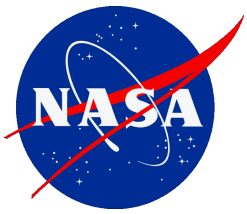
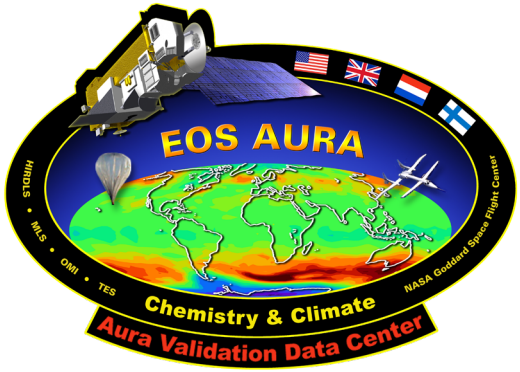
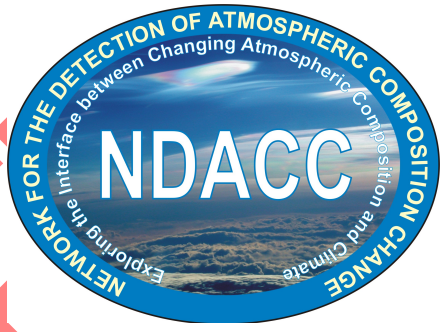


National Aeronautics and
Space Administration

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/NDACC data reporting requirements for Fourier Transform Interferometers
See Also:	Bojkov *et al.*, 2002, 2006

Table of Contents

1 Overview

This document outlines data reporting requirements for the Fourier Transform Interferometer (FTIR) systems 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) 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, the instrument names of the different FTIR systems to appear in the filenames are based on the primary measured entity [GAS] to be reported in the file (note the convention that each FTIR file reports profile and/or vertical column data for a single molecule [GAS]):

Table 2.1: Examples of FTIR instrument filenames

Primary Measured Entity [GAS]	AVDC Instrument Name
Ozone	FTIR.O3
HCl	FTIR.HCl
ClONO2	FTIR.ClONO2
CO	FTIR.CO
N_2O	FTIR.N2O
HNO_3	FTIR.HNO3
HCN	FTIR.HCN

2.2 Variable Reporting

Each measured primary entity [GAS] requires a mandatory set of 26 variables to be reported within a FTIR.[GAS] file. A description of the variables is given in Table 2.2.

Notes:

For archiving in NDACC, daily mean values are reported, together with a typical averaging kernel (AVK).

If a user requires individual data granules for satellite validation purposes, including individual AVK data, he/she must contact the instrument PI. For these cases, FTIR files require 26 mandatory variables (refer to Table 2.2).

Table 2.2: FTIR mandatory variables with recommended variable attribute entries.

#	Variable	Units[a] (VAR_UNIT)	Numeric type (VAR_DATA_TYPE)	Formatting (VIS_FORMAT)	Fill value (VAR_FILL_VALUE)	Comment
1	LATITUDE.INSTRUMENT	Deg	REAL	F9.2	-90000.00	*Inst. geolocation*
2	LONGITUDE.INSTRUMENT	deg	REAL	F9.2	-90000.00	*Inst. geolocation*
3	ALTITUDE.INSTRUMENT	m	LONG	I6	-90000	*Inst. geolocation*
4	DATETIME	MJD2000	DOUBLE	F16.9	-90000.000000000	*Weighted Meas. time*
5	ALTITUDE	km	REAL	E11.3	-9.000E+004	*Retrieval altitude vector*
6	PRESSURE_INDEPENDENT	hPa	REAL	E12.4	-9.0000E+004	*Effective pressure at each altitude*
7	TEMPERATURE_INDEPENDENT	K	REAL	F9.2	-90000.00	*Effective temperature at each altitude*
8	AIR.MASS_INDEPENDENT	molec m-2	REAL	F10.3	-90000.000	*Vector of vertical air masses associated with the layers set by the altitude vector*
9	PRESSURE.SURFACE_INDEPENDENT;	hPa	REAL	E12.4	-9.0000E+004	*Surface/ground pressure*
10	TEMPERATURE.SURFACE_INDEPENDENT	K	REAL	F9.2	-90000.00	*Surface/ground temperature*
11	[GAS].MIXING.RATIO_ABSORPTION.SOLAR or [GAS].MIXING.RATIO_ABSORPTION.LUNAR	ppv	REAL	E12.4	-9.0000E+004	*Retrieved target vertical profile in VMR units*
12	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_INTEGRATION.TIME or [GAS].MIXING.RATIO_ABSORPTION.LUNAR_INTEGRATION.TIME	ppv	REAL	E12.4	-9.0000E+004	*Retrieved target integration time*
13	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_UNCERTAINTY.RANDOM or [GAS].MIXING.RATIO_ABSORPTION.LUNAR_UNCERTAINTY.RANDOM	ppv2	REAL	E12.4	-9.0000E+004	*Sx or error covariance matrix of retrieved target profile, NOT including the smoothing error.*
14	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_UNCERTAINTY.SYSTEMATIC or [GAS].MIXING.RATIO_ABSORPTION.LUNAR_UNCERTAINTY.SYSTEMATIC	ppv2	REAL	E12.4	-9.0000E+004	*Systematic error covariance matrix associated with the retrieved vertical profile (expressed in same units as the profile)*
15	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_AVK[b] or [GAS].MIXING.RATIO_ABSORPTION.LUNAR_AVK[b]	DIMENSIONLESS	REAL	E12.4	-9.0000E+004	*A or Averaging kernel matrix for retrieved target profile (expressed in same units as the profile)*
16	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_APRIORI[b] or [GAS].MIXING.RATIO_ABSORPTION.LUNAR_APRIORI[b]	ppv	REAL	E12.4	-9.0000E+004	*A priori target vertical profile in VMR units*
17	H2O.MIXING.RATIO_ABSORPTION.SOLAR					

Table 2.2: continued

#	Variable	Units[a] (VAR_UNIT)	Numeric type (VAR_DATA_TYPE)	Formatting (VIS_FORMAT)	Fill value (VAR_FILL_VALUE)	Comment
18	ALTITUDE.BOUNDARIES	km	REAL	E10.3	-90000.000	*Altitude boundaries for the partial column profile (see algorithm issues below)*
19	[GAS].COLUMN.VERTICAL.PARTIAL_ABSORPTION.SOLAR or [GAS].COLUMN.VERTICAL.PARTIAL_ABSORPTION.LUNAR	molec m-2	REAL	E12.4	-9.0000E+004	*Partial column profile*
20	[GAS].COLUMN.VERTICAL.PARTIAL_ABSORPTION.SOLAR _APRIORI[b] Or [GAS].COLUMN.VERTICAL.PARTIAL_ABSORPTION.LUNAR_APRIORI[b]	molec m-2	REAL	E12.4	-9.0000E+004	*Partial column profile apriori*
21	[GAS].COLUMN.VERTICAL_ABSORPTION.SOLAR Or [GAS].COLUMN.VERTICAL_ABSORPTION.LUNAR	molec m-2	REAL	E12.4	-9.0000E+004	*Total column of target, corresponding to retrieved profile*
22	[GAS].COLUMN.VERTICAL_ABSORPTION.SOLAR _APRIORI[b] or [GAS].COLUMN.VERTICAL_ABSORPTION.LUNAR_APRIORI[b]	molec m-2	REAL	E12.4	-9.0000E+004	*Total a priori column of target, corresponding to a priori profile*
23	[GAS].COLUMN.VERTICAL_ABSORPTION.SOLAR_UNCERTAINTY.RANDOM or [GAS].COLUMN.VERTICAL_ABSORPTION.LUNAR_UNCERTAINTY.RANDOM	molec m-2	REAL	E12.4	-9.0000E+004	*Random uncertainty on the retrieved partial columns (expressed in same units as the column)*
24	[GAS].COLUMN.VERTICAL_ABSORPTION.SOLAR UNCERTAINTY.SYSTEMATIC Or [GAS].COLUMN.VERTICAL_ABSORPTION.LUNAR_UNCERTAINTY.SYSTEMATIC	molec m-2	REAL	E12.4	-9.0000E+004	*Systematic uncertainty on the retrieved partial columns (expressed in same units as the column)*
25	H2O.COLUMN.VERTICAL_ABSORPTION.SOLAR					
26	ANGLE.SOLAR_ZENITH.ASTRONOMICAL	deg	REAL	F9.2	-90000.00	*Only if individual measurements reported*
27	ANGLE.SOLAR_AZIMUTH	deg	REAL	F9.2	-90000.00	*Only if individual measurements reported*

[a] The units are given here as examples; equivalent standard units like ppbv instead of ppv, or molec cm-2 instead of molec m-2, may be used, on the condition that the corresponding VAR_SI_CONVERSION, VAR_DATA_TYPE, VAR_FILL_VALUE and VIS_FORMAT attributes are completed properly.

[b] The averaging kernel and a priori measurements are included in each file, so users have the option to convolve higher resolution datasets to the FTIR resolution.

Note, to accommodate the PROFITT level-based and SFIT2 layer-based algorithm outputs, an ALTITUDE and an ALTITUDE.BOUNDARIES vector (1-dimensional, or 1× N) have been added.

In the case of SFIT2, ALTITUDE contains the output altitude vector (i.e., the centre altitudes of the layers, N in number). The target gas mixing ratio profile, the partial columns, as well as pressure, temperature, are referenced to this ALTITUDE vector. The ALTITUDE.BOUNDARIES vector provides the additional information about the layer boundaries; it is a variable dependent on ALTITUDE (must have the same size). The lowermost boundary is set equal to ALTITUDE.INSTRUMENT.

In the case of PROFITT, ALTITUDE contains the level altitudes (N+1 in number). The target gas mixing ratio profile, the partial columns, as well as pressure, temperature, are referenced to this ALTITUDE vector. As the number of partial columns is one less than the number of levels, it is proposed to set the highest partial column equal to 0 – BRB: fill would be better. In this case, it is not necessary to provide the ALTITUDE.BOUNDARIES vector, because it would be identical to ALTITUDE, therefore, ALTITUDE.BOUNDARIES is an optional variable.

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.

The AVDC/NDACC variable equivalencies with the variable definitions of the EC funded UFTIR project (De Mazière, 2006) are listed in Table A of Appendix A. The UFTIR definitions are compatible with the Envisat Cal/Val guidelines (Bojkov *et al.*, 2002).

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 granularity for FTIR measurements for archiving in NDACC is defined by the *a priori* information, but not larger than one file per year: all data retrieved with the same a priori profile and associated a priori error covariance matrix (the latter one is not reported in the file) are reported in the same file. For example, if the a priori information in the retrieval changes on a monthly basis, then monthly data files will be generated. If the a priori information is constant throughout the year, then yearly data files will be created. The most common granularities will therefore be monthly, seasonal or yearly.

3 Metadata

3.1 Global Attributes

Each FTIR.[GAS] file requires one set of **Global Attributes**. These have been grouped in to three categories describing the file contents, namely **Originator Attributes**, **Dataset Attributes** and **File Attributes**. An example of global attributes for an FTIR ozone measurement at Jungfraujoch (PI and data submittor: M. De Mazière, BIRA.IASB; Data analysis: Corinne Vigoroux, 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	Vigoroux; 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.IASBG001	*Refer to standard*
DATA_LEVEL	D2	*Refer to standard*
DATA_VARIABLES	LATITUDE.INSTRUMENT LONGITUDE.INSTRUMENT ALTITUDE.INSTRUMENT DATETIME ALTITUDE PRESSURE_INDEPENDENT TEMPERATURE.AIR_INDEPENDENT *AIR.MASS_INDEPENDENT* PRESSURE.SURFACE_INDEPENDENT TEMPERATURE.SURFACE_INDEPENDENT CH4.MIXING.RATIO_ABSORPTION.SOLAR CH4.MIXING.RATIO_ABSORPTION.SOLAR_INTEGRATION.TIME CH4.MIXING.RATIO_ABSORPTION.SOLAR_UNCERTAINTY.RANDOM CH4.MIXING.RATIO_ABSORPTION.SOLAR_UNCERTAINTY.SYSTEMATIC CH4.MIXING.RATIO_ABSORPTION.SOLAR_AVK CH4.MIXING.RATIO_ABSORPTION.SOLAR_APRIORI H2O.MIXING.RATIO_ABSORPTION.SOLAR ALTITUDE.BOUNDARIES 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_UNCERTAINTY.RANDOM CH4.COLUMN.VERTICAL_ABSORPTION.SOLAR_UNCERTAINTY.SYSTEMATIC H2O.COLUMN.VERTICAL_ABSORPTION.SOLAR ANGLE.SOLAR_AZIMUTH ANGLE.SOLAR_ZENITH.ASTRONOMICAL	*Note: Angles to be added only for individual data*
DATA_START_DATE	1681	*ISO8601*
DATA_FILE_VERSION	001	
DATA_MODIFICATIONS	None	*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_d2_20040808t000000z_001.hdf	*Naming convention*
FILE_GENERATION_DATE	20050512T143444Z	*ISO8601*
FILE_ACCESS	HYMN; NDACC	*Project dependent*
FILE_PROJECT_ID	AOID9999	*Project dependent*
FILE_ASSOCIATION	NDACC	*Project dependent*
FILE_META_VERSION	02R023; IDLCR8HDF	*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	O3.MIXING.RATIO_ABSORPTION.SOLAR _AVK	*Refer to standard*
VAR_DESCRIPTION	Typical averaging kernel matrix (AVK) of the retrieved vertical profile of O3, 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;ALTITUDE	*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	O3 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*

3.3 Metadata updates

Minor metadata updates and clarifications have been incorporated into the original Envisat Cal/Val metadata guidelines (Bojkov *et al.*, 2002). A detailed description of these changes[a] can be found in the AVDC addendum (Bojkov *et al.*, 2006).

[a] ESA has committed to synchronizing the Envisat Cal/Val metadata requirements to NASA's AVDC.

Table 3.3: Summary of metadata changes.

Attribute Name	Attribute Type	Change	Comment
DATA_TYPE	Global Attribute	DATA_LEVEL	*New name for clarity*
DATA_FILE_VERSION	Global Attribute	Additional entry formats allowed	*Now can also describe processing version. For example v8, 5.01, etc.*
FILE_META_VERSION	Global Attribute	Requires 2 mandatory entries	*Attribute entries are the metadata version and the conversion tool name.*
VAR_MONOTONE	Variable Attribute	Removed	
VIS_SCALE_TYPE	Variable Attribute	Entry change	*If VIS_PLOT_TYPE set to NONE, then VIS_SCALE_TYPE must be set to NONE;NONE*
VIS_SCALE_MIN/MAX	Variable Attribute	Entry change	*If VIS_PLOT_TYPE set to NONE, then VIS_SCALE_MIN and VIS_SCALE_MAX must be set to NONE*

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
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 Version History

20060908 Include UFTIR variable information and equivalences.

20060921 Typographical corrections in Tables 2.2, 3.2 and 3.3.

2008 Final

7 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

Appendix

A. UFTIR variable equivalencies

The AVDC/NDACC variable equivalencies with the variable requirements of the EC funded UFTIR project (De Mazière, 2006) are listed in Table A.

Table A: UFTIR variable equivalencies.

#	AVDC/NDACC Variable Names	UFTIR Variable Names
1	LATITUDE.INSTRUMENT	LATITUDE.INSTRUMENT
2	LONGITUDE.INSTRUMENT	LONGITUDE.INSTRUMENT
3	ALTITUDE.INSTRUMENT	ALTITUDE.INSTRUMENT
4	DATETIME	DATETIME
5	ALTITUDE	ALTITUDE
6	PRESSURE_INDEPENDENT	PRESSURE_APRIORI
7	TEMPERATURE_INDEPENDENT	TEMPERATURE.AIR_APRIORI
8	AIR.MASS_INDEPENDENT	AIR.CONCENTRATION_APRIORI
9	PRESSURE.SURFACE_INDEPENDENT	PRESSURE_INSITU
10	TEMPERATURE.SURFACE_INDEPENDENT	TEMPERATURE.AIR_INSITU
11	[GAS].MIXING.RATIO_ABSORPTION.SOLAR	[GAS].CONCENTRATION_VERTICAL.SOLAR
12	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_UNCERTAINTY.RANDOM	[GAS].CONCENTRATION_VERTICAL.SOLAR_UNCERTAINTY.RANDOM
13	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_AVK	[GAS].CONCENTRATION.AVK_VERTICAL.SOLAR
14	[GAS].MIXING.RATIO_ABSORPTION.SOLAR_APRIORI	[GAS].CONCENTRATION_APRIORI
15	[GAS].COLUMN.VERTICAL_ABSORPTION.SOLAR	[GAS].COLUMN_VERTICAL.SOLAR
16	[GAS].COLUMN.VERTICAL_ABSORPTION.SOLAR _APRIORI	[GAS].COLUMN_APRIORI
17	ANGLE.SOLAR_ZENITH.ASTRONOMICAL	ANGLE.SOLAR_ZENITH_ASTRONOMICAL
18	ANGLE.SOLAR_AZIMUTH	ANGLE.SOLAR_AZIMUTH