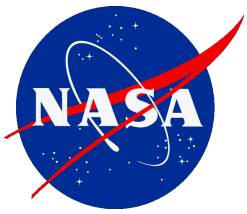
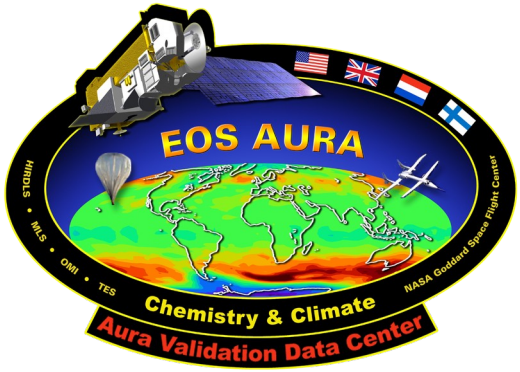
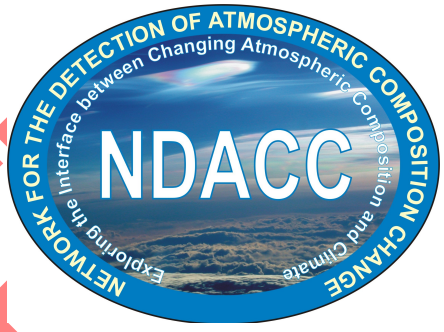


National Aeronautics and
Space Administration

Goddard Space Flight Center
Greenbelt, MD





AVDC/NDACC FTIR Data Reporting Guidelines

NASA GEST Work Activity 610-75-262

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Abstract:	This document describes the AVDC/EVDC/NDACC data reporting requirements for Fourier Transform Infrared Spectrometers in the NDACC-IRWG
See Also:	Bojkov *et al.*, 2002, 2006

Table of Contents

1 Overview

This document outlines data reporting requirements for the Fourier Transform Infrared (FTIR) Spectrometers of the Network for the Detection of Atmospheric Composition Change (NDACC, formerly called NDSC or Network for the Detection of Stratospheric Change). These guidelines were developed by the Infrared Working Group (IRWG) of NDACC and the Aura Validation Data Center (AVDC) to facilitate the submission of FTIR datasets in the AVDC/Envisat HDFv4 file formulation (Bojkov *et al.*, 2002) to the AURA Validation Data Center (AVDC), the Envisat Validation Data Center (EVDC) and the NDACC Data Handling Facility (DHF).

2 Guidelines

2.1 Instrument Naming

Although FTIR spectrometer systems have the capability to measure multiple atmospheric entities simultaneously, we adopt the convention that each file reports data for a single target gas. Therefore, the different files are distinguished by the instrument name that appears in the filename and that is a concatenation of the instrument name (FTIR) + primary measured target gas [GAS] reported in the file, as shown in Table 2.1

Table 2.1: Examples of instrument identifications in the filename and the attribute DATA_SOURCE

Primary Measured Entity [GAS]	Instrument Name
O_3	FTIR.O3
HCl	FTIR.HCl
$ClONO_2$	FTIR.ClONO2
CO	FTIR.CO
N_2O	FTIR.N2O
HNO_3	FTIR.HNO3
HCN	FTIR.HCN
CH_4	FTIR.CH4
HF	FTIR.HF
C_2H_6	FTIR.C2H6

2.2 Variable Reporting

Each measured primary entity [GAS] requires a mandatory set of 28 variables to be reported within a FTIR.[GAS] file. A description of the variables is given in Table 2.2. Notice that all variables are mandatory for the submission of vertical profile data. If only total column data are reported, then the variables 12 and 14 to 19 need not be reported.

Individual data will be reported, each with its own random and systematic error estimates and averaging kernels. As such the same data files that are archived in NDACC can be used for satellite validation purposes and any other applications.

Table 2.2: FTIR mandatory (except where noted 'optional' in the comments) variables with recommended variable attribute entries.

Variable number	Variable Name	Units	Data Type	Data Format	Fill Value	Variable Description	Mandatory (x) or Optional (o)
1	DATETIME	MJD2000	DOUBLE	F16.9	-90000	Effective meas. time	x
2	LATITUDE.INSTRUMENT	deg	REAL	F9.2	-90000	Inst. geolocation	x
3	LONGITUDE.INSTRUMENT	deg	REAL	F9.2	-90000	Inst. geolocation; preferentially positive East	x
4	ALTITUDE.INSTRUMENT	km	REAL	F10.3	-90000	Inst. geolocation	x
5	SURFACE.PRESSURE_INDEPENDENT	hPa	REAL	E12.4	-9.00E+04	Surface/ground pressure	x
6	SURFACE.TEMPERATURE_INDEPENDENT	K	REAL	F10.3	-90000	Surface/ground temperature	x
7	ALTITUDE.LAYER.INDEX or ALTITUDE.LEVEL.INDEX	DIMENSIONLESS	LONG	I6	-90000	Index of the retrieval altitude layers, if layer-based retrieval or of the retrieval levels if level-based retrieval	x
8	ALTITUDE.BOUNDARIES	km	REAL	F10.3	-90000	2D matrix with on each row the lower and upper boundaries of the layers for which the partial columns are reported. In layer-based retrieval, these are equal to the lower and upper boundaries of the respective retrieval layers	X
9	ALTITUDE	km	REAL	F10.3	-90000	Retrieval effective altitude vector	X
10	PRESSURE_INDEPENDENT	hPa	REAL	E12.4	-9.00E+04	Effective air pressure at each	x

Variable number	Variable Name	Units	Data Type	Data Format	Fill Value	Variable Description	Mandatory (x) or Optional (o)
						altitude	
11	TEMPERATURE_INDEPENDENT	K	REAL	F10.3	-90000	Effective air temperature at each altitude	X
12	[GAS].MIXING.RATIO_ABSORPTION.SOLAR or [GAS].MIXING.RATIO_ABSORPTION.LUNAR	ppmv or ppbv or pptv	REAL	E12.4	-9.00E+04	Retrieved target vertical profile in VMR units	O
13	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_APRIORI or [GAS].MIXING.RATIO_ABSORPTION.LUNAR_APRIORI	ppmv or ppbv or pptv	REAL	E12.4	-9.00E+04	A priori target vertical profile in VMR units	X
14	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_AVK or [GAS].MIXING.RATIO_ABSORPTION.LUNAR_AVK	DIMENSIONLESS	REAL	E12.4	-9.00E+04	A or Averaging kernel matrix for retrieved target profile (expressed in VMR/VMR units)	x if [GAS].MIXING.RATIO_ABSORPTION.SOLAR (LUNAR) is provided
15	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_INTEGRATION.TIME or [GAS].MIXING.RATIO_ABSORPTION.LUNAR_INTEGRATION.TIME	s	REAL	E12.4	-9.00E+04	Duration of the measurement corresponding to the retrieved datapoint	x if [GAS].MIXING.RATIO_ABSORPTION.SOLAR (LUNAR) is provided
16	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_UNCERTAINTY.RANDOM or [GAS].MIXING.RATIO_ABSORPTION.LUNAR_UNCERTAINTY.RANDOM	ppmv2 or ppbv2 or pptv2	REAL	E12.4	-9.00E+04	Total random error covariance matrix associated with the retrieved vertical profile (expressed in same units as the profile) (without smoothing error!)	x if [GAS].MIXING.RATIO_ABSORPTION.SOLAR (LUNAR) is provided
17	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_UNCERTAINTY.SYSTEMATIC or [GAS].MIXING.RATIO_ABSORPTION.LUNAR_UNCERTAINTY.SYSTEMATIC	ppmv2 or ppbv2 or pptv2	REAL	E12.4	-9.00E+04	Total systematic error covariance matrix associated with the retrieved vertical profile (expressed in same units as the profile)	x if [GAS].MIXING.RATIO_ABSORPTION.SOLAR (LUNAR) is provided
18	[GAS].COLUMN.VERTICAL.PARTIAL_ABSORPTION.SOLAR or [GAS].COLUMN.VERTICAL.PARTIAL_ABSORPTION.LUNAR	molec cm-2 (or a unit scaled by 1E3*n, ex. Pmolec cm-2)	REAL	E12.4	-9.00E+04	Vertical profile of partial columns per layer	x if [GAS].MIXING.RATIO_ABSORPTION.SOLAR (LUNAR) is provided
19	[GAS].COLUMN.VERTICAL.PARTIAL_ABSORPTION.SOLAR _APRIORI or [GAS].COLUMN.VERTICAL.PARTIAL_ABSORPTION.LUNAR_APRIORI	molec cm-2 (or a unit scaled by 1E3*n, ex. Pmolec cm-2)	REAL	E12.4	-9.00E+04	Vertical profile of a priori partial columns per layer	x if [GAS].MIXING.RATIO_ABSORPTION.SOLAR (LUNAR) is

Variable number	Variable Name	Units	Data Type	Data Format	Fill Value	Variable Description	Mandatory (x) or Optional (o) provided
20	[GAS].COLUMN.VERTICAL_ABSORPTION.SOLAR or [GAS].COLUMN.VERTICAL_ABSORPTION.LUNAR	molec cm-2 (or a unit scaled by 1E3*n, ex. Pmolec cm-2)	REAL	E12.4	-9.00E+04	Total vertical column of target gas	X
21	[GAS].COLUMN.VERTICAL_ABSORPTION.SOLAR _APRIORI or [GAS].COLUMN.VERTICAL_ABSORPTION.LUNAR_APRIORI	molec cm^{-2} (or a unit scaled by 1E3*n, ex. Pmolec cm^{-2})	REAL	E12.4	-9.00E+04	A priori total vertical column of target gas	X
22	[GAS].COLUMN.VERTICAL_ABSORPTION.SOLAR _AVK or [GAS].COLUMN.VERTICAL_ABSORPTION.LUNAR_AVK	DIMENSIONLESS	REAL	E12.4	-9.00E+04	Averaging kernel matrix associated with the total vertical column of the target gas (in molec cm-2/molec cm-2 units)	X
23	[GAS].COLUMN.VERTICAL_ABSORPTION.SOLAR_UNCERTAINTY.RANDOM or [GAS].COLUMN.VERTICAL_ABSORPTION.LUNAR_UNCERTAINTY.RANDOM	molec cm^{-2} (or a unit scaled by 1E3*n, ex. Pmolec cm^{-2})	REAL	E12.4	-9.00E+04	Total random uncertainty on the retrieved total column (expressed in same units as the column) (without smoothing error)	x
24	[GAS].COLUMN.VERTICAL_ABSORPTION.SOLAR UNCERTAINTY.SYSTEMATIC or [GAS].COLUMN.VERTICAL_ABSORPTION.LUNAR_UNCERTAINTY.SYSTEMATIC	molec cm^{-2} (or a unit scaled by 1E3*n, ex. Pmolec cm^{-2})	REAL	E12.4	-9.00E+04	Total systematic uncertainty on the retrieved partial columns (expressed in same units as the column)	x
25	ANGLE.SOLAR_ZENITH.ASTRONOMICAL or ANGLE.LUNAR_ZENITH.ASTRONOMICAL	deg	REAL	F9.2	-90000	The solar (or lunar) astronomical zenith angle at which the measurement was taken	x
26	ANGLE.SOLAR_AZIMUTH or ANGLE.LUNAR_AZIMUTH	deg	REAL	F9.2	-90000	The solar (or lunar) azimuth angle at which the measurement was taken	x
27	H2O.MIXING.RATIO_ABSORPTION.SOLAR or H2O.MIXING.RATIO_ABSORPTION.LUNAR	ppmv or ppbv or pptv	REAL	E12.4	-9.00E+04	Vertical profile of H2O adopted in the target gas retrieval, in VMR units	x
28	H2O.COLUMN.VERTICAL_ABSORPTION.SOLAR or H2O.COLUMN.VERTICAL_ABSORPTION.LUNAR	molec cm^{-2} (or a unit scaled by	REAL	E12.4	-9.00E+04	Total vertical column of H2O	x

Variable number	Variable Name	Units	Data Type	Data Format	Fill Value	Variable Description	Mandatory (x) or Optional (o)
		1E3*n, ex. Pmolec cm^{-2})				adopted in the target gas retrieval	

Note:
The [GAS].MIXING.RATIO_ABSORPTION.SOLAR (LUNAR)_UNCERTAINTY.RANDOM and [GAS].MIXING.RATIO_ABSORPTION.SOLAR (LUNAR)_UNCERTAINTY.SYSTEMATIC are the full posteriori error covariance matrices.

Note

To accommodate variable altitude retrieval grids from one reported data point to another, however always with the same number of retrieval levels (PROFFIT retrieval code) or layers (SFIT2 retrieval code), the ALTITUDE.LEVEL.INDEX and ALTITUDE.LAYER.INDEX vectors have been introduced, espectively. The retrieval altitude grid (variable ALTITUDE) is then referenced to this variable.

In the case of SFIT2, ALTITUDE contains the output altitude vector (i.e., the centre altitudes of the retrieval layers, N in number). The target gas mixing ratio profile and the pressure and temperature profiles are referenced to this ALTITUDE vector. The ALTITUDE.BOUNDARIES vector provides the additional information about the layer boundary altitudes; it is a variable dependent on ALTITUDE (its first dimension must have size N; its second dimension has size 2). It provides the boundaries of the layers for which the vertical partial columns of the target gas are reported ([GAS].COLUMN.VERTICAL.PARTIAL_ABSORPTION.SOLAR (LUNAR)).

In the case of PROFFIT, ALTITUDE contains the N altitude levels upon which the target gas mixing ratio profile is retrieved and reported; also the pressure and temperature profiles are reported on this altitude grid. The ALTITUDE.BOUNDARIES vector has again size (N,2); the boundary altitudes are equal to the successive level altitudes. As the number of partial columns between the levels is one less than the number of levels, the highest partial column is set to zero.

To avoid end-user confusion, it is essential to explain the interpretation of the dependences of the geophysical parameters (mixing ratio, pressure, temperature, and partial columns) on the altitudes in the VAR_DESCRIPTION variable.

2.3 Variable Fill Values

The variable fill value is a number inserted as a substitute data element if a data element of a variable is missing or erroneous. Special care must be given to the number of positions reported for the data format (VIS_FORMAT) to also accommodate the fill value. In most cases the reported variable fill value will be -90000, with precision and format as defined by VIS_FORMAT, as shown in the examples in Table 2.3 (and Table 2.2).

Table 2.3: Fill value examples

Variable numeric type (VAR_DATA_TYPE)	Formatting (VIS_FORMAT)	Fill value (VAR_FILL_VALUE)
REAL	F9.2	-90000.00
REAL	E10.2	-9.00E+004
DOUBLE	E11.3	-9.000E+004
LONG	I6	-90000

2.4 File Granularity

The choice of the file granularity for archiving FTIR measurements in NDACC is left to the data provider, but it is forbidden that the file covers more than 1 year of data. It is possible now to store in the same file data retrieved with different a priori profiles, and therefore different averaging kernels and uncertainty estimates, as all individual data are reported. The most common granularities will be monthly, seasonal (3 months) or yearly.

3 Metadata

3.1 Global Attributes

Each FTIR.[GAS] file requires one set of **Global Attributes**. These have been grouped into three categories describing the file contents, namely **Originator Attributes**, **Dataset Attributes** and **File Attributes**. An example of global attributes for an FTIR methane measurement at Reunion (PI and data submittor: M. De Mazière, BIRA.IASB; Data analysis using SFIT2 (layer based retrieval): Corinne Vigouroux, BIRA.IASB) is given in Table 3.1.

Table 3.1: Global Attributes Example

Global Attribute Label	Global Attribute Value (example)	Comment
PI_NAME	De Maziere; Martine	
PI_AFFILIATION	Belgian Institute for Space Aeronomy;BIRA.IASB	
PI_ADDRESS	Avenue Circulaire, 3;B-1180 Brussels;BELGIUM	
PI_EMAIL	martine@bira-iasb.oma.be	
DO_NAME	Vigouroux; Corinne	
DO_AFFILIATION	Belgian Institute for Space Aeronomy;BIRA.IASB	
DO_ADDRESS	Avenue Circulaire, 3;B-1180 Brussels;BELGIUM	
DO_EMAIL	corinnev@bira-iasb.oma.be	
DS_NAME	De Maziere; Martine	
DS_AFFILIATION	Belgian Institute for Space Aeronomy;BIRA.IASB	
DS_ADDRESS	Avenue Circulaire, 3;B-1180 Brussels;BELGIUM	
DS_EMAIL	martine@bira-iasb.oma.be	
DATA_DESCRIPTION	FTIR vmr vertical profile data of CH4 at Reunion Island (St Denis)	*Free format*
DATA_DISCIPLINE	ATMOSPHERIC.PHYSICS;REMOTE.SENSING;GROUNDBASED	*Refer to standard*
DATA_GROUP	EXPERIMENTAL; PROFILE.STATIONARY	*Refer to standard*
DATA_LOCATION	LA.REUNION	*Refer to standard*
DATA_SOURCE	FTIR.CH4_BIRA.IASB001	*Refer to standard*
DATA_LEVEL	O2	*Refer to standard*
DATA_VARIABLES	DATETIME LATITUDE.INSTRUMENT LONGITUDE.INSTRUMENT ALTITUDE.INSTRUMENT SURFACE.PRESSURE_INDEPENDENT SURFACE.TEMPERATURE_INDEPENDENT ALTITUDE.LAYER.INDEX ALTITUDE.BOUNDARIES ALTITUDE PRESSURE_INDEPENDENT TEMPERATURE_INDEPENDENT CH4.MIXING.RATIO_ABSORPTION.SOLAR CH4.MIXING.RATIO_ABSORPTION.SOLAR_APRIORI CH4.MIXING.RATIO_ABSORPTION.SOLAR_AVK CH4.MIXING.RATIO_ABSORPTION.SOLAR_INTEGRATION.TIME CH4.MIXING.RATIO_ABSORPTION.SOLAR_UNCERTAINTY.RANDOM CH4.MIXING.RATIO_ABSORPTION.SOLAR_UNCERTAINTY.SYSTEMATIC CH4.COLUMN.VERTICAL.PARTIAL_ABSORPTION.SOLAR	

	CH4.COLUMN.VERTICAL.PARTIAL_ABSORPTION.SOLAR_APRIORI CH4.COLUMN.VERTICAL_ABSORPTION.SOLAR CH4.COLUMN.VERTICAL_ABSORPTION.SOLAR_APRIORI CH4.COLUMN.VERTICAL_ABSORPTION.SOLAR_AVK CH4.COLUMN.VERTICAL_ABSORPTION.SOLAR_UNCERTAINTY.RANDOM CH4.COLUMN.VERTICAL_ABSORPTION.SOLAR_UNCERTAINTY.SYSTEMATIC ANGLE.SOLAR_ZENITH.ASTRONOMICAL ANGLE.SOLAR_AZIMUTH H2O.MIXING.RATIO_ABSORPTION.SOLAR H2O.COLUMN.VERTICAL_ABSORPTION.SOLAR	
DATA_START_DATE	20070525T040000Z	*ISO8601*
DATA_STOP_DATE	20071020T150000Z	*ISO8601*
DATA_FILE_VERSION	001	
DATA_MODIFICATIONS	None	*Free format*
DATA_QUALITY	Reference paper Senten et al., ACP, 8, 3483-3508, 2008	*Free format*
DATA_CAVEATS	None	*Free format*
DATA_RULES_OF_USE	please contact M. De Mazière	*Free format*
DATA_ACKNOWLEDGEMENT	EU projects UFTIR and HYMN	*Free format*
FILE_NAME	groundbased_ftir.ch4_bira.iasb001_la.reunion_02_20070525t040000z_001.hdf	*Naming convention*
FILE_GENERATION_DATE	20080312T143444Z	*ISO8601*
FILE_ACCESS	HYMN; NDACC	*Project dependent*
FILE_PROJECT_ID	AOID9999	*Project dependent*
FILE_ASSOCIATION	NDACC	*Project dependent*
FILE_META_VERSION	03R014; ASC2HDF version 03R014 20070914T000000Z	*Refer to standard*

3.2 Variable Attributes

Each variable reported in a FTIR.[GAS] file requires one set of **Variable Attributes**. These have been grouped into two categories describing the variable, namely the **Variable Description Attributes** and the **Variable Visualization Attributes**. An example of an attribute set is given in Table 3.2.

Table 3.2: Variable Attributes Example

Attribute Label	Attribute Value	Comment
VAR_NAME	CH4.MIXING.RATIO_ABSORPTION.SOLAR _AVK	*Refer to standard*

VAR_DESCRIPTION	Typical averaging kernel matrix (AVK) of the retrieved vertical profile of CH4, referred to VMR units	*Free format*
VAR_NOTES	Dimension 1 are the AVK rows; dimension 2 are the AVK columns	*Free format*
VAR_DIMENSION	2	
VAR_SIZE	41;41	*The number of elements in each dimension*
VAR_DEPEND	ALTITUDE.LAYER.INDEX;ALTITUDE.LAYER.INDEX	*INDEPENDENT, CONSTANT or a previously given one dimensional variable*
VAR_DATA_TYPE	DOUBLE	*Allowable formats are INTEGER, LONG, REAL, DOUBLE*
VAR_UNITS	DIMENSIONLESS	*Refer to standard for permissible units*
VAR_SI_CONVERSION	0;1.;DIMENSIONLESS	*Refer to standard*
VAR_VALID_MIN	-2.	
VAR_VALID_MAX	2.	
VAR_AVG_TYPE	NONE	*Refer to standard*
VAR_FILL_VALUE	-9.0000E+004	*Needs to be outside VAR_VALID_MIN and VAR_VALID_MAX values*
VIS_LABEL	CH4 VMR averaging kernel	*Free format*
VIS_FORMAT	E12.4	*Needs to accommodate valid minimum, valid maximum and the fill values*
VIS_PLOT_TYPE	XYZ.COLOUR	*Refer to standard*
VIS_SCALE_TYPE	LINEAR;INCREASE	*Refer to standard*
VIS_SCALE_MIN	-2.	*Refer to standard*
VIS_SCALE_MAX	2.	*Refer to standard*

4 HDF4 Implementation

The HDF version 4 (NCSA, 2001) file formulation is limited to: 1) the global attributes containing the file metadata, and 2) the scientific data sets (SDS) model to represent each variable with appropriate variable metadata. A similar file structure has been developed by the AVDC for the HDF 5 type files. A detailed description of the AVDC HDF 4 and the HDF 5 type files is provided by Bojkov *et al.*, 2006.

5 Acronyms

AVDC	Aura Validation Data Center
AVK	Averaging Kernel
Cal/Val	ESA Envisat Calibration and Validation datacenter
DHF	NDACC Data handling Facility
ESA	European Space Agency
EVDC	Envisat Validation Data Center
FTIR	Fourier Transform InfraRed
HDF	Hierarchical Data Format
MJD2000	Modified Julian Date 2000
NCSA	National Center for Supercomputing Applications
NDACC	Network for the Detection of Atmospheric Composition Change
NDSC	Network for the Detection of Stratospheric Change
UFTIR	Time series of Upper Free Troposphere observations from a European ground-based FTIR network

6 References

B.R. Bojkov, De Mazière, M. and R. Koopman, Generic metadata guidelines on atmospheric and oceanographic datasets for the Envisat Calibration and Validation Project, Version 01R001, April 23, 2002. Available for download at http://avdc.gsfc.nasa.gov/Documentation/Metadata/

B.R. Bojkov, Boyd, I., De Mazière, M. and R. Koopman, Addendum to the "Generic metadata guidelines on atmospheric and oceanographic datasets for the Envisat Calibration and Validation Project" as implemented by the Aura Validation Data Center (AVDC), August 31, 2006. Available for download at http://avdc.gsfc.nasa.gov/Documentation/Metadata/

M. De Mazière, Final Report of the EC project UFTIR, Time series of Upper Free Troposphere observations from a European ground-based FTIR network (contract n° EVK2-2002- 00159, 2003-2005), http://www.nilu.no/uftir, 2006.

NCSA, National Center for Supercomputing Applications – HDF 4 home page: http://hdf.ncsa.uiuc.edu/hdf4.html