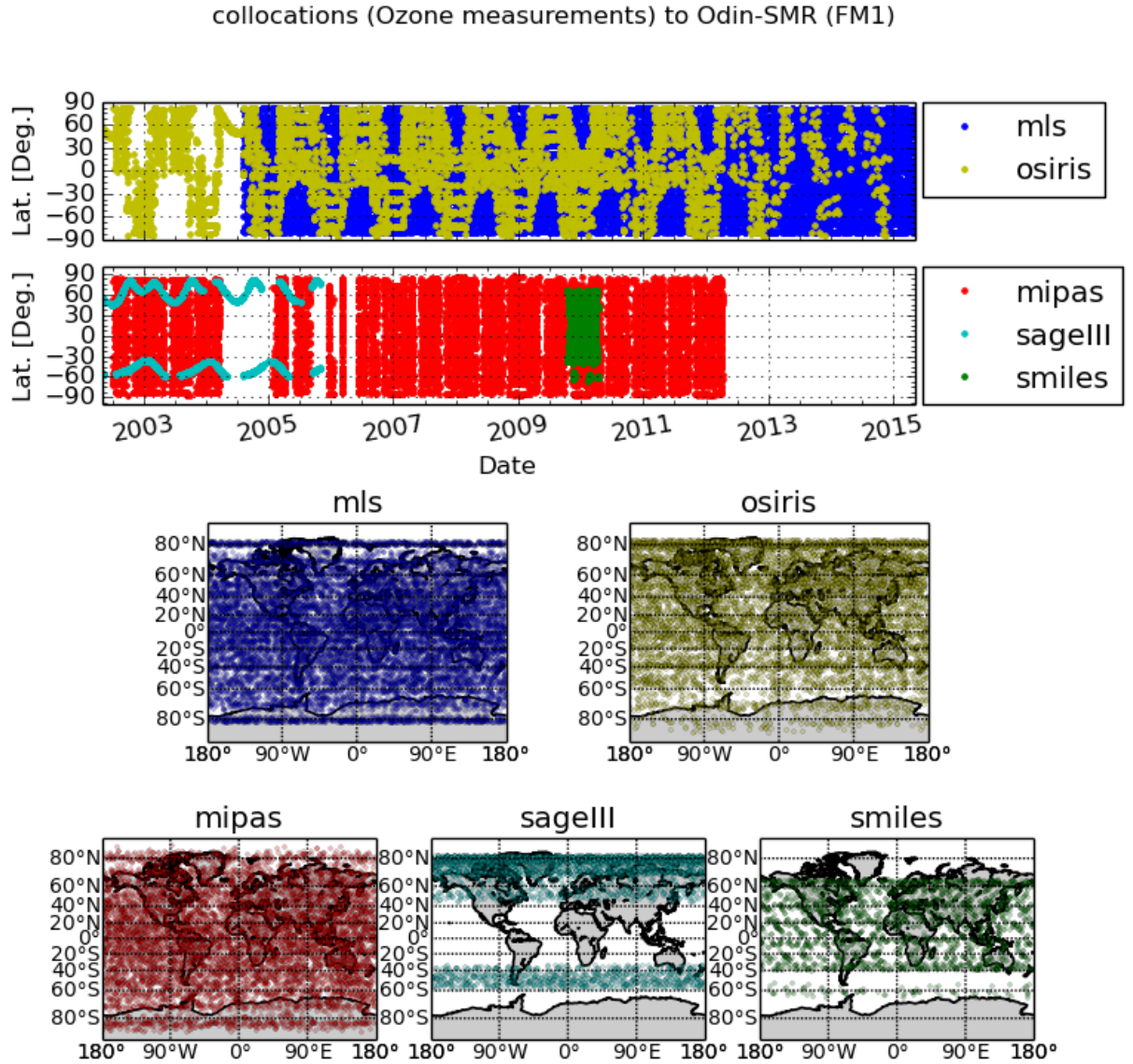


Figure 3.2: Positions of collocations for the various limb instruments and Odin/SMR frequency mode 1 scans, included in the VDS. The upper two panels show the latitude of the collocations as function of time. The bottom panels show the geographical coverage of the collocations between Odin/SMR and the other instruments.

# Chapter 4 | API description

This section describes the API calls used to get data from the VDS. The data is accessed through a hierarchical REST API where deeper URIs return more specific data. All call URIs have a common root `rest_api/<version>`, which has been omitted below for clarity. All GET calls return JSON objects unless otherwise noted. Key/value pairs are listed as name of the key along with the type of the corresponding value within parantheses, followed by a brief description of the contents. See the sections on the different data sources for specifications on the structure of their respective JSON objects.

## 4.1 API calls

### 4.1.1 `vds`

Method: *GET*

Returns object with the following attributes:

- VDS:

A list of objects containing information about colocated scans, grouped by backend and frequency mode. Each object contains the following keys:

- Backend (*String*): The backend for the data
- FreqMode (*Int*): The frequency mode for the data
- URL-allscans (*URI*): A URI for getting a list of all scans from the VDS for the Backend/FreqMode pair
- URL-collocations (*URI*): A URI for getting a more specific list of the data available for the Backend/FreqMode pair

### 4.1.2 `vds/<backend>/<freqmode>`

Method: *GET*

Returns object with the following attributes:

- VDS:

A list of objects containing information about colocated scans for the chosen backend and frequency, grouped by instrument and species. Each object contains the following keys:

- Backend (*String*): The backend for the data
- FreqMode (*Int*): The frequency mode for the data

- Instrument (*String*): The name of the instrument with which the VDS data is collocated
- NumScan (*Int*): Number of collocated scans
- Species (*String*): The species the collocated data considers
- URL (*URI*): A URI for getting a more specific list of the data available for the Instrument/Species pair

#### 4.1.3 `vds/<backend>/<freqmode>/allscans`

Method: *GET*

Returns object with the following attributes:

- VDS:

A list of objects containing detailed information about all the scans in the VDS for the chosen backend and frequency. Each object contains the following keys:

- Info (*Object*): Object containing information about the Odin/SMR scan, such as time and geolocation
- URLS (*Object*): Object containing URIs for getting the Odin/SMR spectra and apriori data for the specific scan, as well as the PTZ data

#### 4.1.4 `vds/<backend>/<freqmode>/<species>/<instrument>`

Method: *GET*

Returns object with the following attributes:

- VDS:

A list of objects containing information about collocated scans for the chosen backend, frequency, species and instrument, grouped by date. Each object contains the following keys:

- Backend (*String*): The backend for the data
- Date (*String*): The date (in ISO format) on which the data was collected
- FreqMode (*Int*): The frequency mode for the data
- Instrument (*String*): The name of the instrument with which the VDS data is collocated
- NumScan (*Int*): Number of collocated scans
- Species (*String*): The species the collocated data considers
- URL (*URI*): A URI for getting a more specific list of the data available for the particular date

#### 4.1.5 `vds/<backend>/<freqmode>/<species>/<instrument>/<date>`

Method: *GET*

Returns object with the following attributes:

- VDS:

A list of objects containing detailed information about the scans for the chosen backend, frequency, instrument, species and date. Each object contains the following keys:

- CollocationInfo (*Object*): Object containing information about the collocated measurement, such as time and geolocation, as well as Delta time and angular distance between the Odin/SMR scan and the collocated data from the selected instrument
- OdinInfo (*Object*): Object containing information about the Odin/SMR scan, such as time and geolocation
- URLS (*Object*): Object containing URIs for getting the Odin/SMR spectra and apriori data for the specific scan, as well as the PTZ data, and the collocated data from the selected instrument

#### 4.1.6 `vds_external/<instrument>/<species>/<date>/<file>/<file_index>`

Method: *GET*

Returns object containing the data for the specified instrument, species and date. See Sect. B for details on their respective data structures.

## 4.2 Example usage

This is a brief example of how to use the VDS API in Python. The basic procedure for navigating the call hierarchy is the same in all major programming languages and browsers.

*# Setup the name space:*

```
import requests
```

*# Start by making a request to the root URI of the VDS API:*

```
r0 = requests.get("http://odin.rss.chalmers.se/rest_api/v4/vds/")
```

*# The request contains the returned JSON object, which in Python is a dictionary, which can be printed or inspected to find out its keys and contents. Let's assume that we have done that, or that we have read the API documentation, so that we know that 'FreqMode' is a key.*

*# Use this to single out the frequency mode of interest, in this case 2:*

```
FM2 = [x for x in r0.json()['VDS'] if x['FreqMode'] == 2][0]
```

*# Make a new request using the URI provided in the JSON object, and single out the species O3 and the instrument MLS:*

```
r1 = requests.get(FM2["URL-collocation"])
O3MLS = [x for x in r1.json()['VDS'] if x['Species'] == 'O3' and
         x['Instrument'] == 'mls'][0]
```

*# Repeat for the new object and a date of interest:*

```
r2 = requests.get(O3MLS['URL'])
day = [x for x in r2.json()['VDS'] if x['Date'] == '2012-09-15'][0]
```

*# To get the detailed information about the collocated scans on that day, we make one more request:*

```
r3 = requests.get(day['URL'])
scanData = r3.json()['VDS']
```

*# scanData contains URIs for getting all the collocated Odin/SMR scans for 2012-09-15, as well as the data from MLS. As a final step, let's request the latter for the first of the collocated scans for our chosen frequency mode, species, instrument and day:*

```
r4 = requests.get(scanData[0]['URLS']['URL-mls-O3'])
mlsData = r4.json()
```

*# Now we have the data at hand and can proceed with crunching it!*



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# Appendix A | Verification dataset figures

The following figures show the positions of scans/profiles for the various datasets included in the VDS for each frequency mode of Odin/SMR.

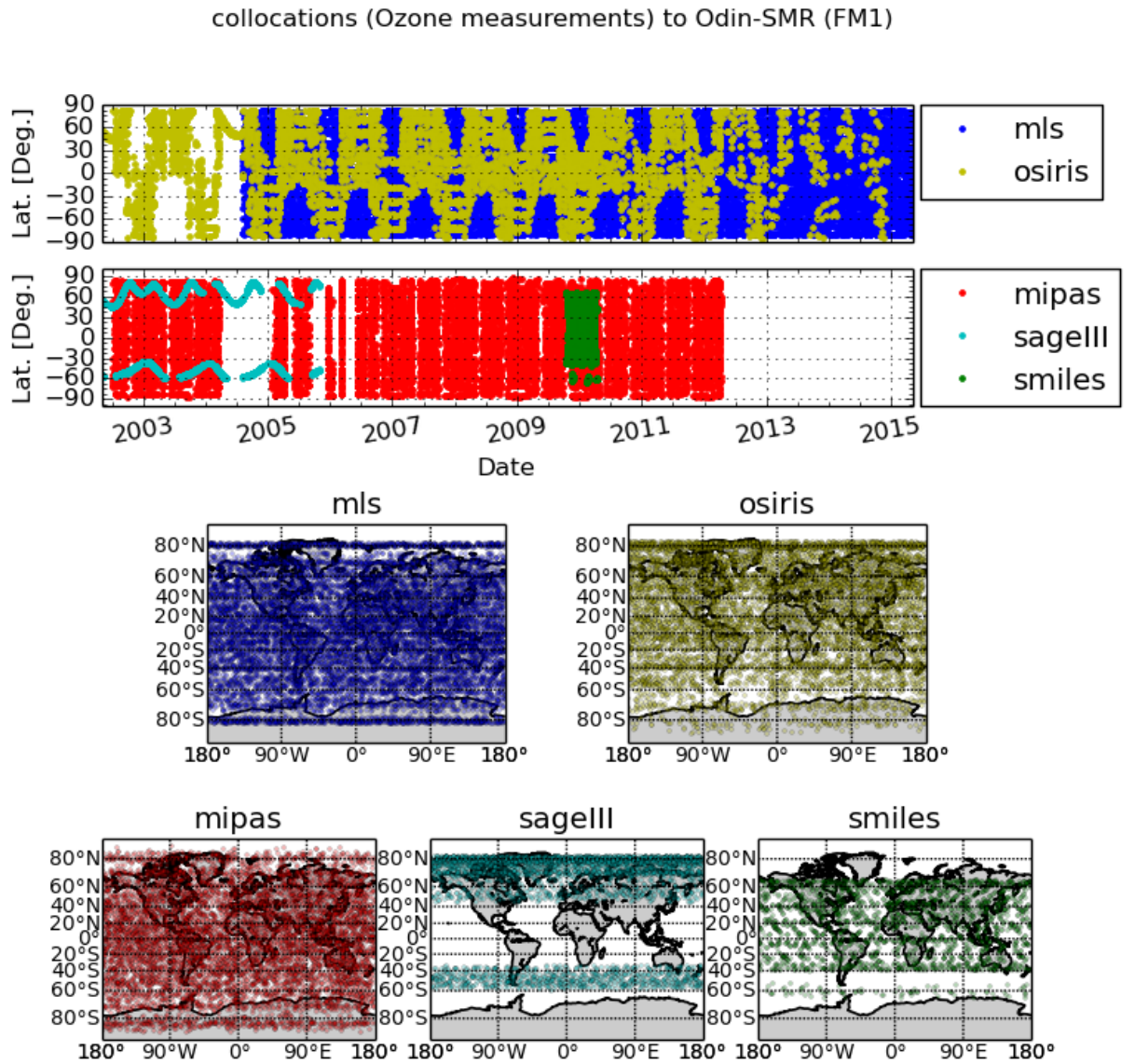


Figure A.1: VDS:Positions of collocated scans for frequency mode 1.

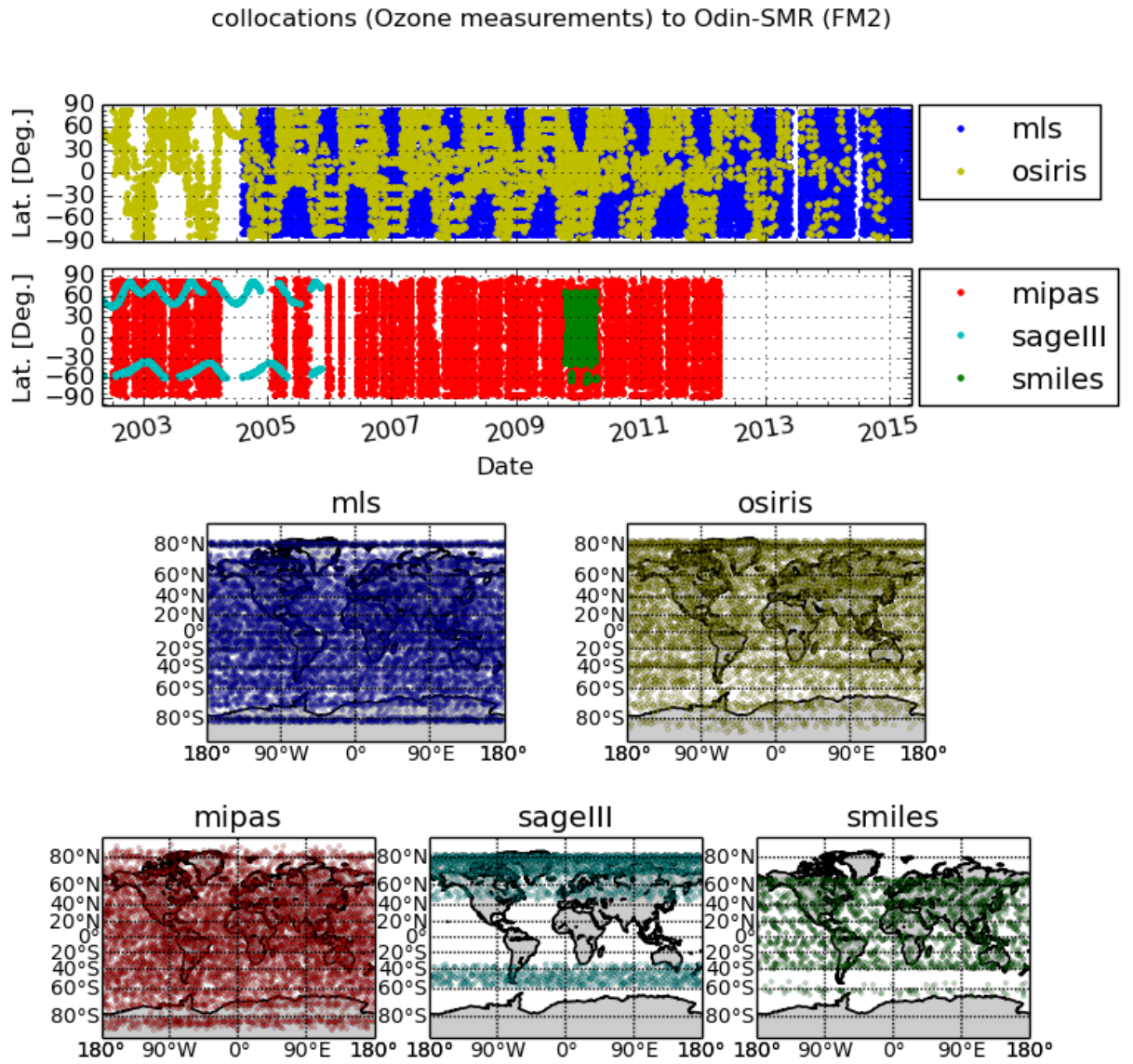


Figure A.2: VDS:Positions of collocated scans for frequency mode 2.

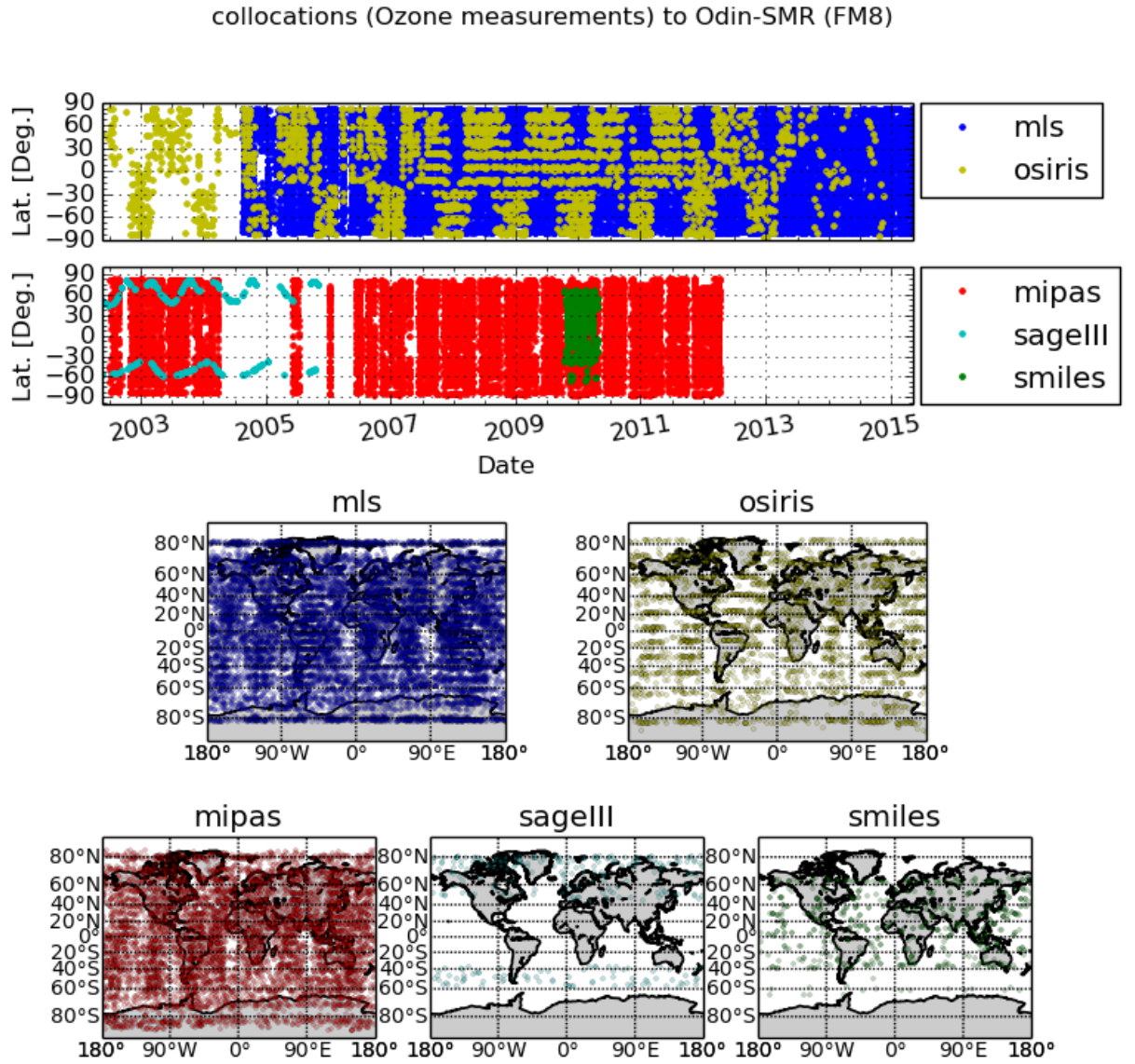


Figure A.3: VDS:Positions of collocated scans for frequency mode 8.



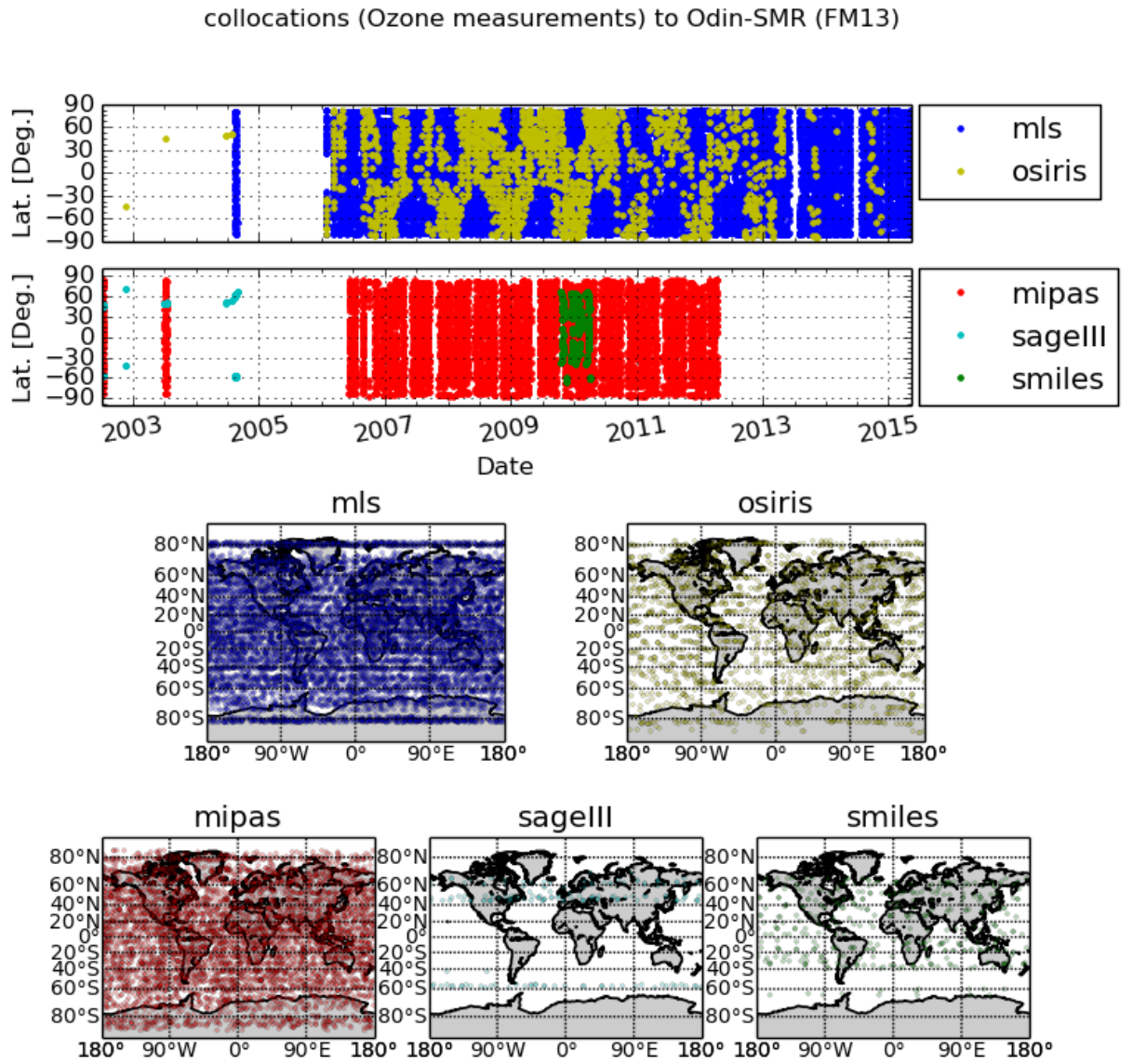


Figure A.4: VDS:Positions of collocated scans for frequency mode 13.

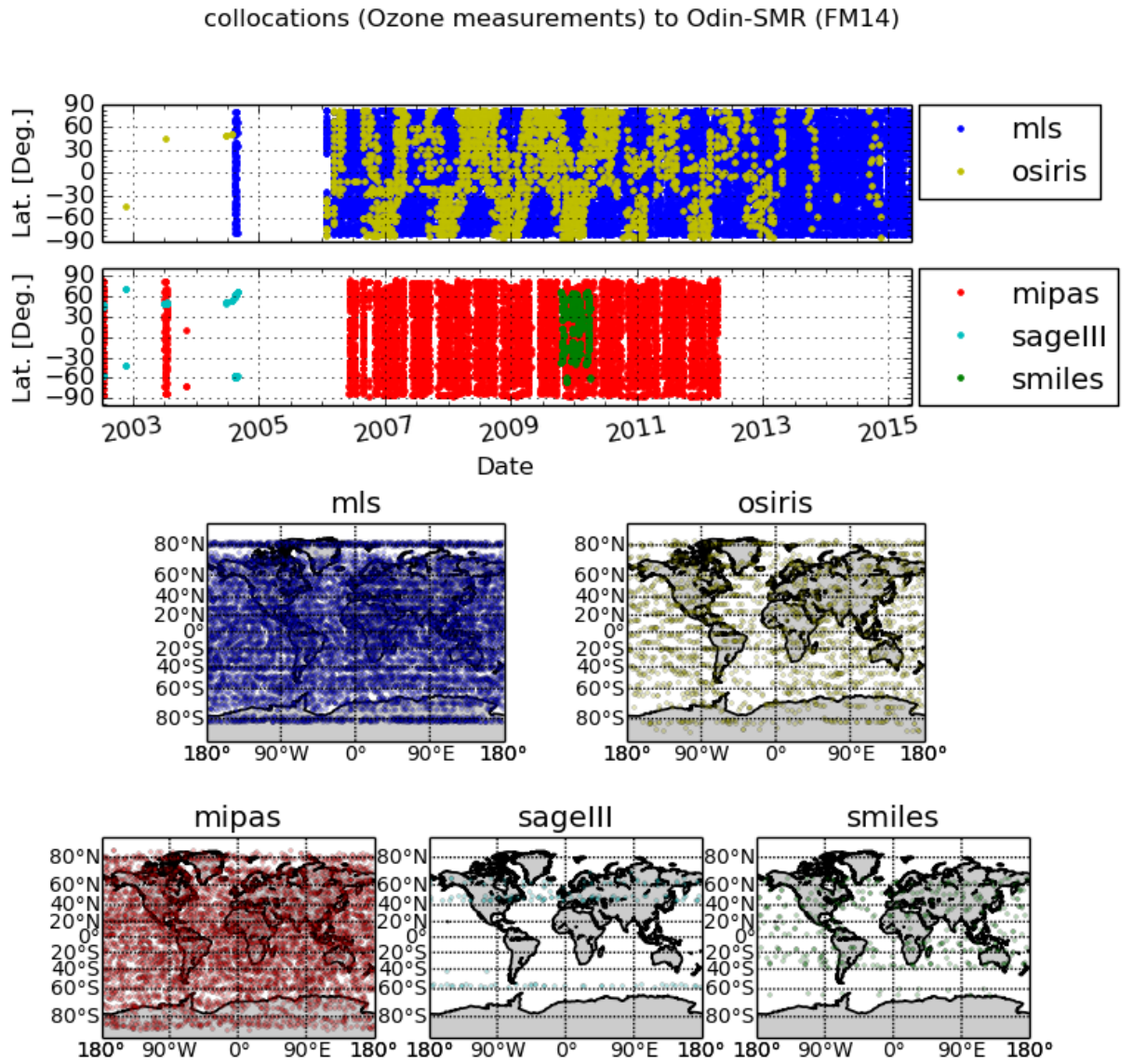


Figure A.5: VDS:Positions of collocated scans for frequency mode 14.

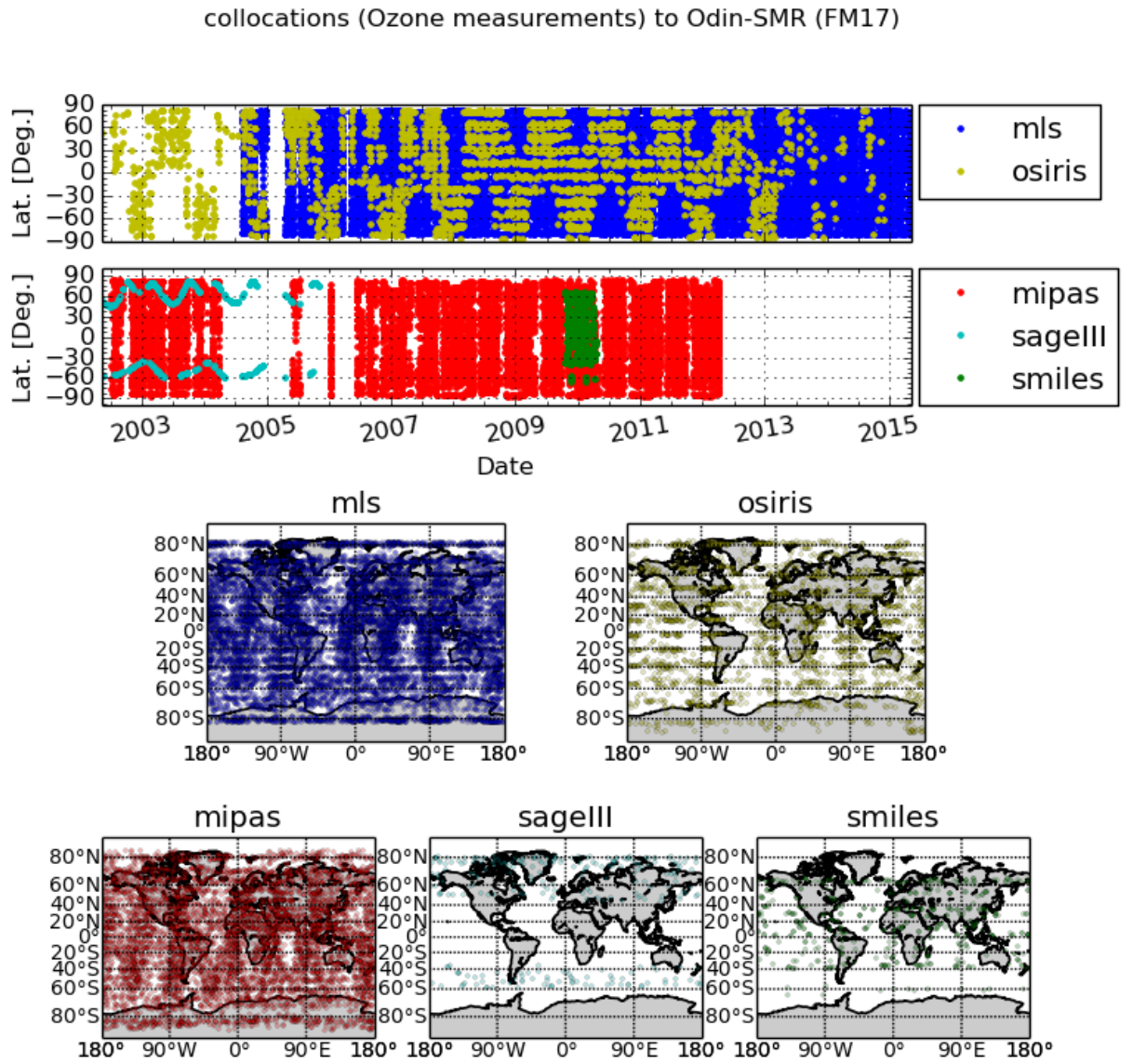


Figure A.6: VDS:Positions of collocated scans for frequency mode 17.



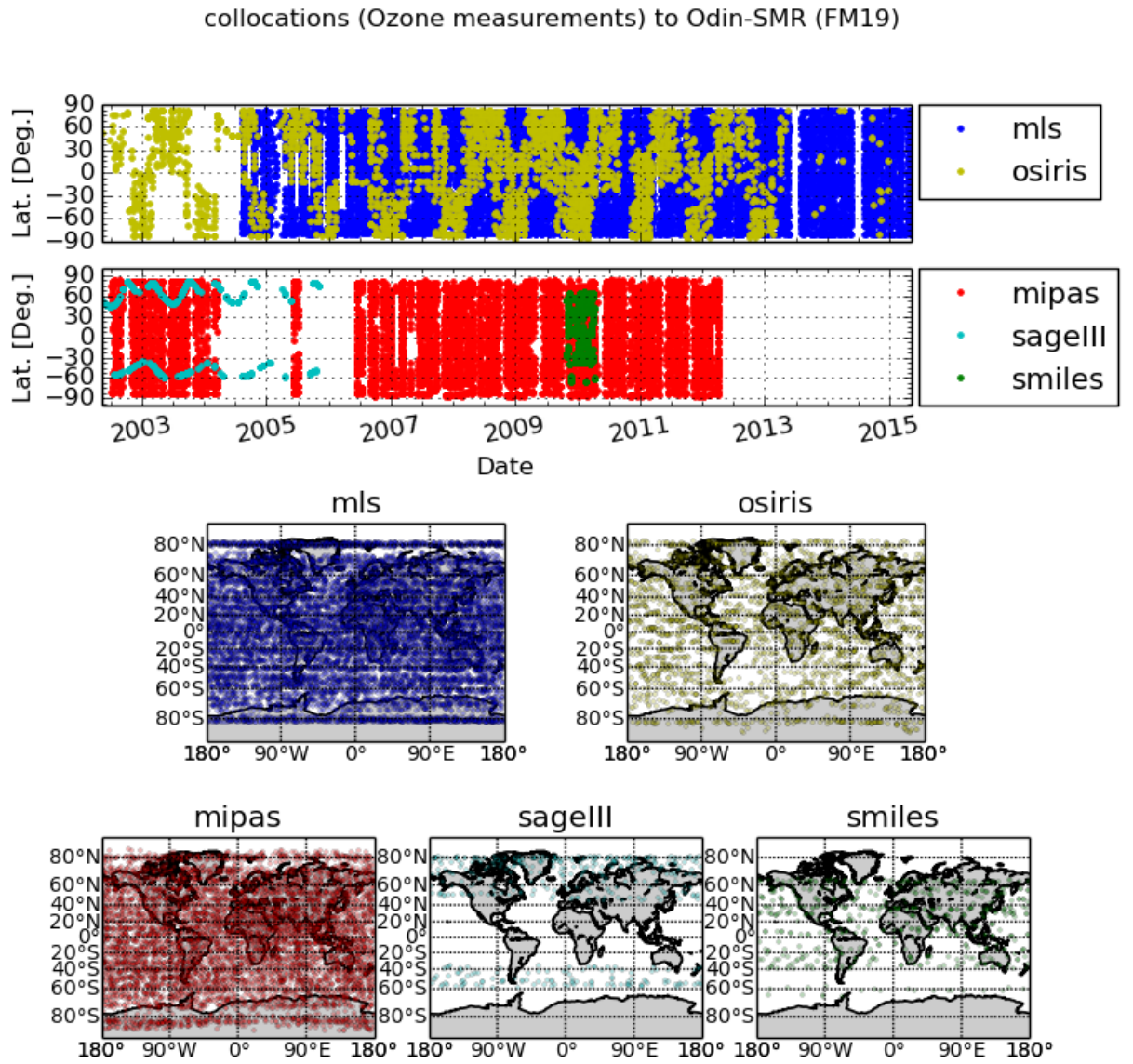


Figure A.7: VDS:Positions of collocated scans for frequency mode 19.

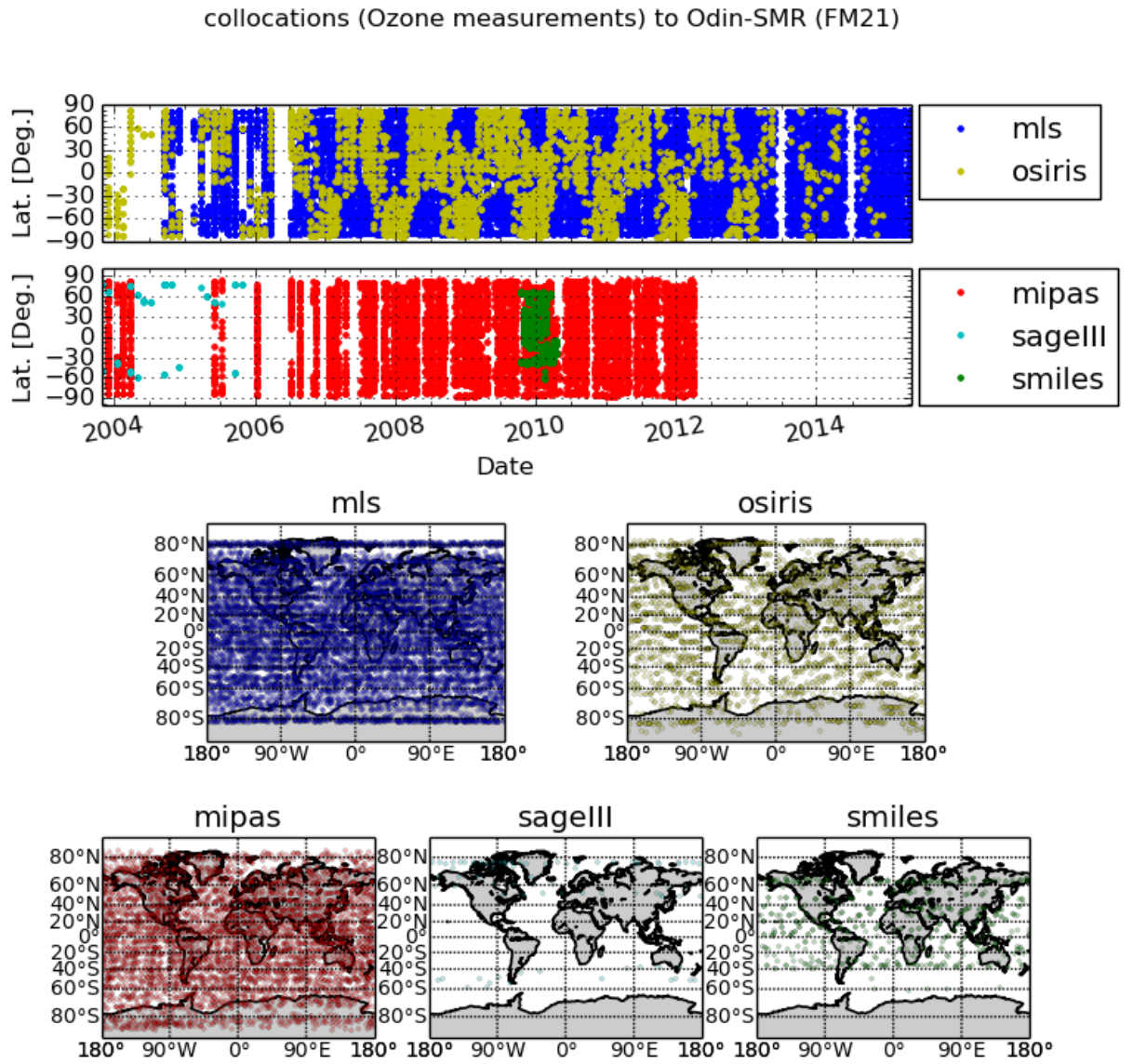


Figure A.8: VDS:Positions of collocated scans for frequency mode 21.

# Appendix B | Data formats for the instruments

## B.1 Aura/MLS

The MLS data collocated with Odin/SMR is accessible through the Odin REST API, see section 4. The data is returned as a JSON object with the following attributes:

- `data_fields` (*Object*): Object containing the data under the following keys:
  - `AscDescMode` (*Int*): 0 for ascending, 1 for descending measurement mode
  - `<Species>` (*Array of doubles*): Concentration profile for `<Species>`
  - `<Species>Precision` (*Array of doubles*): Precision of the concentration profile for `<Species>`
  - `L2gpValue` (*Array of doubles*): Concentration profile for `<Species>`
  - `L2gpPrecision` (*Array of doubles*): Precision of the concentration profile for `<Species>`
  - `Quality` (*Double*): Quality; larger is generally better
  - `Status` (*Int*): Status code; use with caution if non-zero, don't use of odd
  - `Convergence` (*Double*): Convergence of retrieval algorithms; values near unity indicate good convergence
- `geolocation_fields` (*Object*): Object containing the geolocation of the data under the following keys:
  - `ChunkNumber` (*Int*): Number of chunks used in retrieval
  - `Latitude` (*Double*): Latitude for the observation
  - `Longitude` (*Double*): Longitude for the observation
  - `LineOfSightAngle` (*Double*): Line of sight angle for the observation
  - `LocalSolarTime` (*Double*): Local solar time for the observation
  - `MJD` (*Double*): Time for the observation in MJD
  - `Time` (*Double*): Time for the observation in TAI units
  - `OrbitGeodeticAngle` (*Double*): The geodetic angle of the orbit at the time observation
  - `SolarZenithAngle` (*Double*): The solar zenith angle for the observation
  - `Pressure` (*Array of doubles*): Pressure profile for the observation

## B.2 ENVISAT/MIPAS

The MIPAS data collocated with Odin/SMR is accessible through the Odin REST API, see section 4. The data is returned as a JSON object with the following attributes:

- *MJD (Double)*: Time in MJD for the observation
- *time (Double)*: Time of the observation in days since 1970-01-01T00:00:00
- *altitude (Array of doubles)*: Altitudes for the observation
- *latitude (Double)*: Latitude for the observation
- *longitude (Double)*: Longitude for the observation
- *los (Array of doubles)*: Line of sight angles for the observation
- *sza (Double)*: Sun zenith angle for the observation
- *geo\_id (Array of strings)*: Geolocation identifier
- *sub\_id (Array of strings)*: Sub-project identifier
- *pressure (Array of doubles)*: Pressure profile for the observation
- *temperature (Array of doubles)*: Temperature profile for the observation
- *chi2 (Double)*:  $\chi^2$  of retrieval
- *dof (Double)*: Degrees of freedom of target retrieval
- *eta (Array of doubles)*: Engineering tangent altitude
- *eta\_indices (Array of ints)*: Indices of used engineering tangent altitude
- *rms (Double)*: Root mean square of residual
- *target (Array of doubles)*: Target profiles
- *target\_noise\_error (Array of doubles)*: Noise error of target profiles
- *visibility (Array of ints)*: Visibility of altitude; 0 indicates obscured, 1 indicates visible
- *akm\_diagonal (Array of doubles)*: Diagonal elements of averaging kernel
- *vr\_akdiag (Array of doubles)*: Vertical resolution (altitude grid spacing divided by averaging kernel diagonal)
- *vr\_col (Array of doubles)*: Vertical resolution (FWHM of averaging kernel columns)
- *vr\_row (Array of doubles)*: Vertical resolution (FWHM of averaging kernel rows)

## B.3 ISS/JEM/SMILES

The SMILES data collocated with Odin/SMR is accessible through the Odin REST API, see section 4. The data is returned as a JSON object with the following attributes:

- `data_fields` (*Object*): Object containing the data under the following keys:
  - `Apriori` (*Array of doubles*): A priori profile
  - `AprioriError` (*Array of doubles*): A priori error
  - `L2Value` (*Array of doubles*): Retrieved profile
  - `L2Precision` (*Array of doubles*): Calculation error; negative values indicate un-useful data
  - `AveragingKernel` (*Two-dimensional array of doubles*): Averaging kernel
  - `Baseline<N>` (*Array of doubles*): Coefficients of continuum
  - `Baseline<n>Precision` (*Array of doubles*): Baseline errors of coefficients of continuum
  - `Convergence` (*Double*): Convergence status
  - `CorrLength` (*Double*): Correlative length of a priori
  - `CostFunctionY` (*Array of doubles*): Cost function of spectra for each altitude
  - `CostFunctionYAll` (*Double*): Cost function of spectra
  - `DifferenceY` (*Array of doubles*): Normalised HCl difference between scan and zonal mean profile
  - `DifferenceYAll` (*Double*): Maximum normalised HCl difference between scan and zonal mean profile
  - `FOVInterference` (*Int*): Field-of-view interference flag; -1 indicates no information, 0 indicates no interference, larger than 0 indicates source of interference
  - `InformationValue` (*Array of doubles*): Information value
  - `MaxNumIteration` (*Int*): Maximum convergence number
  - `NumIterPerform` (*Int*): Convergence loop number and result
  - `MeasurementError` (*Array of doubles*): Measurement error
  - `PrecisionWOSignal` (*Array of doubles*): Calculation error without signal information
  - `Pressure` (*Array of doubles*): Pressure profile for the observation
  - `Temperature` (*Array of doubles*): Temperature profile for the observation
  - `RadianceResidualMax` (*Double*): Maximum radiance residual
  - `RadianceResidualMean` (*Double*): Mean radiance residual
  - `RadianceResidualRMS` (*Double*): Root mean square radiance residual
  - `SeqCount` (*Int*): Sequence counter
  - `AOSUnitNum` (*Double*): Number of observed AOS units
  - `SmoothingError` (*Array of doubles*): Smoothing error
  - `VerticalResolution` (*Array of doubles*): Vertical resolution of the profiles
  - `WaterVapor` (*Array of doubles*): Using water vapour of retrieval

- Status (*Int*): Status information as a bit mask error code; 0 indicates useful information
- geolocation\_fields (*Object*): Object containing the geolocation of the data under the following keys:
  - AscendingDescending (*Int*): 0 for ascending, 1 for descending measurement mode
  - Latitude (*Double*): Latitude for the observation
  - Longitude (*Double*): Longitude for the observation
  - LineOfSightAngle (*Double*): Azimuth view
  - MJD (*Double*): Time for the observation in MJD
  - Time (*Double*): Time for the observation in seconds from 1958-01-01
  - LocalTime (*Double*): Local time (decimal hour of day) for the observation
  - TimeUTC (*String*): Date and time for the observation in UTC as a string in ISO format
  - SolarZenithAngle (*Double*): The solar zenith angle for the observation
  - Altitude (*Array of doubles*): Representative altitudes (km) for the measured profiles
  - Reserved (*Int*): Reserved field

## B.4 Meteor3M/SAGE III

The SAGE III data collocated with Odin/SMR is accessible through the Odin REST API, see section 4. The data is returned as a JSON object with the following attributes:

- FileName (*String*): Filename is the same as in the original data set
- Instrument (*String*): Name of the instrument
- EventType (*String*): Solar or Lunar (only Solar included in VDS)
- MJDStart (*Double*): Start time in MJD for the observation
- MJDEnd (*Double*): End time in MJD for the observation
- LatStart (*Double*): Start latitude for the observation
- LatEnd (*Double*): End latitude for the observation
- LongStart (*Double*): Start longitude for the observation
- LongEnd (*Double*): End longitude for the observation
- Pressure (*Array of doubles*): Pressure profile for the observation
- Temperature (*Array of doubles*): Temperature profile for the observation
- <Species> (*Array of triplets of doubles*): Profile for <Species> for the observation; each row is a triplet containing concentration, uncertainty, and a quality bit



## B.5 Odin/OSIRIS

The OSIRIS data collocated with Odin/SMR is accessible through the Odin REST API, see section 4. The data is returned as a JSON object with the following attributes (see <http://odin-osiris.usask.ca/sites/default/files/media/pdf/l2dataformat.pdf> for more details):

- `data_fields` (*Object*): Object containing the data under the following keys:
  - `O3` (*Array of doubles*): Measured ozone profiles expressed as volume mixing ratio
  - `O3NumberDensity` (*Array of doubles*): The measured ozone profiles expressed as number density
  - `O3Precision` (*Array of doubles*): The error in the ozone volume mixing ratio
  - `RTModel_AirDensity` (*Array of doubles*): The atmospheric air density profile used in the radiative transfer model
  - `RTModel_Albedo` (*Double*): The ground albedo value used in the radiative transfer code
  - `RTModel_O3Density` (*Array of doubles*): The atmospheric air density profile used in the radiative transfer model
  - `RTModel_O3InitialGuess` (*Array of doubles*): The initial guess of  $O_3$  used in the MART retrieval, expressed as a number density
  - `RTModel_Temperature` (*Array of doubles*): The atmospheric temperature profile used in the radiative transfer model in the inversion algorithms
- `geolocation_fields` (*Object*): Object containing the geolocation of the data under the following keys:
  - `Altitude` (*Array of doubles*): The geometric altitude of the primary swath data products expressed in km. The altitudes are specified with respect to the IAU 1976 reference geoid
  - `Latitude` (*Double*): The nominal latitude of the scan expressed in degrees. This corresponds to the latitude of the tangent point at time Time.
  - `Longitude` (*Double*): The nominal longitude of the scan expressed in degrees. This corresponds to the latitude of the tangent point at time Time
  - `LocalSolarTime` (*Double*): The local solar time at the nominal tangent point expressed in hours
  - `RTModel_Altitude` (*Array of doubles*): The geometric altitude of the model inputs expressed in km. The altitudes are with respect to the IAU 1976 reference geoid
  - `ScanEndLatitude` (*Double*): The latitude of the tangent point in degrees at the end of the scan
  - `ScanEndLongitude` (*Double*): The longitude of the tangent point at the end of the scan
  - `ScanEndTime` (*Double*): The end time of the scan expressed as TAI93 assuming no offset between UTC and TAI93
  - `ScanNo` (*Int*): The unique identification number of this scan

- ScanStartLatitude (*Double*): The latitude of the tangent point in degrees at the start of the scan
- ScanStartLongitude (*Double*): The longitude of the tangent point in degrees at the start of the scan
- ScanStartTime (*Double*): The start time of the scan expressed as TAI93 assuming no offset between UTC and TAI93
- ScanUpFlag (*Int*): Indicates if the scan was going up (1) or going down (0)
- SolarAzimuthAngle (*Double*): The solar azimuth angle expressed in degrees at the nominal tangent point of the scan
- SolarScatteringAngle (*Double*): The solar scattering angle expressed in degrees at the nominal tangent point of the scan
- SolarZenithAngle (*Double*): The solar zenith angle expressed in degrees at the nominal tangent point of the scan
- Time (*Double*): The nominal time of the scan in UTC expressed as TAI93 assuming no offset between UTC and TAI93. This corresponds to the instant when the tangent point of the OSIRIS look vector was at 25 km
- MJD (*Double*): Time for the observation in MJD

## B.6 Odin/SMR 2.1

The Odin/SMR 2.0/2.1 data collocated with Odin/SMR is accessible through the Odin REST API, see section 4. The data is returned as a JSON object with the following attributes (see <http://amazonite.rss.chalmers.se:8280/OdinSMR/the-odin-level-2-data-format> for more details):

- Data (*Object*): Object containing the data under the following keys:
  - Altitudes (*Array of doubles*): Retrieval altitude for the selected species
  - Profiles (*Array of doubles*): Measured profile for the selected species (VMR)
  - MeasResp (*Array of doubles*): Measurement response
  - MeasError (*Array of doubles*): Retrieval error due to errors in the measurement
  - SmoothingError (*Array of doubles*): Retrieval error due to the error between true and a priori states
  - TotalError (*Array of doubles*): Total retrieval error
  - ID2 (*Array of ints*): Index used to identify the data in the original HDF file
- Geolocation (*Object*): Object containing the geolocation of the data under the following keys:
  - Year (*Int*): Year for the scan
  - Month (*Int*): Month for the scan
  - Day (*Int*): Day for the scan
  - Hour (*Int*): Hour for the scan
  - Min (*Int*): Minute for the scan
  - Secs (*Int*): Second for the scan



- Ticks (*Double*): Ticks of the scan
- MJD (*Double*): Time for the scan in MJD
- LST (*Double*): Local (mean) sidereal time
- Time (*Double*): Time for the scan in TAI93 units
- Latitude (*Double*): Reference latitude for the scan
- StartLat (*Double*): Geodetic start latitude for the scan
- EndLat (*Double*): Geodetic end latitude for the scan
- Longitude (*Double*): Reference longitude for the scan
- StartLong (*Double*): Geodetic start longitude for the scan
- EndLong (*Double*): Geodetic end longitude for the scan
- StartTan (*Double*): Start tangent altitude for the scan
- EndTan (*Double*): End tangent altitude for the scan
- SunZD (*Double*): Average solar zenith angle for the scan in degrees
- Nspecies (*Int*): Number of species in the scan
- Quality (*Int*): Quality bit flag
- ScanNo (*Int*): Scan number
- ID1 (*Int*): Index used to identify the scan in the original HDF file
- OrbitFilename (*String*): Full orbit filename (without .HDF for ) including the spectrometer that was used
- Source (*String*): Observation mode
- ZPTSource (*String*): Source file for the temperature and pressure profiles
- Version1b (*String*): Version of the Level1b processing chain used to create the Level1b file
- Version2 (*String*): Version of the Level2 processing chain used to chreat the Level2 file