3.3.2.3. NXcanSAS

Status:

application definition, extends NXobject, version 1.0

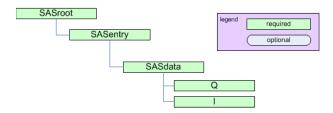
Description:

Implementation of the canSAS standard to store reduced small-angle scattering data of any dimension.

For more details, see:

- http://www.cansas.org/
- http://www.cansas.org/formats/canSAS1d/1.1/doc/
- <u>http://cansas-org.github.io/canSAS2012/</u>
- <u>https://github.com/canSAS-org/NXcanSAS_examples</u>

The minimum requirements for *reduced* small-angle scattering data as described by canSAS are summarized in the following figure:



The minimum requirements for *reduced* small-angle scattering data. (<u>full image</u>) See <u>below</u> for the minimum required information for a NeXus data file written to the NXcanSAS specification.

Implementation of canSAS standard in NeXus

This application definition is an implementation of the canSAS standard for storing both one-dimensional and multi-dimensional *reduced* small-angle scattering data.

- NXcanSAS is for reduced SAS data and metadata to be stored together in one file.
- Reduced SAS data consists of $I(ec{Q})$ or $I(|ec{Q}|)$
- External file links are not to be used for the reduced data.
- A good practice/practise is, at least, to include a reference to how the data was acquired and processed. Yet this is not a requirement.
- There is no need for NXcanSAS to refer to any raw data.

The canSAS data format has a structure similar to NeXus, not identical. To allow canSAS data to be expressed in NeXus, yet identifiable by the canSAS standard, an additional group attribute <u>canSAS_class</u> was introduced. Here is the mapping of some common groups.

group (*)	NX_class	canSAS_class	
sasentry	NXentry	SASentry	
sasdata	NXdata	SASdata	
sasdetector	NXdetector	SASdetector	

group (*)	NX_class	canSAS_class
sasinstrument	NXinstrument	SASinstrument
sasnote	NXnote	SASnote
sasprocess	NXprocess	SASprocess
sasprocessnote	NXcollection	SASprocessnote
sastransmission	NXdata	SAStransmission_spectrum
sassample	NXsample	SASsample
sassource	NXsource	SASsource

(*) The name of each group is a suggestion, not a fixed requirement and is chosen as fits each data file. See the section on defining <u>NXDL group and field names</u>.

Refer to the NeXus Coordinate System drawing (<u>NeXus Coordinate Systems</u>) for choice and direction of x, y, and z axes.

The minimum required information for a NeXus data file written to the NXcanSAS specification.

1 2	NXcanSAS HDF5 data file entry : NXentry		
3	<pre>@NX_class = "NXentry"</pre>		
4	<pre>@canSAS_class = "SASentry"</pre>		
5	@version = "1.0"		
6	definition = "NXcanSAS"		
7	<pre>run = "<see documentation="" the="">"</see></pre>		
8	<pre>title = "something descriptive yet short"</pre>		
9	data : NXdata		
10	@NX_class = "NXdata"		
11	@canSAS_class = "SASdata"		
12	@signal = "I"		
13	<pre>@I_axes = "<see documentation="" the="">"</see></pre>		
14	<pre>@Q_indices : NX_INT = <see documentation="" the=""></see></pre>		
15	I : NX_NUMBER		
16	<pre>@units = <see documentation="" the=""></see></pre>		
17	Q : NX_NUMBER		
18	<pre>@units = NX_PER_LENGTH</pre>		

Symbols:

No symbol table

Groups cited:

<u>NXaperture</u>, <u>NXcollection</u>, <u>NXcollimator</u>, <u>NXdata</u>, <u>NXdetector</u>, <u>NXentry</u>, <u>NXinstrument</u>, <u>NXnote</u>, <u>NXprocess</u>, <u>NXsample</u>, <u>NXsource</u>

Structure:

(entry): (required) NXentry

Place the canSAS <u>SASentry</u> group as a child of a NeXus <u>NXentry</u> group (when data from multiple techniques are being stored) or as a replacement for the <u>NXentry</u> group.

Note: It is required for all numerical objects to provide a *units* attribute that describes the engineering units. Use the Unidata UDunits [1] specification as this is compatible with various community standards.

[1] The UDunits specification also includes instructions for derived units.

@default: (optional) <u>NX_CHAR</u>

Declares which <u>NXdata</u> group contains the data to be shown by default. It is needed to resolve ambiguity when more than one <u>NXdata</u> group exists. The value is the name of the default <u>NXdata</u> group. Usually, this will be the name of the first *SASdata* group.

@canSAS_class: (required) NX CHAR

Official canSAS group: SASentry

Obligatory value: SASentry

@version: (required) <u>NX_CHAR</u>

Describes the version of the canSAS standard used to write this data. This must be a text (not numerical) representation. Such as:

@version="1.0"

Obligatory value: 1.0

definition: (required) <u>NX_CHAR</u>

Official NeXus NXDL schema to which this subentry conforms.

Obligatory value: NXcanSAS

title: (required) NX_CHAR

Title of this *SASentry*. Make it so that you can recognize the data by its title. Could be the name of the sample, the name for the measured data, or something else representative.

```
run: (required) NX CHAR
```

Run identification for this *SASentry*. For many facilities, this is an integer, such as en experiment number. Use multiple instances of <u>run</u> as needed, keeping in mind that HDF5 requires unique names for all entities in a group.

@name: (optional) <u>NX_CHAR</u>

Optional string attribute to identify this particular *run*. Could use this to associate (correlate) multiple *SASdata* elements with *run* elements.

(data): (required) NXdata

A SASData group contains a single reduced small-angle scattering data set that can be represented as $I(\vec{Q})$ or $I(|\vec{Q}|)$.

Q can be either a vector ($ec{Q}$) or a vector magnitude ($|ec{Q}|$)

The name of each *SASdata* group must be unique within a SASentry group. Suggest using names such as sasdata01.

NOTE: For the first *SASdata* group, be sure to write the chosen name into the *SASentry/@default* attribute, as in:

SASentry/@default="sasdata01"

A SASdata group has several attributes:

- I_axes
- Q_indices
- Mask_indices

To indicate the dependency relationships of other varied parameters, use attributes similar to @Mask_indices (such as @Temperature_indices or @Pressure_indices).

@canSAS_class: (required) NX_CHAR

Official canSAS group: NXcanSAS (applications); SASdata

Obligatory value: SASdata

@signal: (required) NX_CHAR

Name of the default data field.

Obligatory value:

• I: For canSAS SASdata, this is always "I".

@I_axes: (required) NX CHAR

String array that defines the independent data fields used in the default plot for all of the dimensions of the *signal* field (the *signal* field is the field in this group that is named by the <u>signal</u> attribute of this group). One entry is provided for every dimension of the I data object. Such as:

@I_axes="Temperature", "Time", "Pressure", "Q", "Q"

Since there are five items in the list, the intensity field of this example \underline{I} must be a five-dimensional array (rank=5).

@Q_indices: (required) NX INT

Integer or integer array that describes which indices (of the I data object) are used to reference the $\underline{0}$ data object. The items in this array use zero-based indexing. Such as:

@Q_indices=1,3,4

which indicates that \underline{Q} requires three indices from the I data object: one for time and two for Q position. Thus, in this example, the \underline{Q} data is time-dependent: $\vec{Q}(t)$.

@Mask_indices: (optional) <u>NX_CHAR</u>

Integer or integer array that describes which indices (of the I data object) are used to reference the <u>Mask</u> data object. The items in this array use zero-based indexing. Such as:

@Mask_indices=3,4

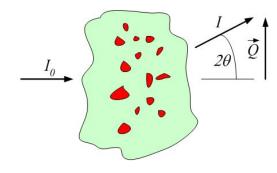
which indicates that Q requires two indices from the I data object for Q position.

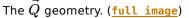
@timestamp: (optional) <u>NX_DATE_TIME</u>

ISO-8601 time [2]

Q: (required) <u>NX_NUMBER</u> {units=<u>NX_PER_LENGTH</u>}

Array of Q data to accompany I.





Q may be represented as either the three-dimensional scattering vector \vec{Q} or the magnitude of the scattering vector, $|\vec{Q}|$.

$$ert ec Q ert = (4\pi/\lambda) sin(heta)$$

When we write Q, we may refer to either or both of $|\vec{Q}|$ or \vec{Q} , depending on the context.

@uncertainties: (optional) NX_CHAR

(optional: for numerical arrays)

Names the dataset (in this SASdata group) that provides the uncertainty to be used for data analysis. The name of the dataset containing the Q uncertainty is flexible. The name must be unique in the SASdata group.

Such as:

@uncertainties="0_uncertainties"

The *uncertainties* field will have the same *shape* (dimensions) as the Q field.

These values are the estimates of uncertainty of each Q. By default, this will be interpreted to be the estimated standard deviation. In special cases, when a standard deviation cannot possibly be used, its value can specify another measure of distribution width.

There may also be a subdirectory (optional) with constituent components.

Note

To report distribution in reported Q values, use the <u>@resolutions</u> attribute. It is possible for both <u>@resolutions</u> and <u>uncertainties</u> to be reported.

@resolutions: (optional) NX_CHAR

(optional: for numerical arrays)

Names the dataset (in this SASdata group) containing the Q resolution. The name of the dataset containing the Q resolution is flexible. The name must be unique in the SASdata group.

The *resolutions* field will have the same *shape* (dimensions) as the Q field.

Generally, this is the principal resolution of each Q. Names the data object (in this SASdata group) that provides the Q resolution to be used for data analysis. Such as:

@resolutions="Qdev"

To specify two-dimensional resolution for slit-smearing geometry, such as (dQw, dQl), use a string array, such as:

@resolutions="dQw", "dQl"

There may also be a subdirectory (optional) with constituent components.

This pattern will demonstrate how to introduce further as-yet unanticipated terms related to the data.

By default, the values of the resolutions data object are assumed to be one standard deviation of any function used to approximate the resolution function. This equates to the width of the gaussian distribution if a Gaussian is chosen. See the @resolutions_description attribute.

Note

To report uncertainty in reported Q values, use the <u>@uncertainties</u> attribute. It is possible for both <u>@resolutions</u> and <u>uncertainties</u> to be reported.

@resolutions_description: (optional) NX_CHAR

(optional) Generally, this describes the $Q \ \underline{\texttt{@resolutions}}$ data object. By default, the value is assumed to be "Gaussian". These are suggestions:

- Gaussian
- Lorentzian
- Square : note that the full width of the square would be ~2.9 times the standard deviation specified in the vector
- Triangular
- Sawtooth-outward : vertical edge pointing to larger Q
- Sawtooth-inward vertical edge pointing to smaller Q
- Bin : range of values contributing (for example, when 2-D

detector data have been reduced to a 1-D I(|Q|) dataset)

For other meanings, it may be necessary to provide further details such as the function used to assess the resolution. In such cases, use additional datasets or a <u>NXnote</u> subgroup to include that detail.

I: (required) <u>NX_NUMBER</u>

Array of intensity (I) data.

The intensity may be represented in one of these forms:

absolute units: $d\Sigma/d\Omega(Q)$ differential cross-section per unit volume per unit solid angle (such as: 1/cm/sr or 1/m/sr)

absolute units: $d\sigma/d\Omega(Q)$ differential cross-section per unit atom per unit solid angle (such as: cm^2 or m^2)

arbitrary units: I(Q) usually a ratio of two detectors but units are meaningless (such as: a.u. or counts)

This presents a few problems for analysis software to sort out when reading the data. Fortunately, it is possible to analyze the *units* to determine which type of intensity is being reported and make choices at the time the file is read. But this is an area for consideration and possible improvement.

One problem arises with software that automatically converts data into some canonical units used by that software. The software should not convert units between these different types of intensity indiscriminately.

A second problem is that when arbitrary units are used, then the set of possible analytical results is restricted. With such units, no meaningful volume fraction or number density can be determined directly from I(Q).

In some cases, it is possible to apply a factor to convert the arbitrary units to an absolute scale. This should be considered as a possibility of the analysis process.

Where this documentation says *typical units*, it is possible that small-angle data may be presented in other units and still be consistent with NeXus. See the <u>NeXus Data Units</u> section.

@uncertainties: (optional) NX_CHAR

(optional: for numerical arrays)

Names the dataset (in this SASdata group) that provides the uncertainty of I to be used for data analysis. The name of the dataset containing the I uncertainty is flexible. The name must be unique in the SASdata group.

Generally, this is the estimate of the uncertainty of each I. Typically the estimated standard deviation.

Idev is the canonical name from the 1D standard. The NXcanSAS standard allows for the name to be described using this attribute. Such as:

```
@uncertainties="Idev"
     @scaling_factor: (optional) NX CHAR
          (optional) Names the field (a.k.a. dataset) that contains a factor to
          multiply I. By default, this value is unity. Should an uncertainty be
          associated with the scaling factor field, the field containing that
          uncertainty would be designated via the uncertainties attribute.
          Such as:
            I : NX NUMBER
                @uncertainties="Idev" : NX CHAR
                @scaling factor="I scaling" : NX CHAR
            Idev : NX NUMBER
            I scaling : NX NUMBER
                @uncertainties="I scaling dev" : NX CHAR
            I_scaling_dev : NX_NUMBER
          The exact names for I_scaling and I_scaling_dev are not defined
          by NXcanSAS. The user has the flexibility to use names different
          than those shown in this example.
Idev: (optional) NX NUMBER
     Estimated uncertainty (usually standard deviation) in I. Must have the
     same units as I.
     When present, the name of this field is also recorded in the uncertainties
     attribute of I, as in:
      I/@uncertainties="Idev"
Qdev: (optional) <u>NX_NUMBER</u> {units=<u>NX_PER_LENGTH</u>}
     Estimated Q resolution (usually standard deviation). Must have the
     same units as Q.
     When present, the name of this field is also recorded in the resolutions
     attribute of Q, as in:
      0/@resolutions="0dev"
     or:
      Q/@resolutions="dQw", "dQl"
dQw: (optional) <u>NX NUMBER</u> {units=<u>NX PER LENGTH</u>}
     Q resolution along the axis of scanning (the high-resolution slit width
     direction). Useful for defining resolution data from slit-smearing
     instruments such as Bonse-Hart geometry. Must have the same units as
     Q.
     When present, the name of this field is also recorded in the resolutions
     attribute of Q, as in:
```

Q/@resolutions="dQw", "dQl"

dQI: (optional) <u>NX_NUMBER</u> {units=<u>NX_PER_LENGTH</u>}

Q resolution perpendicular to the axis of scanning (the low-resolution *slit length* direction). Useful for defining resolution data from slit-smearing instruments such as Bonse-Hart geometry. Must have the same units as Q.

When present, the name of this field is also recorded in the *resolutions* attribute of Q, as in:

Q/@resolutions="dQw", "dQl"

Qmean: (optional) <u>NX_NUMBER</u> {units=<u>NX_PER_LENGTH</u>}

Mean value of Q for this data point. Useful when describing data that has been binned from higher-resolution data.

It is expected that \underline{Q} is provided and that both \underline{Q} and \underline{Qmean} will have the same units.

ShadowFactor: (optional) <u>NX_CHAR</u> {units=<u>NX_DIMENSIONLESS</u>}

A numerical factor applied to pixels affected by the beam stop penumbra. Used in data files from NIST/NCNR instruments.

See: J.G. Barker and J.S. Pedersen (1995) J. Appl. Cryst. 28, 105-114.

(instrument): (optional) NXinstrument

Description of the small-angle scattering instrument.

Consider, carefully, the relevance to the SAS data analysis process when adding subgroups in this **NXinstrument** group. Additional information can be added but will likely be ignored by standardized data anlysis processes.

The NeXus <u>NXbeam</u> base class may be added as a subgroup of this **NXinstrument** group *or* as a subgroup of the **NXsample** group to describe properties of the beam at any point downstream from the source.

@canSAS_class: (required) NX CHAR

Official canSAS group: NXcanSAS (applications); SASinstrument

Obligatory value: SASinstrument

(aperture): (optional) NXaperture

<u>NXaperture</u> is generic and limits the variation in data files.

Possible NeXus base class alternatives are: <u>NXpinhole</u> or <u>NXslit</u>.

@canSAS_class: (required) <u>NX_CHAR</u>

Official canSAS group: NXcanSAS (applications); SASaperture

Obligatory value: SASaperture

shape: (required) NX_CHAR

describe the type of aperture (pinhole, 4-blade slit, Soller slit, ...)

x_gap: (optional) <u>NX_NUMBER</u> {units=<u>NX_LENGTH</u>}

opening along the x axis

y_gap: (optional) <u>NX_NUMBER</u> {units=<u>NX_LENGTH</u>}

opening along the y axis

(collimator): (optional) NXcollimator

Description of a collimating element (defines the divergence of the beam) in the instrument.

To document a slit, pinhole, or the beam, refer to the documentation of the NXinstrument group above.

@canSAS_class: (required) NX_CHAR

Official canSAS group: NXcanSAS (applications); SAScollimation

Obligatory value: SAScollimation

length: (optional) <u>NX_NUMBER</u> {units=<u>NX_LENGTH</u>}

Amount/length of collimation inserted (as on a SANS instrument)

distance: (optional) <u>NX_NUMBER</u> {units=<u>NX_LENGTH</u>}

Distance from this collimation element to the sample

(detector): (optional) NXdetector

Description of a detector in the instrument.

@canSAS_class: (required) <u>NX_CHAR</u>

Official canSAS group: NXcanSAS (applications); SASdetector

Obligatory value: SASdetector

name: (required) NX_CHAR

Identifies the name of this detector

SDD: (optional) <u>NX_NUMBER</u> {units=<u>NX_LENGTH</u>}

Distance between sample and detector.

Note: In NXdetector, the <u>distance</u> field records the distance to the previous component ... most often the sample. This use is the same as <u>SDD</u> for most SAS instruments but not all. For example, Bonse-Hart cameras have one or more crystals between the sample and detector.

We define here the field <u>SDD</u> to document without ambiguity the distance between sample and detector.

slit_length: (optional) <u>NX_NUMBER</u> {units=<u>NX_PER_LENGTH</u>}

Slit length of the instrument for this detector, expressed in the same units as Q.

x_position: (optional) <u>NX_NUMBER</u> {units=<u>NX_LENGTH</u>}

Location of the detector in \boldsymbol{x}

y_position: (optional) <u>NX_NUMBER</u> {units=<u>NX_LENGTH</u>}

Location of the detector in y

roll: (optional) <u>NX_NUMBER</u> {units=<u>NX_ANGLE</u>}

Rotation of the detector about the z axis (roll)

pitch: (optional) <u>NX_NUMBER</u> {units=<u>NX_ANGLE</u>}

Rotation of the detector about the x axis (roll)

yaw: (optional) <u>NX_NUMBER</u> {units=<u>NX_ANGLE</u>}

Rotation of the detector about the y axis (yaw)

beam_center_x: (optional) NX_FLOAT {units=NX_LENGTH}

Position of the beam center on the detector.

This is the x position where the direct beam would hit the detector plane. This is a length, not a pixel position, and can be outside of the actual detector. The value can any real number (positive, zero, or negative).

beam_center_y: (optional) NX_FLOAT {units=NX_LENGTH}

Position of the beam center on the detector.

This is the y position where the direct beam would hit the detector plane. This is a length, not a pixel position, and can be outside of the actual detector. The value can any real number (positive, zero, or negative).

x_pixel_size: (optional) NX_FLOAT {units=NX_LENGTH}

Size of each detector pixel. If it is scalar all pixels are the same size

y_pixel_size: (optional) NX_FLOAT {units=NX_LENGTH}

Size of each detector pixel. If it is scalar all pixels are the same size

(source): (optional) NXsource

Description of the radiation source.

@canSAS_class: (required) <u>NX_CHAR</u>

Official canSAS group: NXcanSAS (applications); SASsource

Obligatory value: SASsource

radiation: (required) NX_CHAR

Name of the radiation used. Note that this is **not** the name of the facility!

Any of these values:

- Spallation Neutron Source
- Pulsed Reactor Neutron Source
- Reactor Neutron Source
- Synchrotron X-ray Source
- Pulsed Muon Source
- Rotating Anode X-ray
- Fixed Tube X-ray
- UV Laser
- Free-Electron Laser
- Optical Laser
- Ion Source
- UV Plasma Source
- neutron
- x-ray
- muon
- electron
- ultraviolet
- visible light
- positron
- proton

beam_shape: (optional) <u>NX_CHAR</u>

Text description of the shape of the beam (incident on the sample).

incident_wavelength: (optional) <u>NX_NUMBER</u>
{units=<u>NX_WAVELENGTH</u>}

wavelength () of radiation incident on the sample

wavelength_min: (optional) <u>NX_NUMBER</u> {units=<u>NX_WAVELENGTH</u>}

Some facilities specify wavelength using a range. This is the lowest wavelength in such a range.

wavelength_max: (optional) <u>NX_NUMBER</u> {units=<u>NX_WAVELENGTH</u>}

Some facilities specify wavelength using a range. This is the highest wavelength in such a range.

incident_wavelength_spread: (optional) <u>NX_NUMBER</u>

{units=<u>NX_WAVELENGTH</u>}

Some facilities specify wavelength using a range. This is the width (FWHM) of such a range.

beam_size_x: (optional) <u>NX_NUMBER</u> {units=<u>NX_LENGTH</u>}

Size of the incident beam along the x axis.

beam_size_y: (optional) <u>NX_NUMBER</u> {units=<u>NX_LENGTH</u>}

Size of the incident beam along the y axis. (sample): (optional) NXsample Description of the sample. @canSAS class: (required) NX CHAR Official canSAS group: NXcanSAS (applications); SASsample Obligatory value: SASsample name: (required) NX CHAR **ID**: Text string that identifies this sample. thickness: (optional) NX FLOAT {units=NX LENGTH} Thickness of this sample transmission: (optional) <u>NX_NUMBER</u> {units=<u>NX_DIMENSIONLESS</u>} Transmission (I/I_0) of this sample. There is no *units* attribute as this number is dimensionless. Note: the ability to store a transmission spectrum, instead of a single value, is provided elsewhere in the structure, in the SAStransmission spectrum element. temperature: (optional) <u>NX_NUMBER</u> {units=<u>NX_TEMPERATURE</u>} Temperature of this sample. details: (optional) NX CHAR Any additional sample details. x_position: (optional) NX_NUMBER {units=NX_LENGTH} Location of the sample in x**y position**: (optional) <u>NX NUMBER</u> {units=<u>NX LENGTH</u>} Location of the sample in yroll: (optional) NX NUMBER {units=NX ANGLE} Rotation of the sample about the z axis (roll) pitch: (optional) <u>NX_NUMBER</u> {units=<u>NX_ANGLE</u>} Rotation of the sample about the x axis (roll) yaw: (optional) <u>NX_NUMBER</u> {units=<u>NX_ANGLE</u>} Rotation of the sample about the y axis (yaw) (process): (optional) NXprocess Description of a processing or analysis step.

Add additional fields as needed to describe value(s) of any variable, parameter, or term related to the *SASprocess* step. Be sure to include *units* attributes for all numerical fields.

@canSAS_class: (required) <u>NX_CHAR</u>

Official canSAS group: NXcanSAS (applications); SASprocess

Obligatory value: SASprocess

name: (optional) NX CHAR

Optional name for this data processing or analysis step

date: (optional) <u>NX_DATE_TIME</u>

Optional date for this data processing or analysis step. [2]

[2] (<u>1</u>, <u>2</u>, <u>3</u>)

ISO-8601 standard time representation.

NeXus dates and times are reported in ISO-8601 (e.g., yyyy-mmddThh:mm:ss) or modified ISO-8601 (e.g., yyyy-mm-dd hh:mm:ss).

See: <u>http://www.w3.org/TR/NOTE-datetime</u> or <u>http://en.wikipedia.org</u> /wiki/ISO_8601 for more details.

description: (optional) <u>NX_CHAR</u>

Optional description for this data processing or analysis step

term: (optional) NX CHAR

Specifies the value of a single variable, parameter, or term (while defined here as a string, it could be a number) related to the *SASprocess* step.

Note: The name *term* is not required, it could take any name, as long as the name is unique within this group.

(note): (optional) <u>NXnote</u>

Any additional notes or subprocessing steps will be documented here.

An **NXnote** group can be added to any NeXus group at or below the **NXentry** group. It is shown here as a suggestion of a good place to *consider* its use.

(collection): (optional) NXcollection

Describes anything about SASprocess that is not already described.

Any content not defined in the canSAS standard can be placed at this point.

Note: The name of this group is flexible, it could take any name, as long as it is unique within the **NXprocess** group.

@canSAS_class: (required) <u>NX_CHAR</u>

Official canSAS group: NXcanSAS (applications); SASprocessnote

Obligatory value: SASprocessnote

(collection): (optional) NXcollection

Free form description of anything not covered by other elements.

@canSAS_class: (required) <u>NX_CHAR</u>

Official canSAS group: NXcanSAS (applications); SASnote

Obligatory value: SASnote

(data): (optional) NXdata

The SAStransmission_spectrum element

This describes certain data obtained from a variable-wavelength source such as pulsed-neutron source.

The name of each *SAStransmission_spectrum* group must be unique within a SASentry group. Suggest using names such as sastransmission_spectrum01.

@canSAS_class: (required) NX_CHAR

Official canSAS group: NXcanSAS (applications); SAStransmission_spectrum

Obligatory value: SAStransmission_spectrum

@signal: (required) NX_CHAR

Name of the default data field.

Obligatory value:

• T: For SAStransmission_spectrum, this is always "T".

@T_axes: (required) NX_CHAR

Obligatory value:

• $\underline{\mathsf{T}}$: the wavelengths field (as a dimension scale) corresponding to this transmission

@name: (required) <u>NX_CHAR</u>

Identify what type of spectrum is being described. It is expected that this value will take either of these two values:

value meaning

sample	measurement with the sample and container
can	measurement with just the container

@timestamp: (optional) <u>NX_DATE_TIME</u>

ISO-8601 time [2]

lambda: (required) <u>NX_NUMBER</u> {units=<u>NX_WAVELENGTH</u>}

Wavelength of the radiation.

This array is of the same shape as \underline{T} and \underline{T} dev.

T: (required) <u>NX_NUMBER</u> {units=<u>NX_DIMENSIONLESS</u>}

Transmission values (I/I_0) as a function of wavelength.

This array is of the same shape as <u>lambda</u> and <u>Tdev</u>.

@uncertainties: (required) NX_CHAR

Names the dataset (in this SASdata group) that provides the uncertainty of each transmission T to be used for data analysis. The name of the dataset containing the T uncertainty is expected to be Tdev.

Typically:

@uncertainties="Tdev"

Tdev: (required) <u>NX_NUMBER</u> {units=<u>NX_DIMENSIONLESS</u>}

Estimated uncertainty (usually standard deviation) in $T. \mbox{ Must have the same units as } T.$

This is the field is named in the *uncertainties* attribute of *T*, as in:

T/@uncertainties="Tdev"

This array is of the same shape as <u>lambda</u> and <u>T</u>.

NXDL Source:

https://github.com/nexusformat/definitions/blob/master/applications/NXcanSAS.nxdl.xml