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[DOCUMENTATION/ GEOMS DATA REPORTING/ FTIR](#)

Fourier Transform Infrared Spectroscopy (FTIR) template description

Document history

Version	Date	Comments
006	Oct 04, 2010	GEOMS FTIR template
005	Nov 05, 2009	GEOMS FTIR template
004	Sep 14, 2009	AVDC/NDACC FTIR reporting guidelines
003	Feb 21, 2008	AVDC/NDACC FTIR reporting guidelines
002	Sep 21, 2006	AVDC/NDACC FTIR reporting guidelines
001	Jun 14, 2005	Draft AVDC/NDACC FTIR reporting guidelines

Authors

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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 compliant to the Generic Earth Observation Metadata Standard (GEOMS) to the Aura Validation Data Center (AVDC), the Envisat Validation Data Center (EVDC) and the NDACC Data Handling Facility (DHF).

Template description

- 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 [GEOMS-TE-FTIR-DS](#).
- Variable Reporting**
 Each measured primary entity [GAS] requires a mandatory set of variables to be reported within a FTIR.[GAS] file. A description of the variables is given in Table [GEOMS-TE-FTIR-VA](#). Notice that all variables are mandatory for the submission of vertical profile data. If only total column data are reported, then some variables 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.

- Additional Notes**
 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, respectively. 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 center 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 dependencies of the geophysical parameters (mixing ratio, pressure, temperature, and partial columns) on the altitudes in the VAR_DESCRIPTION variable.

- **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.

- **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.

- **Metadata - 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 submitter: M. De Mazière, BIRA.IASB; Data analysis using SFIT2 (layer based retrieval): Corinne Vigouroux, BIRA.IASB) is given in Table [GEOMS-EX-FTIR-GA](#).

- **Metadata - 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 [GEOMS-EX-FTIR-VA](#).

Templates and examples

- 1 [GEOMS-TE-FTIR-DS](#) FTIR data sources
- 2 [GEOMS-TE-FTIR-GA](#) FTIR Global Attributes Template
- 3 [GEOMS-TE-FTIR-VA](#) FTIR Variable Attributes Template
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- 5 [GEOMS-EX-FTIR-VA](#) FTIR Variable Attributes Example

GEOMS-TE-FTIR-DS (*FTIR data sources*)

Instrument/Model type Comment

- 0 FTIR.C2H6
- 1 FTIR.CCI2F2
- 2 FTIR.CCI3F
- 3 FTIR.CH4
- 4 FTIR.CHF2CI
- 5 FTIR.CIONO2
- 6 FTIR.CO
- 7 FTIR.CO2
- 8 FTIR.COF2
- 9 FTIR.H2CO
- 10 FTIR.H2O
- 11 FTIR.HCI
- 12 FTIR.HCN
- 13 FTIR.HCOOH
- 14 FTIR.HF
- 15 FTIR.HNO3
- 16 FTIR.N2O
- 17 FTIR.NO
- 18 FTIR.NO2
- 19 FTIR.O3
- 20 FTIR.OCS
- 21 FTIR.SF6

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GEOMS-TE-FTIR-GA (*FTIR Global Attributes Template*)

Download in CSV format [GEOMS-TE-FTIR-GA.csv](#) (last updated: October 04, 2010).

#	Variable name	Variable value	Comment	Req
0	PI_NAME		Refer to GEOMS document	x
1	PI_AFFILIATION		Refer to GEOMS document	x

2	PI_ADDRESS		Refer to GEOMS document	x
3	PI_EMAIL		Refer to GEOMS document	x
4	DO_NAME		Refer to GEOMS document	x
5	DO_AFFILIATION		Refer to GEOMS document	x
6	DO_ADDRESS		Refer to GEOMS document	x
7	DO_EMAIL		Refer to GEOMS document	x
8	DS_NAME		Refer to GEOMS document	x
9	DS_AFFILIATION		Refer to GEOMS document	x
10	DS_ADDRESS		Refer to GEOMS document	x
11	DS_EMAIL		Refer to GEOMS document	x
12	DATA_DESCRIPTION		Free format	x
13	DATA_DISCIPLINE	ATMOSPHERIC.PHYSICS;REMOTE.SENSING;GROUNDBASED	Refer to GEOMS document	x
14	DATA_GROUP	EXPERIMENTAL;PROFILE.STATIONARY	Refer to GEOMS document	x
15	DATA_LOCATION		Refer to GEOMS document	x
16	DATA_SOURCE	FTIR.[GAS]_[DATA_SOURCE] DATETIME; LATITUDE.INSTRUMENT; LONGITUDE.INSTRUMENT; ALTITUDE.INSTRUMENT; SURFACE.PRESSURE_INDEPENDENT; SURFACE.TEMPERATURE_INDEPENDENT; ALTITUDE.BOUNDARIES; ALTITUDE; PRESSURE_INDEPENDENT; TEMPERATURE_INDEPENDENT; INTEGRATION.TIME; [GAS].MIXING.RATIO_ABSORPTION.[SOLAR LUNAR]; [GAS].MIXING.RATIO_ABSORPTION.[SOLAR LUNAR]_APRIORI;	Refer to GEOMS document	x
17	DATA_VARIABLES	[GAS].MIXING.RATIO_ABSORPTION.[SOLAR LUNAR]_AVK; [GAS].MIXING.RATIO_ABSORPTION.[SOLAR LUNAR]_UNCERTAINTY.RANDOM; [GAS].MIXING.RATIO_ABSORPTION.[SOLAR LUNAR]_UNCERTAINTY.SYSTEMATIC; [GAS].COLUMN.PARTIAL_ABSORPTION.[SOLAR LUNAR]; [GAS].COLUMN.PARTIAL_ABSORPTION.[SOLAR LUNAR]_APRIORI; [GAS].COLUMN_ABSORPTION.[SOLAR LUNAR]; [GAS].COLUMN_ABSORPTION.[SOLAR LUNAR]_APRIORI; [GAS].COLUMN_ABSORPTION.[SOLAR LUNAR]_AVK; [GAS].COLUMN_ABSORPTION.[SOLAR LUNAR]_UNCERTAINTY.RANDOM; [GAS].COLUMN_ABSORPTION.[SOLAR LUNAR]_UNCERTAINTY.SYSTEMATIC; ANGLE.SOLAR_ZENITH.ASTRONOMICAL; ANGLE.SOLAR_AZIMUTH; H2O.MIXING.RATIO_ABSORPTION.SOLAR; H2O.COLUMN_ABSORPTION.SOLAR		x
18	DATA_START_DATE		Refer to GEOMS document	x
19	DATA_STOP_DATE		Refer to GEOMS document	x
20	DATA_FILE_VERSION		Refer to GEOMS document	x
21	DATA_MODIFICATIONS		Free format	o
22	DATA_QUALITY		Free format	x
23	DATA_CAVEATS		Free format	o
24	DATA_RULES_OF_USE		Free format	o

25 DATA_ACKNOWLEDGEMENT		Free format	o
26 DATA_TEMPLATE	GEOMS-FTIR-TE-[version number]	Refer to GEOMS document	x
27 DATA_PROCESSOR		Refer to GEOMS document	o
28 FILE_DOI		Refer to GEOMS document	x
29 FILE_NAME		Refer to GEOMS document	x
30 FILE_GENERATION_DATE		Refer to GEOMS document	x
31 FILE_ACCESS		Refer to GEOMS document	x
32 FILE_PROJECT_ID		Refer to GEOMS document	x if file is reported to Envisat Cal/Val
33 FILE_ASSOCIATION		Refer to GEOMS document	x
34 FILE_META_VERSION		Refer to GEOMS document	x

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GEOMS-TE-FTIR-VA (*FTIR Variable Attributes Template*)

Download in CSV format [GEOMS-TE-FTIR-VA.csv](#) (last updated: October 04, 2010).

#	Variable	Unit	Numeric type	Comment	Req
0	DATETIME	MJD2K	DOUBLE	Effective meas. time	x
1	LATITUDE.INSTRUMENT	deg	REAL	Inst. geolocation	x
2	LONGITUDE.INSTRUMENT	deg	REAL	Inst. geolocation; preferentially positive East	x
3	ALTITUDE.INSTRUMENT	km	REAL	Inst. geolocation	x
4	SURFACE.PRESSURE_INDEPENDENT	hPa	REAL	Surface/ground pressure	x
5	SURFACE.TEMPERATURE_INDEPENDENT	K	REAL	Surface/ground temperature	x
6	ALTITUDE.BOUNDARIES	km	REAL	3D 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
7	ALTITUDE	km	REAL	Retrieval effective altitude vector	x
8	PRESSURE_INDEPENDENT	hPa	REAL	Effective air pressure at each altitude	x
9	TEMPERATURE_INDEPENDENT	K	REAL	Effective air temperature at each altitude	x

[Duration of the](#)

10 INTEGRATION.TIME	s	REAL	measurement x if corresponding [GAS].MIXING.RATIO_ABSORPTION.[SOLAR LUNAR] to the retrieved is provided datapoint
11 [GAS].MIXING.RATIO_ABSORPTION.[SOLAR LUNAR]	ppmv or ppbv or pptv	REAL	Retrieved target vertical profile in VMR units
12 [GAS].MIXING.RATIO_ABSORPTION.[SOLAR LUNAR]_APRIORI	ppmv or ppbv or pptv	REAL	A-priori target vertical profile in VMR units
13 [GAS].MIXING.RATIO_ABSORPTION.[SOLAR LUNAR]_AVK	1	REAL	A or Averaging kernel matrix for retrieved target profile (expressed in VMR/VMR units)
14 [GAS].MIXING.RATIO_ABSORPTION.[SOLAR LUNAR]_UNCERTAINTY.RANDOM	ppmv2 or ppbv2 or pptv2	REAL	Total random error covariance matrix associated with the retrieved vertical profile (expressed in same units as the profile) (without smoothing error!)
15 [GAS].MIXING.RATIO_ABSORPTION.[SOLAR LUNAR]_UNCERTAINTY.SYSTEMATIC	ppmv2 or ppbv2 or pptv2	REAL	Total systematic error covariance matrix associated with the retrieved vertical profile (expressed in same units as the profile)
16 [GAS].COLUMN.PARTIAL_ABSORPTION.[SOLAR LUNAR]	molec cm-2 (or a unit scaled by 1E3*n, ex. Pmolec cm-2)	REAL	Vertical profile of partial columns per layer
17 [GAS].COLUMN.PARTIAL_ABSORPTION.[SOLAR LUNAR]_APRIORI	molec cm-2 (or a unit scaled by 1E3*n, ex. Pmolec cm-2)	REAL	Vertical profile of a-priori partial columns per layer
18 [GAS].COLUMN_ABSORPTION.[SOLAR LUNAR]	molec cm-2 (or a unit scaled hv	REAL	Total vertical column of

19	[GAS].COLUMN_ABSORPTION.[SOLAR LUNAR]_APRIORI	~ 1E3*n, ex. Pmolec cm-2) molec cm-2 (or a unit scaled by 1E3*n, ex. Pmolec cm-2)	REAL	target gas A-priori total vertical column x of target gas
20	[GAS].COLUMN_ABSORPTION.[SOLAR LUNAR]_AVK	1	REAL	Averaging kernel matrix associated with the total vertical column x of the target gas (in molec cm-2/molec cm-2 units)
21	[GAS].COLUMN_ABSORPTION.[SOLAR LUNAR]_UNCERTAINTY.RANDOM	molec cm-2 (or a unit scaled by 1E3*n, ex. Pmolec cm-2)	REAL	Total random uncertainty on the retrieved total column (expressed in same units as the column) x (without smoothing error)
22	[GAS].COLUMN_ABSORPTION.[SOLAR LUNAR]_UNCERTAINTY.SYSTEMATIC	molec cm-2 (or a unit scaled by 1E3*n, ex. Pmolec cm-2)	REAL	Total systematic uncertainty on the retrieved partial columns x (expressed in same units as the column)
23	ANGLE.[SOLAR LUNAR]_ZENITH.ASTRONOMICAL	deg	REAL	The solar (or lunar) astronomical zenith angle at x which the measurement was taken
24	ANGLE.[SOLAR LUNAR]_AZIMUTH	deg	REAL	The solar (or lunar) azimuth angle at which x the measurement was taken
25	H2O.MIXING.RATIO_ABSORPTION.[SOLAR LUNAR]	ppmv or ppbv or pptv	REAL	Vertical profile of H2O adopted in the x target gas retrieval, in VMR units
26	H2O.COLUMN_ABSORPTION.[SOLAR LUNAR]	molec cm-2 (or a unit scaled by hv	REAL	Total vertical column of H2O adopted in the x

~
1E3*n,
ex.
Pmolec
cm-2)

target gas
retrieval

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GEOMS-EX-FTIR-GA (FTIR Global Attributes Example)

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#	Variable name	Variable value	Comment
0	PI_NAME	De Maziere;Martine	
1	PI_AFFILIATION	Belgian Institute for Space Aeronomy;BIRA.IASB	
2	PI_ADDRESS	Avenue Circulaire, 3;B-1180 Brussels;BELGIUM	
3	PI_EMAIL	martine@bira-iasb.oma.be	
4	DO_NAME	Vigouroux;Corinne	
5	DO_AFFILIATION	Belgian Institute for Space Aeronomy;BIRA.IASB	
6	DO_ADDRESS	Avenue Circulaire, 3;B-1180 Brussels;BELGIUM	
7	DO_EMAIL	corinnev@bira-iasb.oma.be	
8	DS_NAME	De Maziere;Martine	
9	DS_AFFILIATION	Belgian Institute for Space Aeronomy;BIRA.IASB	
10	DS_ADDRESS	Avenue Circulaire, 3;B-1180 Brussels;BELGIUM	
11	DS_EMAIL	martine@bira-iasb.oma.be	
12	DATA_DESCRIPTION	FTIR vmr vertical profile data of CH4 at Reunion Island (St Denis)	Free format
13	DATA_DISCIPLINE	ATMOSPHERIC.PHYSICS;REMOTE.SENSING;GROUNDBASED	Refer to GEOMS document
14	DATA_GROUP	EXPERIMENTAL;PROFILE.STATIONARY	Refer to GEOMS document
15	DATA_LOCATION	LA.REUNION	Refer to GEOMS document
16	DATA_SOURCE	FTIR.CH4_BIRA.IASB001	Refer to GEOMS document
17	DATA_VARIABLES	DATETIME; LATITUDE.INSTRUMENT; LONGITUDE.INSTRUMENT; ALTITUDE.INSTRUMENT; SURFACE.PRESSURE_INDEPENDENT; SURFACE.TEMPERATURE_INDEPENDENT; ALTITUDE.BOUNDARIES; ALTITUDE; PRESSURE_INDEPENDENT; TEMPERATURE_INDEPENDENT; INTEGRATION.TIME; CH4.MIXING.RATIO_ABSORPTION.SOLAR; CH4.MIXING.RATIO_ABSORPTION.SOLAR_APRIORI; CH4.MIXING.RATIO_ABSORPTION.SOLAR_AVK; CH4.MIXING.RATIO_ABSORPTION.SOLAR_UNCERTAINTY.RANDOM; CH4.MIXING.RATIO_ABSORPTION.SOLAR_UNCERTAINTY.SYSTEMATIC; CH4.COLUMN.PARTIAL_ABSORPTION.SOLAR; CH4.COLUMN.PARTIAL_ABSORPTION.SOLAR_APRIORI; CH4.COLUMN_ABSORPTION.SOLAR; CH4.COLUMN_ABSORPTION.SOLAR_APRIORI; CH4.COLUMN_ABSORPTION.SOLAR_AVK; CH4.COLUMN_ABSORPTION.SOLAR_UNCERTAINTY.RANDOM; CH4.COLUMN_ABSORPTION.SOLAR_UNCERTAINTY.SYSTEMATIC; ANGLE.SOLAR_ZENITH.ASTRONOMICAL; ANGLE.SOLAR_AZIMUTH; H2O.MIXING.RATIO_ABSORPTION.SOLAR; H2O.COLUMN_ABSORPTION.SOLAR	
18	DATA_START_DATE	20070525T040000Z	ISO8601
19	DATA_STOP_DATE	20071020T150000Z	ISO8601
20	DATA_FILE_VERSION	001	Refer to GEOMS document
21	DATA_MODIFICATIONS	None	Free format
22	DATA_QUALITY		Reference paper Senten et al.
23	DATA_CAVEATS	None	Free format
24	DATA_RULES_OF_USE	please contact M. De Mazière	Free format
25	DATA_ACKNOWLEDGEMENT	EU projects UFTIR and HYMN	Free format
26	DATA_TEMPLATE	GEOMS-FTIR-TE-006	Refer to GEOMS document
27	DATA_PROCESSOR	FTIRproc-v1.0	Refer to GEOMS document
28	FILE_DOI		Currently left empty. Definition yet to come.
29	FILE_NAME	groundbased_ftir.ch4_bira.iasb001_la.reunion_02_20070525t040000z_001.hdf	Naming convention

30 FILE_GENERATION_DATE	20080312T143444Z	ISO8601
31 FILE_ACCESS	HYMN;NDACC	Project dependent
32 FILE_PROJECT_ID	AOID9999	Project dependent
33 FILE_ASSOCIATION	NDACC	Project dependent
34 FILE_META_VERSION	04R001;IDLCR8HDF	Refer to GEOMS document

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GEOMS-EX-FTIR-VA (*FTIR Variable Attributes Example*)

Download in CSV format [GEOMS-EX-FTIR-VA.csv](#) (last updated: October 04, 2010).

#	Variable name	Variable value	Comment
0	VAR_NAME	CH4.MIXING.RATIO_ABSORPTION.SOLAR_AVK	Refer to GEOMS document
1	VAR_DESCRIPTION	Typical averaging kernel matrix (AVK) of the retrieved vertical profile of CH4, referred to VMR units	Free format
2	VAR_NOTES	Dimension 1 are the AVK rows; dimension 2 are the AVK columns	Free format
3	VAR_SIZE	41;41	The number of elements in each dimension
4	VAR_DEPEND	ALTITUDE;ALTITUDE	INDEPENDENT, CONSTANT or a previously given one dimensional variable
5	VAR_DATA_TYPE	DOUBLE	Allowable formats are REAL, DOUBLE, BYTE, SHORT, INTEGER
6	VAR_UNITS	1	Refer to GEOMS document
7	VAR_SI_CONVERSION	0;1.;1	Refer to GEOMS document
8	VAR_VALID_MIN	-2.	
9	VAR_VALID_MAX	2.	
10	VAR_FILL_VALUE	-9.0000E+004	

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 Last Updated: October 04, 2010



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