CanSAS 1-D Data Format, v1.0

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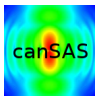
Preface



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Note

Provide a note here describing CanSAS and the initiative to establish a standard file format. Note that the data files must adhere to the XML rules which includes being well-formed (including the use of closing tags). See `http://www.w3schools.com/xml/xml_syntax.asp` for more details. Files that can be validated against cansas1d.xsd are deemed to be valid cansas1d/1.0 data files.

The name "canSAS" stands for "Collective Action for Nomadic Small-Angle Scatterers.

This work is the initiative of the CanSAS 1D Data Formats Working Group, established at the canSAS-V workshop, NIST, Gaithersburg, Maryland, USA from October 29th to 31st 2007. It derives many of its foundations from previous works such as the SASXML format, a joint collaboration between ISIS and ILL.

The home page of the CanSAS 1D Data Formats Working Group[1] describes the members, timelines, and current status. There is a discussion[2] page for some matters that preceded this revision.

Disclaimer

This description is meant to inform the community how to arrange information within the structure of the XML files and to define the spelling of the terms to be used. However, should the information in this document and the cansas1d/1.0 SAS XML Schema [3] differ, the XML Schema will be deemed to have the most correct description of the standard.

[1] http://www.smallangles.net/wgwiki/index.php/1D_Data_Formats_Working_Group
[2] http://www.smallangles.net/wgwiki/index.php/Talk:1D_Data_Formats_Working_Group
[3] http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/cansas1d.xsd

Chapter 1

Wiki Manual

1.1 Objective

One of the first aims of the canSAS (Collective Action for Nomadic Small-Angle Scatterers) forum of users, software developers, and facility staff was to discuss better sharing of SAS data analysis software. CanSAS [1] identified that a significant need within the SAS community can be satisfied by a robust, self-describing, text-based, standard format to communicate reduced one-dimensional small-angle scattering data, "I(Q)", between users of our facilities. Our goal has been to define such a format that leaves the data file instantly human-readable, editable in the simplest of editors, and importable by simple text import filters in programs that need not recognise advanced structure in the file nor require advanced programming interfaces. The file should contain both the primary data of "I(Q)" and also any other descriptive information (metadata) about the sample, measurement, instrument, processing, or analysis steps.

The cansas1d/1.0 standard meets the objectives for a 1D standard, incorporating metadata about the measurement, parameters and results of processing or analysis steps. Even multiple measurements (related or unrelated) may be included within a single XML file.

1.1.1 Status

Version 1.0 was tagged from the subversion repository on 2009-05-12 as no changes were committed since January 2009. Use this command to checkout the tagged release.

```
svn checkout http://svn.smallangles.net/svn/canSAS/1dwg/tags/v1.0 cansas1dwg-1.0
```

1.2 General Layout of the XML Data

The canSAS 1-D standard for reduced 1-D SAS data is implemented using XML files. A single file can contain SAS data from a single experiment or multiple experiments. All types of relevant data ("I(Q)", metadata) are described for each experiment. More details are provided below.

1.2.1 Overview

The basic elements of the cansas1d/1.0 standard are shown in the following table. After an XML header, the root element of the file is SASroot which contains one or more SASentry elements, each of which describes a single experiment (data set, time-slice, step in a series, new sample, etc.). Details of the `SASentry` element are also shown in the next figure. See cansas1d.xml [2] for

[1] http://www.smallangles.net/canSAS
[2] http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/cansas1d.xml

an example XML file. Examples, Case Studies, and other background information are below. More discussion can be found on the canSAS 1D Data Formats Working Group [3] page and its discussion [4] page. A glossary defining the details about each specific field (XPath string, XML elements and attributes) is provided.

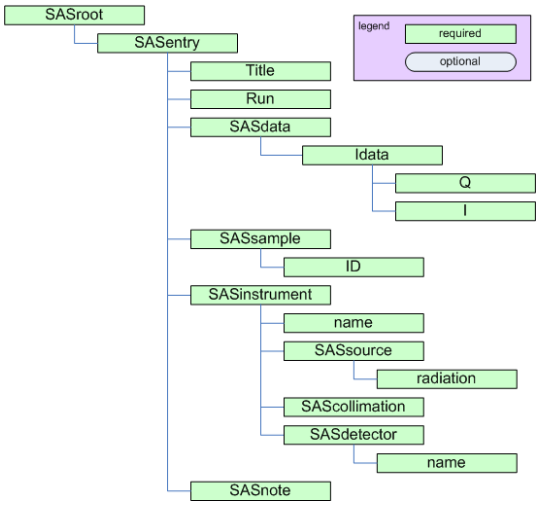


Figure 1.1: block diagram of minimum elements required for cansas1d/1.0 standard

- SASroot: the root element of the file (after the XML header)
- SASentry: describes a single experiment (data set, time-slice, step in a series, new sample, etc.)
- block diagrams
- cansas1d.xml example XML file
- discussion of this format: basic more
- Seek outside help for XML
- Definition of terms: Details about each specific field (XPath string, XML elements and attributes)

1.2.1.1 Basic elements of the cansas1d/1.0 standard

Table 1.1: Basic elements of the CanSAS 1-D standard

Element	Description
XML Header	descriptive info required at the start of every XML file
SASroot	root element of XML file
SASentry	data set, time-slice, step in a series, new sample, etc.
`Title`	for this particular `SASentry`
`Run`	run number or ID number of experiment
`{any}`	any non-cansas1d/1.0 element can be used at this point
`SASdata`	this is where the reduced 1-D SAS data is stored
`Idata`	a single data point in the dataset
`{any}`	any non-cansas1d/1.0 element can be used at this point
`SASsample`	description of the sample
`SASinstrument`	description of the instrument

[3] http://www.smallangles.net/wgwiki/index.php/1D_Data_Formats_Working_Group

[4] http://www.smallangles.net/wgwiki/index.php/Talk:1D_Data_Formats_Working_Group

Table 1.1: (continued)

Element	Description
SASsource	description of the source
SAScollimation	description of the collimation
SASdetector	description of the detector
SASprocess	for each processing or analysis step
SASnote	anything at all

1.2.1.2 Required XML file header

```
<?xml version="1.0"?>
<?xml-stylesheet type="text/xsl" href="cansasxml-html.xsl" ?>
<SASroot version="1.0"
    xmlns="cansas1d/1.0"
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
    xsi:schemaLocation="cansas1d/1.0
    http://svn.smallangles.net/svn/canSAS/1dwg/trunk/cansas1d.xsd">
```

1.2.2 Rules

1. canSAS1d/1.0 XML data files will adhere to the standard if they can successfully [[cansas1d_documentation#Validation_of_XML_
   | validate]] against the established XML Schema cansas1d.xsd
2. $Q=(4 \pi / \lambda) \sin(\theta)$

   where \lambda is the wavelength of the radiation

   and 2\theta is the angle through which the detected radiation has been scattered.

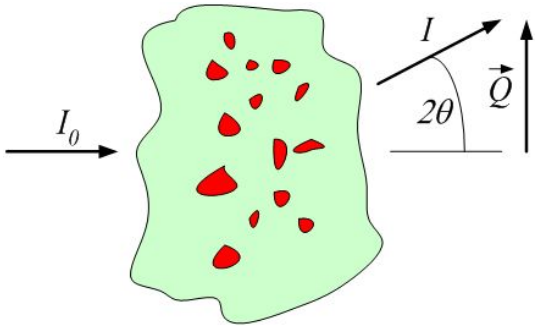


Figure 1.2: definition of Q geometry for small-angle scattering

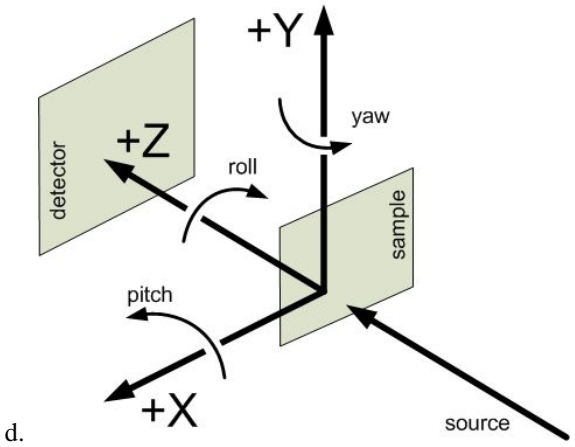
3. units to be given in standard SI abbreviations (eg, m, cm, mm, nm, K) with the following exceptions:
   a. um=micrometres
   b. C=celsius
   c. A=Angstroms
   d. percent=%.
   e. fraction
   f. a.u.=arbitrary units

g. none=no units are relevant (such as dimensionless)

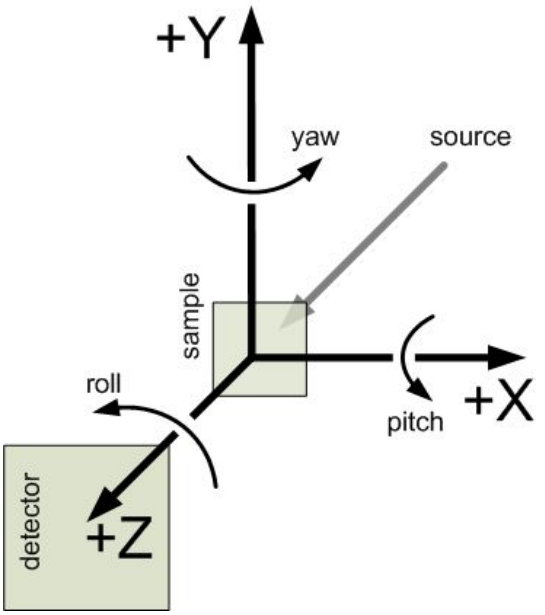
4. where reciprocal units need to be quoted the format shall be "1/abbreviation"
5. when raised to a power, use similar to "A^3" or "1/m^4" (and not "A3" or "m-4")
6. axes:
    a. z is along the flight path (positive value in the direction of the detector)
    b. x is orthogonal to z in the horizontal plane (positive values increase to the right when viewed towards the incoming radiation)
    c. y is orthogonal to z and x in the vertical plane (positive values increase upwards)

Table 1.2:

d.



as viewed from source



as viewed from detector

Figure 1.3: definition of translation and orientation geometry as viewed from the detector towards the source

7. orientation (angles) describes one-axis rotations (rotations about multiple axes require more information):
    a. roll is about z
    b. pitch is about x
    c. yaw is about y
8. Unicode characters MUST NOT be used
9. Binary data is not supported

1.2.3 Compatibility of Geometry Definitions

Note: translation and orientation geometry used by canSAS are consistent with:

- http://en.wikipedia.org/wiki/Cartesian_coordinate_system

- http://en.wikipedia.org/wiki/Right-hand_rule
- http://www.nexusformat.org/Coordinate_Systems
- http://mcstas.risoe.dk/documentation/tutorial/node6.html
- http://webhost5.nts.jhu.edu/reza/book/kinematics/kinematics.htm

The translation and orientation geometry definitions used here are different than those used by **SHADOW** [5] where the y and z axes are swapped and the direction of x is changed.

Note
How does this relate to *McStas* conventions?

1.2.4 Converting data into the XML format

The canSAS/xmlWriter [6] is a WWW form to translate three-column ASCII text data into the canSAS1d/1.0 XML format. This form will help you in creating an XML file with all the required elements in the correct places. The form requests the SAS data of Q, I, and Idev (defined elsewhere on this page) and some basic metadata (title, run, sample info, ...). Press the `<nowiki>Submit</nowiki>` button and you will receive a nicely formatted WWW page with the SAS data. If you then choose "View page source" (from one of your browser menus), you will see the raw XML of the canSAS1d/1.0 XML format and you can copy/paste this into an XML file.

The SAS data that you paste into the form box is likely to be copied directly from a 3-column ASCII file from a text editor. Line breaks are OK, they will be treated as white-space as will tabs and commas. Do not be concerned that the data looks awful in the form entry box, just check the result to see that it comes out OK.

1.3 Documentation and Definitions

- **Documentation**: [[cansas1d_documentation]] (this page)
- **Definitions**: [[cansas1d_definition_of_terms]]
- **Block diagrams**: [[cansas1d_block_diagrams]]

1.3.1 XML Schema

The [http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/cansas1d.xsd cansas1d.xsd] [http://www.w3schools.com/xsd XML Schema] defines the rules for the XML file format ([http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/cansas1d.xsd TRAC], [http://svn.smallangles.net/svn/canSAS/1dwg/trunk/cansas1d.xsd SVN]) and is used to validate any XML file for adherence to the format.

1.3.2 XML Stylesheets

- "'cansasxml-html.xsl"': [http://www.w3schools.com/xsl/ XSLT stylesheets] can be used to extract metadata or to convert into another file format. The default canSAS stylesheet [[http://svn.smallangles.net/svn/canSAS/1dwg/trunk/cansasxml-html.xsl cansasxml-html.xsl]] should be copied into each folder with canSAS XML data file(s). It can be used to display the data in a supporting WWW browser (such as Firefox or Internet Explorer) or to import into Microsoft Excel (with the added XML support in Excel). (See the excellent write-up by Steve King, ISIS, at http://www.isis.rl.ac.uk/archive/LargeScale/LOQ/xml/cansas_xml_fo for an example.) By default, MS Windows binds "'*.xml"' files to start Internet Explorer. Double-clicking on a canSAS XML data file with the [http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/cansasxml-html.xsl "'cansasxml-html.xsl"'] stylesheet in the same directory will produce a WWW page with the SAS data and selected metadata.

[5] http://www.nanotech.wisc.edu/shadow
[6] http://www.smallangles.net/canSAS/xmlWriter/

- Suggestions for support software that writes canSAS1d/1.0 XML data files:
  - be sure to update to the latest SVN repository revision (command: `svn update`)
  - check the output directory to see if it contains the default XSLT file.
  - copy the latest XSLT file to the output directory if either:
    * the output directory contains an older revision
    * the output directory does not have the default XSLT file
  - The most recent XSLT file can be identified by examining the file for the "'$ Revision: "' string. For example: `# $Revision: 111 $` is version 111.

1.3.3 Examples and Case Studies

- [http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/cansas1d.xml cansas1d.xml] basic example: Note that, for clarity, only one row of data is shown. This is probably a very good example to use as a starting point for creating XML files with a text editor.
- [http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/bimodal-test1.xml bimodal-test1.xml]: Simulated SAS data to test size distribution calculation routines.
- [[Glassy_Carbon_Round_Robin | Glassy Carbon Round Robin]]: Glassy carbon samples measured at several facilities worldwide.
- [[cansas1d_casestudy_collagen | dry chick collagen]]: illustrates the minimum information necessary to meet the requirements of the standard format
- [[cansas1d_casestudy_af1410 | AF1410 steel]]: SANS study using magnetic contrast variation (with multiple samples and multiple data sets for each sample), the files can be viewed from TRAC (no description yet): [http://svn.smallangles.net/trac/canSAS/brows http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/examples/af1410/]
- [http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/cansas1d-template.xml cansas1d-template.xml]: This is used to test all the rules in the XML Schema. This is probably not a very good example to use as a starting point for creating XML files with a text editor since it tests many of the special-case rules.

1.3.3.1 XML layout for multiple experiments

Each experiment is described with a single "'SASentry"' element. The fragment below shows how multiple experiments can be included in a single XML file. Full examples of canSAS XML files with multiple experiments include:

- ISIS LOQ SANS instrument: http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/W1W2.XML
- AF1410 steel SANS contrast variation study from NIST: http://svn.smallangles.net/svn/canSAS/1dwg/trunk/examples/af1410/cs_af1410.xml

Here is a brief sketch of how a file would be arranged with multiple SASentry elements and multiple SASdata elements.

```
<?xml version="1.0"?>
<?xml-stylesheet type="text/xsl" href="cansasxml-html.xsl" ?>
<SASroot version="1.0"
      xmlns="cansas1d/1.0"
      xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
      xsi:schemaLocation="cansas1d/1.0 http://svn.smallangles.net/svn/canSAS/1dwg/trunk/ ↩
          cansas1d.xsd"
      >
      <SASentry name="071121.dat#S22">
            <!-\- contents of the first experiment in the file go here -\->
      </SASentry>
      <SASentry name="example temperature series">
           <!-\- example with two SAS data sets related to the same sample -\->
```

```
            <Title>title of this series</Title>
            <Run name="run1">42-001</Run>
            <Run name="run2">42-002</Run>
            <SASdata name="run1">
                 <!-\- data from 42-001 run comes here -\->
            </SASdata>
            <SASdata name="run2">
                 <!-\- data from 42-002 run comes here -\->
            </SASdata>
            <!-\- other elements come here for this entry -\->
       </SASentry>
       <SASentry name="other sample">
            <!-\- any number of additional experiments can be included, as desired -\->
            <!-\- SASentry elements in the same XML file do not have to be related -\->
       </SASentry>
</SASroot>
```

1.3.4 Foreign Elements

To allow for inclusion of elements that are not defined by the cansas1d.xsd XML Schema, XML "foreign elements" are permitted at select locations in the cansas1d/1.0 format. Please refer to the references (and others) [[#Help_for_XML | below]] for deeper discussions on foreign elements.

There is one example that demonstrates the use of a foreign namespace: http://svn.smallangles.net/trac/canSAS/browser/1dwg/-data/Glassy%20Carbon/ISIS/GLASSYC_C4G8G9_withTL.xml This example uses a foreign namespace to record the transmission spectra related to the acquisition of the SANS data at a time-of-flight facility. Look for the `<transmission_spectrum xmlns="urn:transmission:spectrum">` element at line 153. The foreign namespace given (`urn:transmission:spectrum`) becomes the default for just the `transmission_spectrum` element.

Also refer to canSAS TRAC ticket #47 for an example of arranging the content in **SASprocessnote** to avoid the use of foreign namespace elements.

1.3.5 Support tools for Visualization & Analysis software

Support for importing canSAS1d/1.0 files exists for these languages:

Note
Refactor the wiki pages here and link as appropriate.

- **FORTRAN**
- **IgorPro**
- **Java**
- **Microsoft Excel** Support for Microsoft Excel is provided through the default canSAS stylesheet cansasxml-html.xsl. An excellent description of how to import data from the cansas1d/1.0 format into Excel is available from the ISIS LOQ instrument (http://www.isis.stfc.ac.uk/instruments/loq/loq2470.html). Also note the old WWW site. (http://www.isis.rl.ac.uk/LargeScale/LOQ/lo may still be available.
- **PHP**
- **Python**
- **XSLT** (useful in a web browser)

1.3.6 Software repositories (for canSAS1d/1.0 standard)

- **TRAC**: http://svn.smallangles.net/trac/canSAS/browser/1dwg/tags/v1.0
- **Subversion**: http://svn.smallangles.net/svn/canSAS/1dwg/tags/v1.0

1.4 Validation of XML against the Schema

1. open browser to: http://www.xmlvalidation.com/
2. paste content of candidate XML file (with reference in the header to the XML Schema as shown above) into the form
3. press <validate>
4. paste content of [http://svn.smallangles.net/svn/canSAS/1dwg/trunk/cansas1d.xsd cansas1d.xsd] XSD file into form and press <continue validation>
5. check the results

1.5 Help for XML

The various references for help on XML have been moved to their own wiki page: [[XmlHelp]]

Note
chapter="Other" section="XML Help" xml:id="wiki-XML_Help"

Chapter 2

canSAS1d/1.0 Specification

This is the definitive specification of `canSAS1d/1.0`, the canSAS standard format for storing small-angle scattering data in XML files. The standard is defined using the rules of XML Schema.

Note
More needs to be written here.

Chapter 3

canSAS1d/1.0 Tutorial

This is a tutorial for `canSAS1d/1.0`, the canSAS standard format for storing small-angle scattering data in XML files.

Note
More needs to be written here.

Chapter 4

Elements of the CanSAS XML standard

Starting the description of each element will be the current version control *Revision* and *Date* of the documentation section. There are various elements (tag names) in the canSAS1d/1.0 standard. Each of these is described below.

The *Name* is the XML tag to be used for this element of the standard.

The *Type* may be a *container*, *header*, or *floating-point number*, or *string*.

Elements of type *container* have subelements but no text for themselves. These are similar to the NeXus NXDL `group` type.

Elements of type *floating-point number* are obvious. In most cases, a `unit` attribute is required. This will be noted.

Elements of type *string* are any valid string (non-whitespace) sequence.

Elements of type *header* describe the required XML header lines. Use them without question.

The number of times a particular element may appear is described in the *occurence* column. A value of *[0..1]* indicates the element is optional but may appear one time. A value of *[0..inf]* indicates the element is optional but may appear an infinite number of times (also known as unbounded).

4.1 Required XML Header

$Revision: 127 $ $Date: 2009-09-30 14:01:08 -0500 (Wed, 30 Sep 2009) $

Table 4.1:

Name	Type	Occurrence	Description	Attributes
xml declaration	header	[1..1]	`<?xml version="1.0"?>`	`version="1.0"`
stylesheet	header	[0..1]	`<?xml-stylesheet type="text/xsl" href="example.xsl" ?>` Declares that *example.xsl* (needs to be in the local directory) will be the default stylesheet to an XML visualization tool. Change *example.xsl* to indicate a different stylesheet in the local directory. Refer to W3 Schools XSLT Help for assistance in constructing XSLT files. XML rules actually allow for multiple stylesheet declarations. Explore this possibility as your own adventure.	`type="text/xsl" href="example.xsl"`

Table 4.1: (continued)

SASroot	container	[1..1]	The canSAS reduced 1-D SAS data (cansas1d/1.0) will be in the **SASroot** database. (This is similar to NXroot NXroot used by NeXus.) • **version="1.0"** is required to identify the cansas1d/1.0 standard for SAS data. • **xmlns** sets the default namespace for all elements (with no prefix) in this file. • **xmlns:xsi** sets **xsi** as the prefix for any elements from the governing XML Schema. • **xsi:schemaLocation** associates a suggested URL (where the cansas1d/1.0 XML Schema might be found) with the default namespace string. See Note 1 below	See Note 2 below

4.1.1 Glossary

Note 1: Required header for canSAS1d/1.0 XML files

```
<SASroot version="1.0"
    xmlns="cansas1d/1.0"
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
    xsi:schemaLocation="cansas1d/1.0
        http://svn.smallangles.net/svn/canSAS/1dwg/trunk/cansas1d.xsd">
```

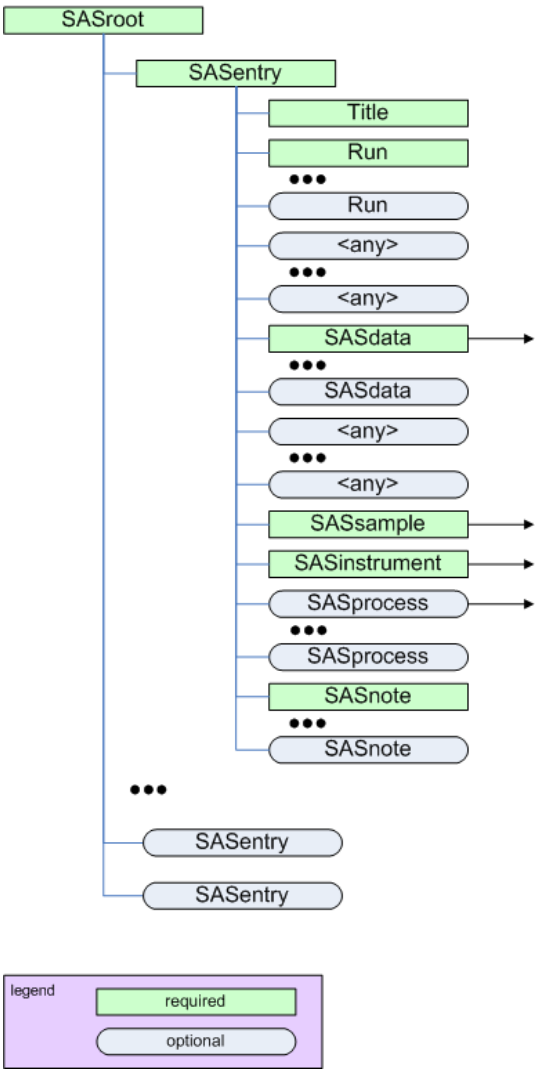
Note 2: Description of attributes in required header for canSAS1d/1.0 XML files

```
version="1.0"
     xmlns="{this-namespace-URI}"
     xmlns:xsi="{URL-of-governing-XML-Schema}"
     xsi:schemaLocation="{this-namespace-URI}  {URL-to-find-XML-Schema}"
```

4.2 SASroot element

$Revision: 128 $ $Date: 2009-09-30 16:33:30 -0500 (Wed, 30 Sep 2009) $

- parent: XML header



The SASroot element

Figure 4.1: The SASroot element

Table 4.2:

Name	Type	Occurrence	Description	Attributes
SASentry	container	[1..inf]	A single SAS scan is reported in a **SASentry**. Include as many **SASentry** elements as desired. They may contain related or unrelated data. **name** is an optional attribute to provide a string for this **SASentry**. (Use of this string is not defined by this standard.)	name=short-name

4.3 SASentry element

$Revision: 128 $ $Date: 2009-09-30 16:33:30 -0500 (Wed, 30 Sep 2009) $

- parent: SASroot

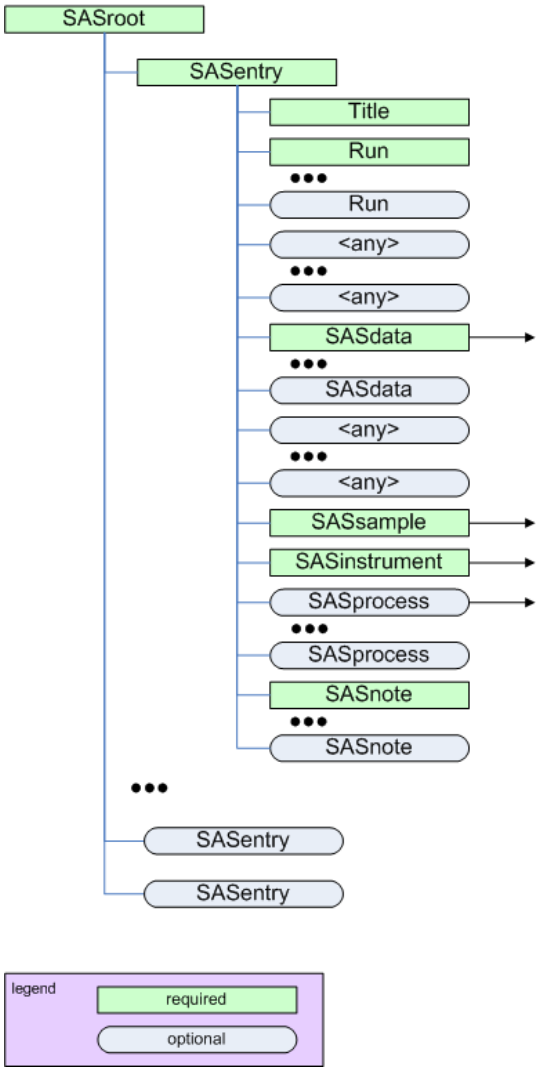


Figure 4.2: The SASentry element

Table 4.3:

Name	Type	Occurrence	Description	Attributes
Title	string	[1..1]	Title of this **SASentry**.	

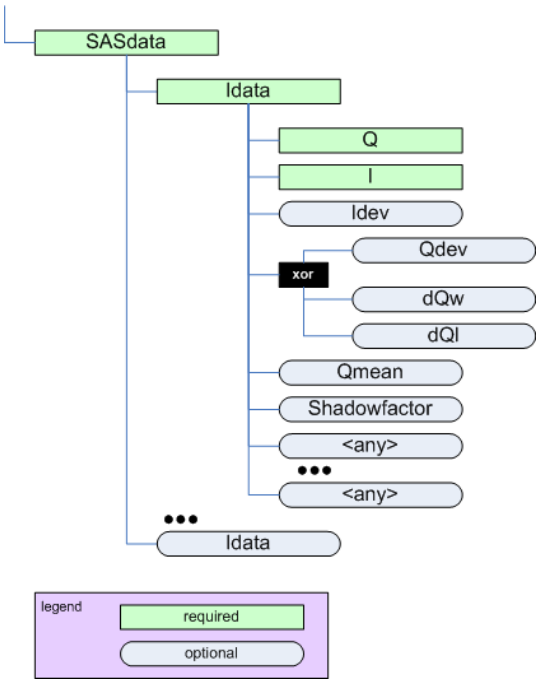
Table 4.3: (continued)

Run	string	[1..inf]	Run identification for this "'SASentry"'. For many facilities, this is an integer. Use multiple instances of **Run** as needed. Note: How to correlate this with "'SASdata"' and "'SASinstrument"' configurations has not yet been defined. **name** is an optional string attribute to identify this particular **Run**. Could use this to associate (correlate) multiple "'SASdata"' elements with **Run** elements. (Give them the same *short-Run-identifier*.)	***name***={short-Run-identifier}
"""{any}"""	container	[0..inf]	Any element(s) not defined in the cansas1d/1.0 standard can be placed at this point. See "{any}" for more details.	***xmlns:{foreign-prefix}***={foreign-namespace}
SASdata	container	[1..inf]	Reduced 1-D SAS data for this "'SASentry"'. Use multiple "'SASdata"' elements to represent multiple frames. Use this to associate (correlate) multiple "'SASdata"' elements with **Run** elements. (Give them the same name.)	***name***={short-Run-identifier}
"""{any}"""	container	[0..inf]	Any element(s) not defined in the cansas1d/1.0 standard can be placed at this point. See "{any}" for more details.	***xmlns:{foreign-prefix}***={foreign-namespace}
SASsample	container	[1..1]	Description of the sample.	***name***={short-SASsample-identifier}
SASinstrument	container	[1..1]	Description of the instrument	
SASprocess	container	[0..inf]	Description of a processing or analysis step.	***name***={short-SASprocess-identifier}
SASnote	container	[1..inf]	Free form description of anything not covered by other elements.	***name***={short-SASnote-identifier}

4.4 SASdata element

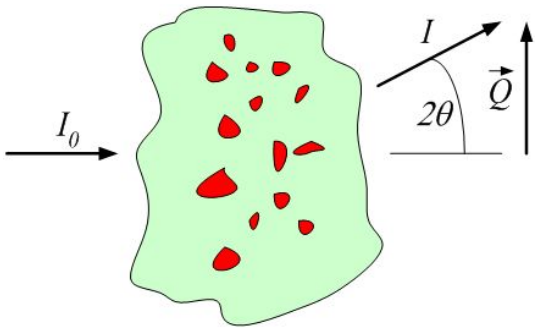
$Revision: 128 $ $Date: 2009-09-30 16:33:30 -0500 (Wed, 30 Sep 2009) $

- parent: SASentry



The SASdata element

Figure 4.3: The SASdata element



Q geometry

Figure 4.4: Q geometry

4.4.1 SASdata

Table 4.4:

Name	Type	Occurrence	Description	Attributes
`Idata`	container	[1..inf]	Idata describes a single SAS data point.	

4.4.2 Idata

Table 4.5:

Name	Type	Occurrence	Description	Attributes
`Q`	floating-point number	[1..1]	$Q=(4 \pi / \lambda) \sin(\theta)$ where λ is the wavelength of the radiation and 2θ is the angle through which the detected radiation has been scattered. The **unit** attribute is required. See rules for units for acceptable values. Either *1/A* or *1/nm* are typical.	**unit**={units}
`I`	floating-point number	[1..1]	Intensity of the detected radiation. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values. One possibility might be*1/cm* for absolute units when the intensity describes a *differential cross-section per unit volume per unit solid angle*. Be aware that there are different types of intensity used in small-angle scattering that may be reported (see the section titled The Intensity Problem). One should be very careful to inspect the **unit** attribute to determine how to handle subsequent data processing, especially in the area of units conversion.	**unit**={units}
`Idev`	floating-point number	[0..1]	Estimated standard deviation of **I**. The **unit** attribute is required. See rules for units for acceptable values. One possibility might be *1/cm*.	**unit**={units}
`Qdev`	floating-point number	[0..1]	Estimated standard deviation of **Q**. (optional: see note below on usage)The **unit** attribute is required. See rules for units for acceptable values. Either *1/A* or *1/nm* are typical.	**unit**={units}
`dQw`	floating-point number	[0..1]	**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. (optional: see note below on usage). The **unit** attribute is required. See rules for units for acceptable values. Either *1/A* or *1/nm* are typical.	**unit**={units}
`dQl`	floating-point number	[0..1]	**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. (optional: see note below on usage)The **unit** attribute is required. See rules for units for acceptable values. Either *1/A* or *1/nm* are typical.	**unit**={units}

Table 4.5: (continued)

`Qmean`	floating-point number	[0..1]	Mean value of **Q** for this datum. Useful when describing data that has been binned from higher-resolution or from area detectors.The **unit** attribute is required. See rules for units for acceptable values. Either *1/A* or *1/nm* are typical.	**unit**={units}
`Shadowfactor`	floating-point number	[0..1]	Describes the adjustment due to the beam stop penumbra. **Caution** This definition needs revision. NIST? **Note** There is no unit attribute.	
`{any}`	container	[0..inf]	Any element(s) not defined in the cansas1d/1.0 standard can be placed at this point. See {any} for more details.	***xmlns:{foreign-prefix}*** ={foreign-namespace}

4.4.3 Notes

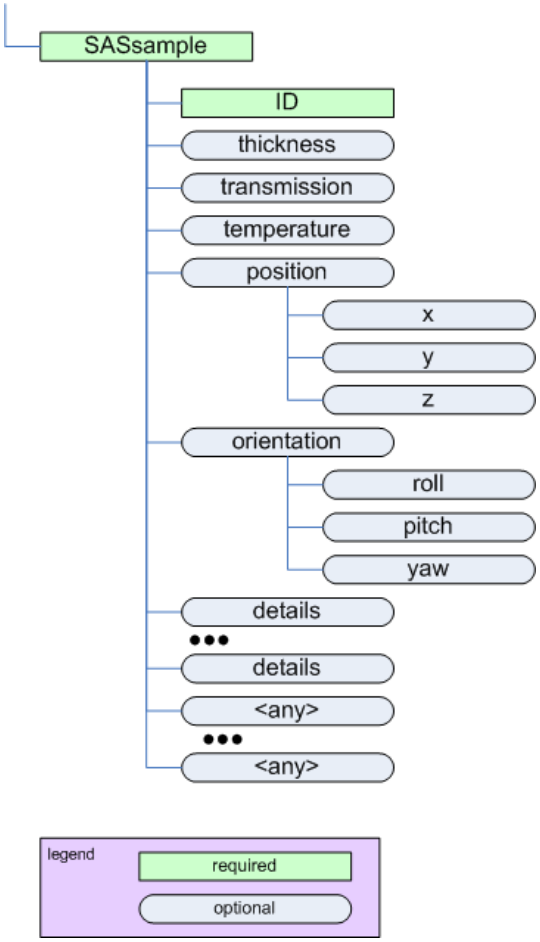
1. When an optional element (***Idev***, ***Qdev***, ...) is used, it must be given in every **Idata** within the enclosing **SASdata**.
2. If either ***dQw*** or ***dQl*** are used, then ***Qdev*** is not permitted to be used.

Note
(The Shadowfactor attribute definition needs revision. NIST?)

4.5 SASsample element

$Revision: 128 $ $Date: 2009-09-30 16:33:30 -0500 (Wed, 30 Sep 2009) $

- parent: SASentry



The SASsample element

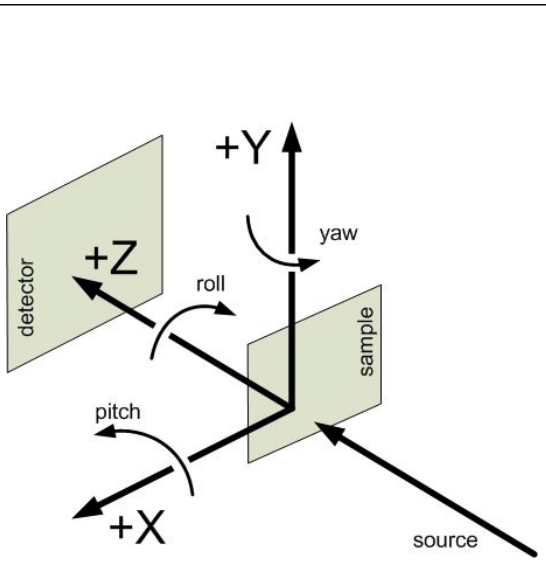
Figure 4.5: The SASsample element

Table 4.6:

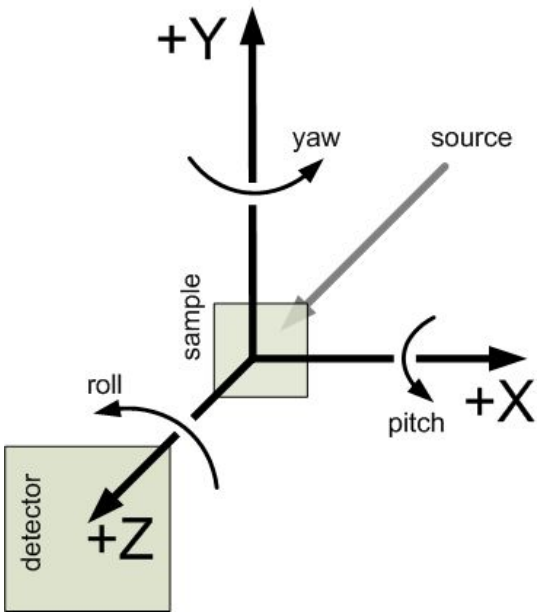
Name	Type	Occurrence	Description	Attributes
ID	string	[1..1]	Text string that identifies this sample.	
thickness	floating-point number	[0..1]	Thickness of this sample. Must specify the unit as an attribute.	**unit**={unit}
transmission	floating-point number	[0..1]	Transmission (1-attenuation) of this sample. Express this as a fraction, not as a percentage. NOTE: there is no unit attribute.	
temperature	floating-point number	[0..1]	Temperature of this sample. Must specify the unit as an attribute.	**unit**={unit}
””””position””””	container	[0..1]	Location in X, Y, and Z of the sample.	
””””orientation””””	container	[0..1]	Orientation (rotation) of the sample.	
details	string	[0..inf]	Any additional sample details.	
””””{any}””””	container	[0..inf]	Any element(s) not defined in the cansas1d/1.0 standard can be placed at this point. See ”{any}” for more details.	***xmlns:{foreign-prefix}***={foreign-namespace}

4.5.1 geometry

Table 4.7:



view from source



view from detector

4.5.2 position

Table 4.8:

Name	Type	Occurrence	Description	Attributes
x	floating-point number	[0..1]	Position of the sample in X. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
y	floating-point number	[0..1]	Position of the sample in Y. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
z	floating-point number	[0..1]	Position of the sample in Z. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values. Note: While Z dimension is allowed by the standard (provided by use of a standard element in the XML Schema), it does not make sense for small-angle scattering.	**unit**={units}

4.5.3 orientation

Table 4.9:

Table 4.9: (continued)

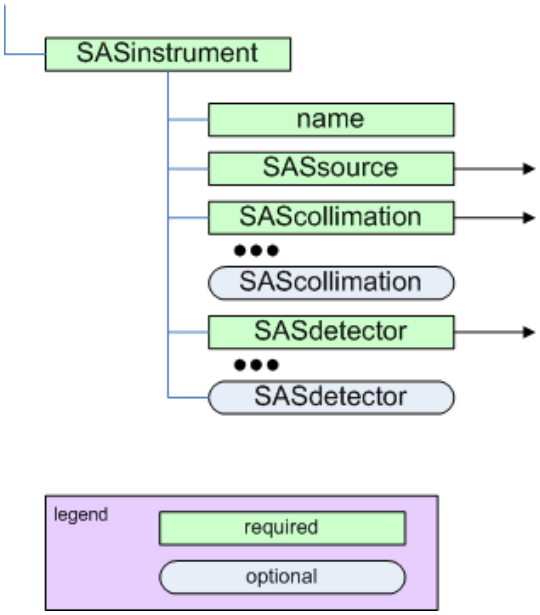
Name	Type	Occurrence	Description	Attributes
roll	floating-point number	[0..1]	Rotation about the *Z* axis (roll). The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
pitch	floating-point number	[0..1]	Rotation about the *X* axis (pitch). The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
yaw	floating-point number	[0..1]	Rotation about the *Y* axis (yaw). The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}

Note
The **orientation** element is intended to describe simple rotations about a single axis rather than a full set of rotations as in a crystallographic context.

4.6 SASinstrument element

$Revision: 128 $ $Date: 2009-09-30 16:33:30 -0500 (Wed, 30 Sep 2009) $

- parent: SASentry



The SASinstrument element

Figure 4.6: The SASinstrument element

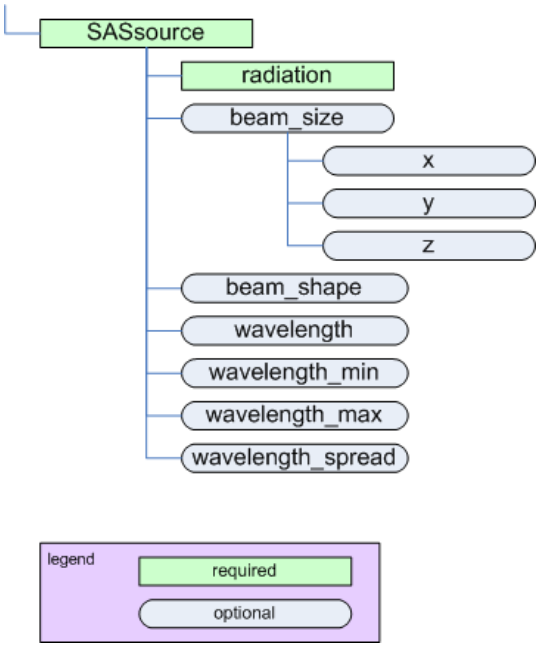
Table 4.10:

Name	Type	Occurrence	Description	Attributes
name	string	[1..1]	Text string that identifies the name of this instrument.	
"'SASsource"'	container	[1..1]	Text string that identifies the name of this source of radiation.	***name***={name}
"'SAScollimation"'	container	[1..inf]	Text string that identifies the name of this instrument collimation.	***name***={name}
"'SASdetector"'	container	[1..inf]	Text string that identifies the name of this detector.	

4.7 SASsource element

$Revision: 128 $ $Date: 2009-09-30 16:33:30 -0500 (Wed, 30 Sep 2009) $

- parent: SASinstrument



The SASsource element

Figure 4.7: The SASsource element

4.7.1 SASsource

Table 4.11:

Name	Type	Occurrence	Description	Attributes

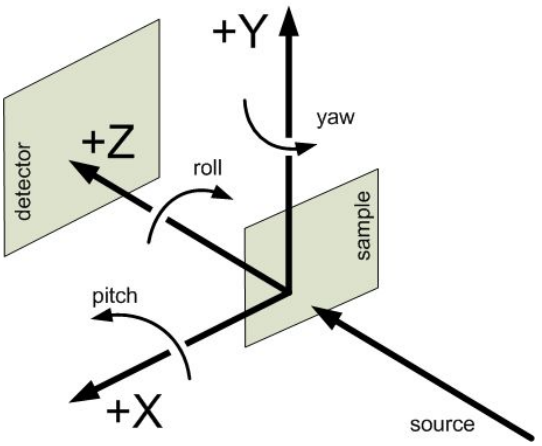
Table 4.11: (continued)

radiation	string	[1..1]	Name of the radiation used. For maximum compatibility with NeXus, use one of the names defined by either *NeXus* `NXsource/type` • 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 or *NeXus* `NXsource/probe` • neutron • x-ray • muon • electron	
””””beam_size””””	container	[0..1]	Physical dimension of the beam (incident on the sample). Note: If beam is round, just use X dimension. Note: While Z dimension is allowed by the standard, it does not make sense for small-angle scattering.	***name***={name}
beam_shape	string	[0..1]	Text description of the shape of the beam (incident on the sample).	
wavelength	floating-point number	[0..1]	wavelength (λ) of radiation incident on the sample.	**unit**={unit}
wavelength_min	floating-point number	[0..1]	Some facilities specify wavelength using a range. The minimum of such a range is given by wavelength_min.	**unit**={unit}
wavelength_max	floating-point number	[0..1]	Some facilities specify wavelength using a range. The maximum of such a range is given by wavelength_max.	**unit**={unit}
wavelength_spread	floating-point number	[0..1]	Some facilities specify the width of the wavelength spectrum. The width of such a range is given by wavelength_spread.	**unit**={unit}

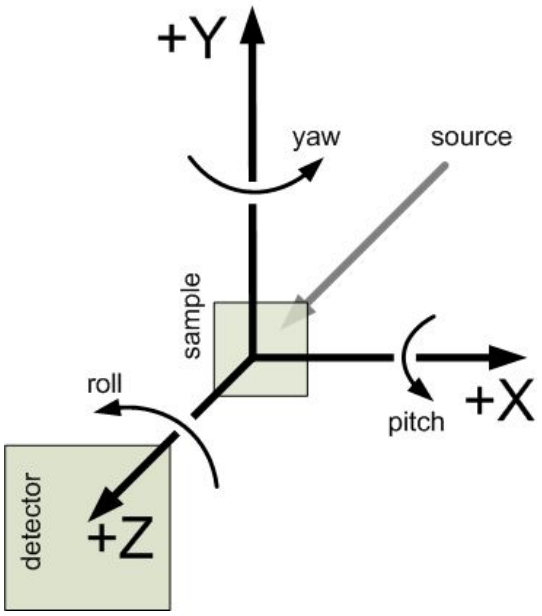
4.7.2 beam_size

Table 4.12:

Table 4.12: (continued)



view from source



view from detector

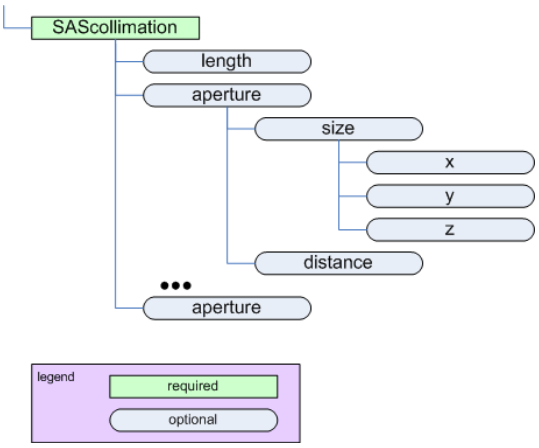
Table 4.13:

Name	Type	Occurrence	Description	Attributes
x	floating-point number	[0..1]	Dimension of the beam in X. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
y	floating-point number	[0..1]	Dimension of the beam in Y. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
z	floating-point number	[0..1]	Dimension of the beam in Z. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values. Note: While Z dimension is allowed by the standard (provided by use of a standard element in the XML Schema), it does not make sense for small-angle scattering.	**unit**={units}

4.8 SAScollimation element

$Revision: 128 $ $Date: 2009-09-30 16:33:30 -0500 (Wed, 30 Sep 2009) $

- parent: SASinstrument



The SAScollimation element

Figure 4.8: The SAScollimation element

4.8.1 SAScollimation

Table 4.14:

Name	Type	Occurrence	Description	Attributes
length	floating-point number	[0..1]	Amount/length of collimation inserted (on a SANS instrument)	***unit***={unit}
””””aperture””””	container	[0..inf]	Description of a slit or aperture. ***name***: Optional name attribute for this aperture. ***type***: Optional text attribute to describe the type aperture (pinhole, 4-blade slit, Soller slit, ...).	***name***={name} ***type***={type}

4.8.2 aperture

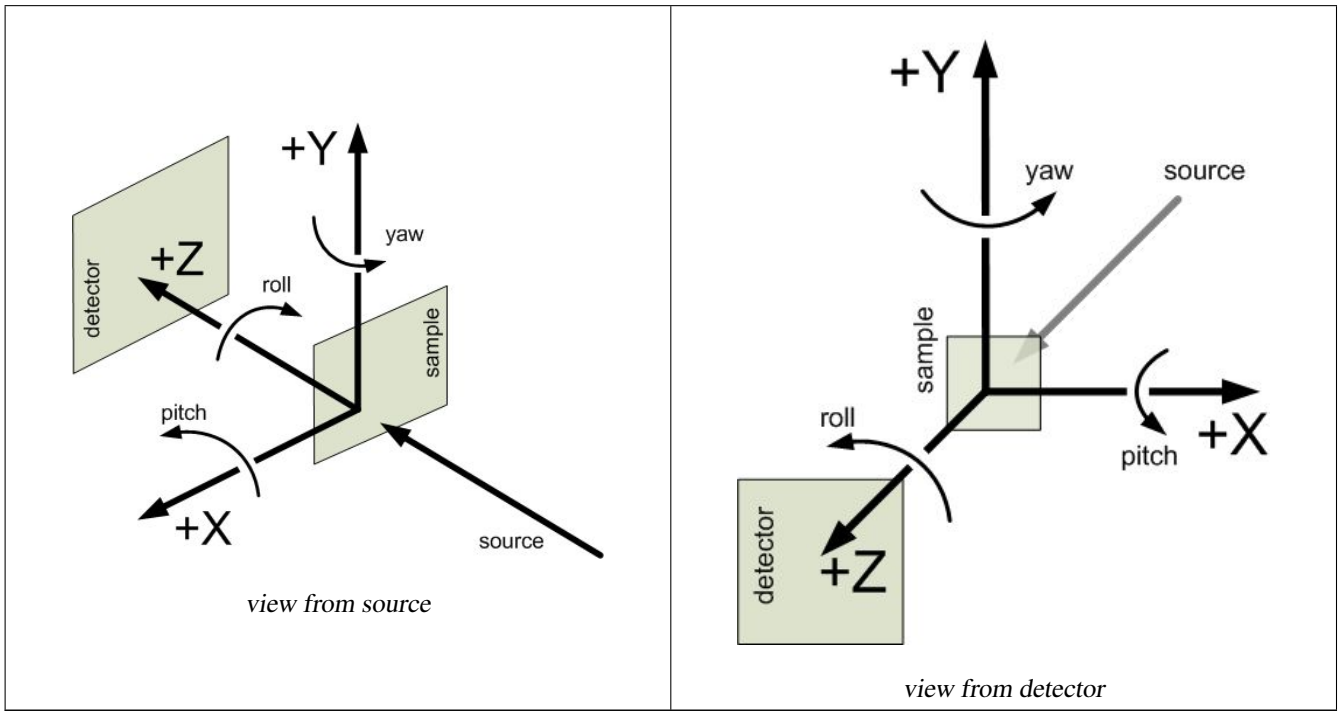
Table 4.15:

Name	Type	Occurrence	Description	Attributes
””””size””””	container	[0..1]	Opening dimensions of this aperture.	***name***={name}
distance	floating-point number	[0..1]	Distance from this collimation element to the sample.	***unit***={unit}

4.8.3 size

Table 4.16:

Table 4.16: (continued)



view from source

view from detector

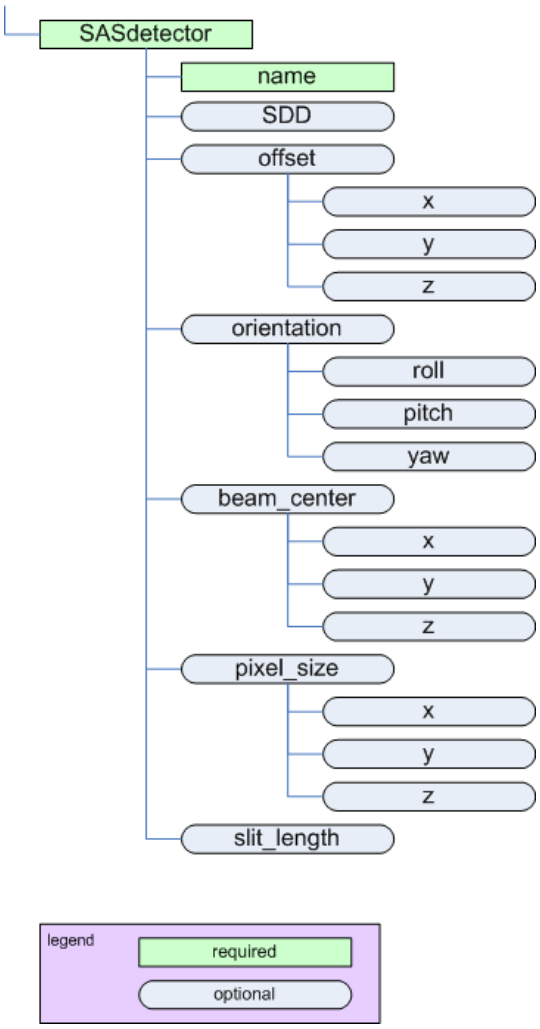
Table 4.17:

Name	Type	Occurrence	Description	Attributes
x	floating-point number	[0..1]	Dimension of the collimation in X. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
y	floating-point number	[0..1]	Dimension of the collimation in Y. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
z	floating-point number	[0..1]	Dimension of the collimation in Z. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values. Note: While Z dimension is allowed by the standard (provided by use of a standard element in the XML Schema), it does not make sense for small-angle scattering.	**unit**={units}

4.9 SASdetector element

$Revision: 128 $ $Date: 2009-09-30 16:33:30 -0500 (Wed, 30 Sep 2009) $

- parent: SASinstrument



The SASdetector element

Figure 4.9: The SASdetector element

4.9.1 SASdetector

Table 4.18:

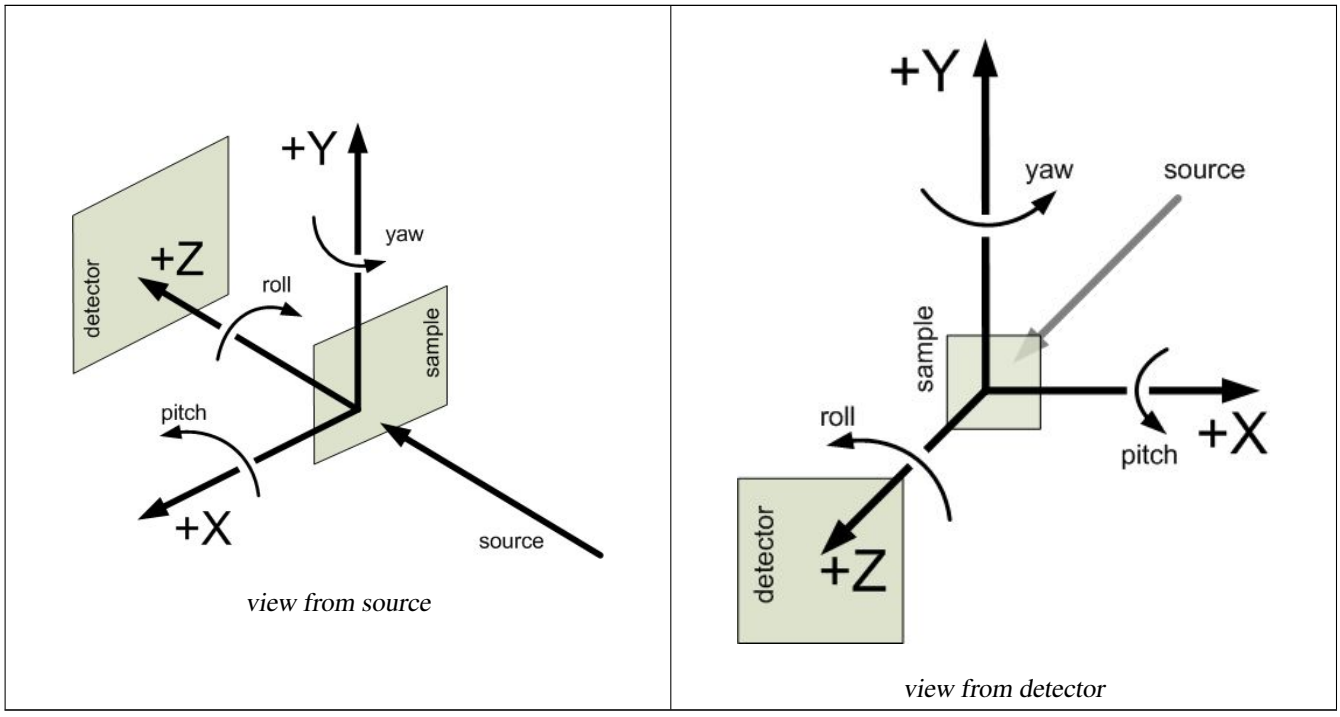
Name	Type	Occurrence	Description	Attributes
name	string	[1..1]	Text string that identifies the name of this detector.	
SDD	floating-point number	[0..1]	Distance between sample and detector.	***unit***={unit}
””””offset””””	container	[0..1]	Offset of this detector position in X, Y, (and Z if necessary).	
””””orientation””””	container	[0..1]	Orientation (rotation) of this detector in roll, pitch, and yaw.	
””””beam_center””””	container	[0..1]	Center of the beam on the detector in X and Y (and Z if necessary).	
””””pixel_size””””	container	[0..1]	Size of detector pixels in X and Y (and Z if necessary).	

Table 4.18: (continued)

slit_length	floating-point number	[0..1]	Slit length of the instrument for this detector. This is expressed in the same units as Q (reciprocal space units).	***unit***={unit}

4.9.2 geometry

Table 4.19:



4.9.3 offset

Table 4.20:

Name	Type	Occurrence	Description	Attributes
x	floating-point number	[0..1]	Offset of the detector position in X. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
y	floating-point number	[0..1]	Offset of the detector position in Y. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
z	floating-point number	[0..1]	Offset of the detector position in Z. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values. Note: While Z is allowed by the standard (provided by use of a standard element in the XML Schema), it does not make sense for small-angle scattering.	**unit**={units}

4.9.4 orientation

Table 4.21:

Name	Type	Occurrence	Description	Attributes
roll	floating-point number	[0..1]	Rotation about the *Z* axis (roll). The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
pitch	floating-point number	[0..1]	Rotation about the *X* axis (pitch). The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
yaw	floating-point number	[0..1]	Rotation about the *Y* axis (yaw). The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}

4.9.5 beam_center

Table 4.22:

Name	Type	Occurrence	Description	Attributes
x	floating-point number	[0..1]	Position of the beam center on the detector in X. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
y	floating-point number	[0..1]	Position of the beam center on the detector in Y. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
z	floating-point number	[0..1]	Position of the beam center on the detector in Z. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values. Note: While Z dimension is allowed by the standard (provided by use of a standard element in the XML Schema), it does not make sense for small-angle scattering.	**unit**={units}

4.9.6 pixel_size

Table 4.23:

Name	Type	Occurrence	Description	Attributes

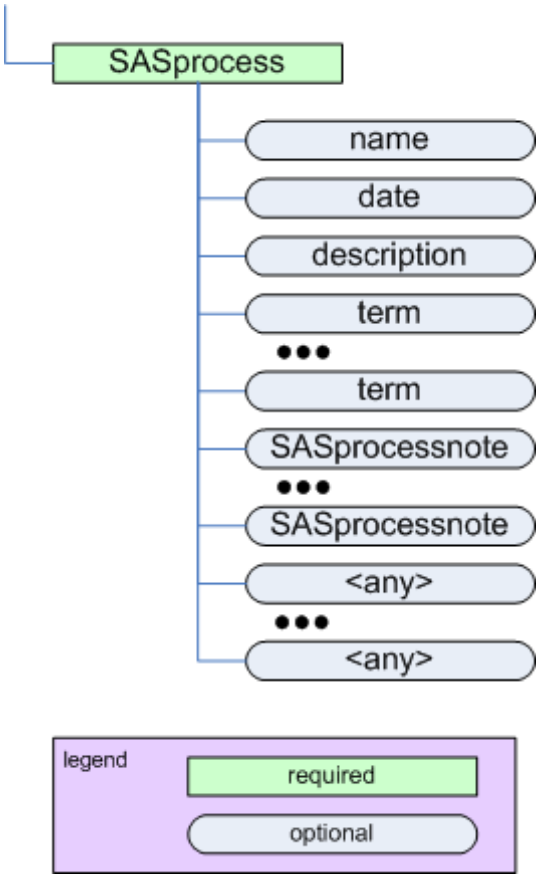
Table 4.23: (continued)

x	floating-point number	[0..1]	Size of a detector pixel in X. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
y	floating-point number	[0..1]	Size of a detector pixel in Y. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values.	**unit**={units}
z	floating-point number	[0..1]	Size of a detector pixel in Z. The **unit** attribute is required. See cansas1d_documentation#Rules for acceptable values. Note: While Z dimension is allowed by the standard (provided by use of a standard element in the XML Schema), it does not make sense for small-angle scattering.	**unit**={units}

4.10 SASprocess element

$Revision: 128 $ $Date: 2009-09-30 16:33:30 -0500 (Wed, 30 Sep 2009) $

- parent: SASentry



The SASprocess element

Figure 4.10: The SASprocess element

Table 4.24:

Name	Type	Occurrence	Description	Attributes
name	string	[0..1]	Optional name for this data processing or analysis step.	
date	string	[0..1]	Optional date for this data processing or analysis step. Use a format which is easily machine-readable such as yyyy-mm-dd hh:mm:ss The format for the date string may be specified at a later date.	
description	string	[0..1]	Optional description for this data processing or analysis step.	
term	string	[0..inf]	This is used to specify 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.	**unit**={unit}
””””SASprocessnote””””	container	[1..inf]	This element is used to describe anything about SASprocess that is not already described.	
””””{any}””””	container	[0..inf]	Any element(s) not defined in the cansas1d/1.0 standard can be placed at this point. See ”{any}” for more details.	***xmlns:{foreign-prefix}***={foreign-namespace}

4.10.1 SASprocessnote

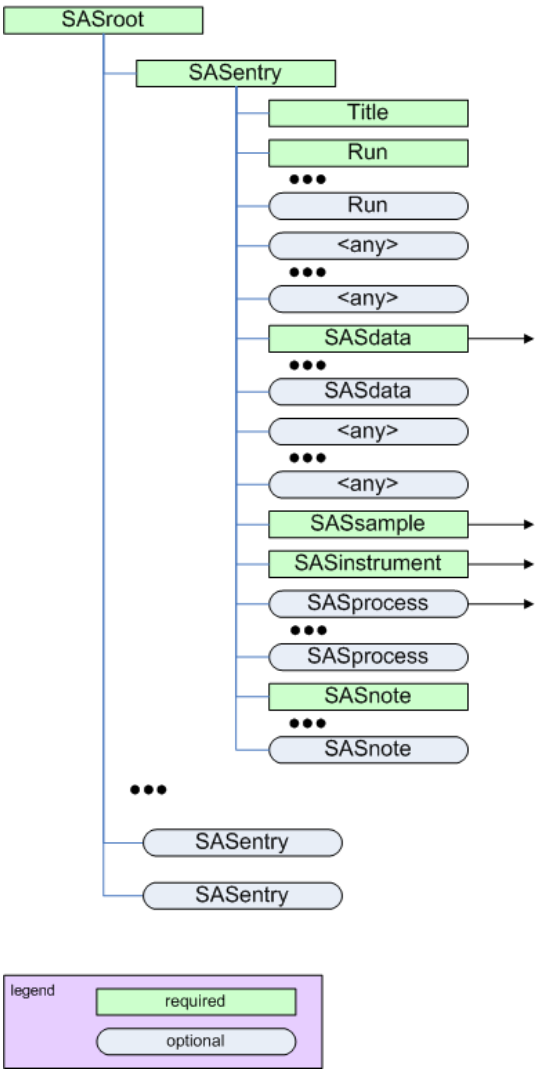
Table 4.25:

Name	Type	Occurrence	Description	Attributes
””””{any}””””	container	[0..inf]	Any element(s) not defined in the cansas1d/1.0 standard can be placed at this point. See ”{any}” for more details.	***xmlns:{foreign-prefix}***={foreign-namespace}

4.11 SASnote element

$Revision: 128 $ $Date: 2009-09-30 16:33:30 -0500 (Wed, 30 Sep 2009) $

- parent: SASentry



The SASroot element

Figure 4.11: The SASroot element

Table 4.26:

Name	Type	Occurrence	Description	Attributes
”””{any}”””	container	[0..inf]	Any element(s) not defined in the cansas1d/1.0 standard can be placed at this point. See ”{any}” for more details.	***xmlns:{foreign-prefix}***={foreign-namespace}

4.12 ”{any}” element

$Revision: 127 $ $Date: 2009-09-30 14:01:08 -0500 (Wed, 30 Sep 2009) $

Table 4.27:

Name	Type	Occurrence	Description	Attributes
{any}	container	[0..inf]	Any element(s) not defined in the cansas1d/1.0 standard can be placed at this point. (These are called *foreign* elements. It is suggested to associate foreign elements with a foreign namespace to differentiate them from the canSAS elements in the XML file.)	***xmlns:{foreign-prefix}*** ={foreign-namespace}

Chapter 5

Bindings and Software Support

Bindings (import/export drivers) and other software support have been created and contributed. These are listed here by the language or software environment.

5.1 Fortran binding

$Revision: 127 $ $Date: 2009-09-30 14:01:08 -0500 (Wed, 30 Sep 2009) $

The development of the FORTRAN language, so beloved of scientists, pre-dates the development of XML. And it shows. FORTRAN is not a language that manipulates strings with ease, and this makes parsing XML decidedly awkward. So unless you *really* have to use FORTRAN, you are probably better off with C/C++ (or something else more 'modern'), see for example Daniel Veillard's LIBXML2 library at http://xmlsoft.org/ or Frank van den Berghen's parser at http://www.applied-mathematics.net/tools/xmlParser.html.

If you have to use a dialect earlier than FORTRAN-90 (F90), then the chances are you will have to code your own parser.

5.1.1 Software Development Kits

For later dialects, there are some SDK's available on the Web:

- F90:
  - XMLPARSE - by Arjen Markus at http://xml-fortran.sourceforge.net/
  - FoX - by Toby White others at http://uszla.me.uk/space/software/FoX/
- For F95:
  - XML - by Mart Rentmeester at http://nn-online.org/code/xml/

5.1.2 canSAS 1-D SAS XML v1.0 support

Steve King[mailto:s.m.king@rl.ac.uk] (ISIS) has provided a F77 routine (*SASXML_G77.F*) that will read CanSAS XML v1.0 files.

5.2 IgorPro binding

$Revision: 127 $ $Date: 2009-09-30 14:01:08 -0500 (Wed, 30 Sep 2009) $

An import tool (binding) for IgorPro has been created (cansasXML.ipf). You can check out the IgorPro working directory from the SVN server (see instructions below).

To use the canSASxml.ipf procedure, you must have the XMLutils XOP IGOR plugin installed. See the Usage Notes below.

Note
Note that this tool is not a true binding in that the structure of the XML file is not replicated in IgorPro data structures. This tool reads the vectors of 1-D SAS data (Q, I, ...) into IgorPro waves (Qsas, Isas, ...). The tool also reads most of the metadata into an IgorPro textWave for use by other support in IgorPro.

Note
Note that the code described here is *not a complete user interface*. (See further comments below.) It is expected that this code will be called by a graphical user interface routine and that routine will handle the work of copying the loaded SAS data in IgorPro from the root:Packages:CS_XMLreader data folder to the destination of choice (including any renaming of waves as desired).

---

file

cansasXML.ipf

author

Pete R. Jemian <jemian@anl.gov>

date

2009-09-02

version

1.11 (**requires** latest XMLutils XOP -- see below)

purpose

implement an IgorPro file reader to read the canSAS 1-D reduced SAS data in XML files adheres to the cansas1d/1.0 standard: http://www.smallangles.net/wgwiki/index.php/cansas1d_documentation

URL

TRAC: http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/IgorPro/cansasXML.ipf

SVN: http://svn.smallangles.net/svn/canSAS/1dwg/trunk/IgorPro/cansasXML.ipf

requires

IgorPro: http://www.wavemetrics.com XMLutils - XOP: http://www.igorexchange.com/project/XMLutils (IGOR.5.04.x-1.x-dev, 2008-Aug-22)

5.2.1 Checkout of support code in Subversion

Subversion (http://subversion.tigris.org/) is a program formanaging software versions. There are command line and GUI clients-for a variety of operating systems. We won't recommend any herebut will show the command lines necessary.

5.2.1.1 XMLutils XOP

The XMLutils XOP, written by Andrew Nelson (ANSTO), is hosted on the IgorExchange (http://www.igorexchange.com/).

One good location to place the checked out XMLutils directoryis in the Wavemetrics directory, next to the Igor Pro Folder

```
svn://svn.igorexchange.com/packages/XMLutils/ XMLutils
```

In the future, to retrieve an updated version of this support, go intothe XMLutils directory (created above) and type the command

```
svn update
```

This will check the repository and update files as needed.If the installer program was updated, you;ll need to run the newinstaller program. It is not necessary to uninstall first.

The installer executables contained in the download will do all the installation for you. They will place the XOP in the folder */User Procedures/motofit/XMLutils*, and create a shortcut/alias to the plugin in /Igor Extensions.Packages from other facilities should place the XOP there as well.

5.2.1.2 cansasXML.ipf

Check out the canSAS 1d SAS XML reader from the subversion repository:

```
svn checkout http://svn.smallangles.net/svn/canSAS/1dwg/trunk cansas-1dwg
```

This will download lots of extra files. The file of interest is in the IgorProdirectory and is called cansasXML.ipf

In the future, to retrieve an updated version of this support, go intothe cansas-1dwg directory (created above) and type the command

```
svn update
```

This will check the repository and update files as needed.

5.2.2 Installation

1. License and Install IgorPro (should have already been done by now)
2. Quit IgorPro if it is running
3. Download XMLutils XOP. Either checkout from subversion (see above) or, with a web browser, go to http://svn.igorexchange.com/
4. Install XMLutils XOP by double-clicking the installer for you operating system.
5. Download cansasXML.ipf. Either checkout from subversion (see above) or, with a web browser, copy cansasXML.ipf from on-line subversion repository: http://svn.smallangles.net/svn/canSAS/1dwg/trunk/IgorPro/cansasXML.ipf
6. Copy cansasXML.ipf file to ...WavemetricsIgor Pro FolderUser Procedures (or file system equivalent)
7. Then, you should be able to restart IgorPro and progress from there

5.2.3 Usage Notes

To use the canSASxml.ipf procedure, you must have the XMLutils XOP IGOR plugin installed. This may be downloaded from the IgorExchange Project site. There are installer executables contained in the download that will do all the installation for you. Each installer will place the XOP in the folder ...WavemetricsIgor Pro FolderUser ProceduresmotofitXMLutils, and create a shortcut/alias to the plugin in ...WavemetricsIgor Pro FolderIgor Extensions.

5.2.4 What it does

Given an XML file, **CS_XmlReader(fileName)** attempts to open the fileand read its contents as if it conformed to the canSAS XML standard forreduced 1-D SAS data (cansas1d/1.0, also known as SASXML). If the file is found to be non-conforming, then **CS_XmlReader(fileName)** returns with anerror code (show below), otherwise it returns **0** that indicates *no error*.All data read by this code is left in the IgorPro data folder ***root:Packages:CS_XMLreader*** for pickup by the calling routine.(Two examples are provided to show how a routine might retrieve the data.)

After opening the XML file (with a file identifier *fileID*), control is passed to **CS_1i_parseXml(fileID)** which then walks through the XMLelements. For each **SASentry** in the file, a new data folder is createdwith the name derived from the Title element (or best effort determination).Efforts are taken to avoid duplication of data folder names (using standard IgorPro routines). For **SASentry** elements that contain more than one SASdataelement, a **SASdata** folder is created for each and the corresponding *I(Q)* is placed in that subfolder. When only one **SASdata** is found, the *I(Q)*data is placed in the main *Title* folder.

5.2.4.1 data columns

Each column of data in the **SASdata/Idata/*** table is placed into a singleIgorPro wave. At present, the code does not check for non-standard data columns.(The capability is built into the code but is deactivated at present).

5.2.4.2 metadata

Additional metadata is collected into a single text wave (*metadata*) where the first columnis an identifier (or *key*) and the second identifier is the *value*. Only those keys with non-empty values are retained in the metadata table.

Caution
The *values* are not checked for characters that may cause trouble when placed in a wave note. This will be the responsibility of the calling routineto *clean these up* if the need arises.

The code checks for most metadata elements and will check for repeated elements where the standard permits.

Here is an example of the metadata for the `cs_collagen_full.xml` case study:

Table 5.1: metadata for the "cs_collagen_full.xml" case study

row: `i`	key: `metadata[i][0]`	value: `metadata[i][1]`
0	xmlFile	cs_collagen_full.xml
1	namespace	cansas1d/1.0
2	Title	dry chick collagen, d = 673 A, 6531 eV, X6B
3	Run	Sep 19 1994 01:41:02 am
4	SASsample/ID	dry chick collagen, d = 673 A, 6531 eV, X6B
5	SASinstrument/name	X6B, NSLS, BNL
6	SASinstrument/SASsource/radiation	X-ray synchrotron
7	SASinstrument/SASsource/wavelength	1.898
8	SASinstrument/SASsource/wavelength/@unit	A
9	SASinstrument/SASdetector/@name	X6B PSD

10	SASnote	`Sep 19 1994 01:41:02 am Elt: 00090 Seconds`
		`ID: No spectrum identifier defined`
		`Memory Size: 8192 Chls Conversion Gain: 1024 Adc Offset: 0000 Chls`
		`dry chick collagen, d = 673 A`
		`6531 eV, X6B`

5.2.4.3 XML foreign namespace elements

These are ignored at this time.

5.2.4.4 XML namespace and header

The routine does a *best-efforts* check to ensure that the givenXML file conforms to the [[cansas1d_documentation#Required_XML_file_h
|required XML file header]]. If you take a minimalist view (*a.k.a.* a shortcut),it is likely that your file may be refused by this and other readers. Pay particular attention to UPPER/lower case in the text **cansas1d/1.0** as this is a **key component** used toindex through the XML file.

5.2.4.5 XML stylesheet processing-instruction is not generated

The *"'XMLutils"'* package does not provide a method to insert the prescribed XML stylesheet processing-instruction into the XML data file.

```
?xml-stylesheet type=text/xsl href=example.xsl ?
```

If this processing-instruction is desired, it must be added to each XML data file by other methods such as use of a text editor or application of an XSLT transformation.

5.2.5 List of Functions

These are (most of) the FUNCTIONS in the cansasXML.ipf code.The only functions of interest are **CS_XmlReader(fileName)**which reads the named XML file and and loads SAS data and the two demonstrationfunctions **prj_grabMyXmlData()** and **prjTest_cansas1d()** together show a usage example.

- **CS_XmlReader(fileName)** : open a canSAS 1-D reduced SAS XML data file
- input: *fileName* (string) name of canSAS XML file (can include file system path name to file)
- returns:
  - 0 successful
  - -1: XML file not found
  - -2: root element is not SASroot with valid canSAS namespace
  - -3: SASroot version is not 1.0
  - -4: no SASentry elements (NOT USED NOW)
  - -5: XOPutils needs upgrade
- CS_1i_parseXml(fileID) : **This is what guides the work**, given a file ID returned from **XMLOpenFile()**, parses that file for SAS data and metadata (1i in the function name signifies this is a function that supports INPUT from version 1.0 XML files)
- CS_1i_getOneSASdata(fileID, Title, SASdataPath) : harvest the data and metadata in the specific SASdata element
- CS_1i_getOneVector(file,prefix,XML_name,Igor_name) : harvest just one column (vector) of data
- CS_1i_GetReducedSASdata(fileID, SASdataPath) : grab the data and put it in the working data folder
- CS_1i_locateTitle(fileID, SASentryPath) : determine the title for this experiment
- CS_appendMetaData(fileID, key, xpath, value) : queries XML file for **xpath**. If **value** is not empty, appends it to **metadata** where *last* is the new last row: metadata[last][0]=key; metadata[last][1]=value
- CS_buildXpathStr(prefix, value) : this function can be used only with very simple XPath constructions

- CS_cleanFolderName(proposal) : given a proposal string, returns a candidate folder name for immediate use
- CS_findElementIndex(matchStr) : looks for element index in structure *W_ElementList* returned from call to **XmlElemList(fileID)**
- CS_getDefaultNamespace(fileID) : returns the string containing the default namespace for the XML file
- CS_registerNameSpaces() : Builds a table of all namespaces used in the XML file and appends **W_ElementList** with full namespace-xpath string for each element.
- CS_simpleXmlListXpath(fileID, prefix, value) : Calls **XMLlistXpath()** with proper namespace prefix attached.
- CS_simpleXmlWaveFmXpath(fileID, prefix, value) : Calls **XMLwaveFmXpath()** with proper namespace prefix attached.
- CS_updateWaveNote(wavName, key, value) : adds (or replaces) definition of *key=value* in the wave note of *wavName*
- CS_XmlStrFmXpath(fileID, prefix, value) : Calls **XmlStrFmXpath()** with proper namespace prefix attached. Trims the result string.
- CS_XPath_NS(simpleStr) : this function adds namespace info as necessary to simpleStr (an XPath)
- TrimWS(str) : Calls **TrimWSL(TrimWSR(str))**
- TrimWSL(str) : Trims white space from left (leading) end of **str**
- TrimWSR(str) : Trims white space from right (trailing) end of **str**
- prjTest_cansas1d() : Demonstration function that calls **CS_XmlReader(fileName)** for many of the test data sets.
- prj_grabMyXmlData() : Demonstration function that moves loaded data from root:Packages:CS_XMLreader to a user's data folder. (In this *example*, that folder is root:PRJ_canSAS.)
- testCollette() : Demonstration function that reads an ISIS/LOQ file and copies the data to the root folder a la COLLETE

5.2.6 Example test case

Here is an example running the test routine **prjTest_cansas1d()**.

```
•prjTest_cansas1d()
XMLopenfile: File(path) to open doesn't exist, or file can't be opened
elmo.xml either not found or cannot be opened for reading
    Completed in 0.00669666 seconds
XMLopenfile: XML file was not parseable
cansasXML.ipf: failed to parse XML
    Completed in 0.0133704 seconds
root element is not SASroot with valid canSAS namespace
    Completed in 0.0134224 seconds
bimodal-test1.xml      identified as: cansas1d/1.0 XML file
    Title: SAS bimodal test1
    Completed in 0.068654 seconds
root element is not SASroot with valid canSAS namespace
    Completed in 0.0172572 seconds
root element is not SASroot with valid canSAS namespace
    Completed in 0.0123102 seconds
root element is not SASroot with valid canSAS namespace
    Completed in 0.00930118 seconds
ISIS_SANS_Example.xml      identified as: cansas1d/1.0 XML file
    Title: standard can 12mm SANS
    Completed in 0.0410387 seconds
W1W2.xml     identified as: cansas1d/1.0 XML file
    Title: standard can 12mm SANS
    Title: TK49 standard 12mm SANS
    Completed in 0.0669074 seconds
```

```
ill_sasxml_example.xml     identified as: cansas1d/1.0 XML file
    Title: ILL-D22 example: 7D1 2mm
    Completed in 0.0332752 seconds
isis_sasxml_example.xml      identified as: cansas1d/1.0 XML file
    Title: LOQ TK49 Standard 12mm C9
    Completed in 0.0388868 seconds
r586.xml     identified as: cansas1d/1.0 XML file
    Title: ILL-D11 example1: 2A 5mM 0%D2O
    Completed in 0.0213737 seconds
r597.xml     identified as: cansas1d/1.0 XML file
    Title: ILL-D11 example2: 2A 5mM 0%D2O
    Completed in 0.0221894 seconds
xg009036_001.xml     identified as: cansas1d/1.0 XML file
    Title: det corrn 5m
    Completed in 0.0286721 seconds
cs_collagen.xml      identified as: cansas1d/1.0 XML file
    Title: dry chick collagen, d = 673 A, 6531 eV, X6B
    Completed in 0.0296247 seconds
cs_collagen_full.xml     identified as: cansas1d/1.0 XML file
    Title: dry chick collagen, d = 673 A, 6531 eV, X6B
    Completed in 0.0751836 seconds
cs_af1410.xml      identified as: cansas1d/1.0 XML file
    Title: AF1410-10 (AF1410 steel aged 10 h)
    Title: AF1410-8h (AF1410 steel aged 8 h)
    Title: AF1410-qu (AF1410 steel aged 0.25 h)
    Title: AF1410-cc (AF1410 steel aged 100 h)
    Title: AF1410-2h (AF1410 steel aged 2 h)
    Title: AF1410-50 (AF1410 steel aged 50 h)
    Title: AF1410-20 (AF1410 steel aged 20 h)
    Title: AF1410-5h (AF1410 steel aged 5 h)
    Title: AF1410-1h (AF1410 steel aged 1 h)
    Title: AF1410-hf (AF1410 steel aged 0.5 h)
    Completed in 0.338425 seconds
XMLopenfile: File(path) to open doesn't exist, or file can't be opened
cansas1d-template.xml either not found or cannot be opened for reading
    Completed in 0.00892823 seconds
1998spheres.xml      identified as: cansas1d/1.0 XML file
    Title: 255 nm PS spheres
    Title: 460 nm PS spheres
    Completed in 2.87649 seconds
XMLopenfile: File(path) to open doesn't exist, or file can't be opened
does-not-exist-file.xml either not found or cannot be opened for reading
    Completed in 0.00404549 seconds
cs_rr_polymers.xml     identified as: cansas1d/1.0 XML file
    Title: Round Robin Polymer A
    Title: Round Robin Polymer B
    Title: Round Robin Polymer C
    Title: Round Robin Polymer D
    Completed in 0.0943477 seconds
s81-polyurea.xml     identified as: cansas1d/1.0 XML file
    Title: S7 Neat Polyurea
    Completed in 0.0361616 seconds
```

5.2.7 Graphical User Interface

At least two groups are working on graphical user interfaces that use the canSAS 1-D SAS XML format binding to IgorPro. The GUIs are intended to be used with their suites of SAS analysis tools (and hide the detailsof using this support code from the user).

NOTE: There is no support yet for writing the data back into the canSAS format. Several details need to be described, and theseare being collected on the discussion page for the XML format

5.2.7.1 Irena tool suite

Jan Ilavsky's **Irena** tool suite (http://usaxs.xor.aps.anl.gov/staff/ilavsky/irena.html) for IgorPro has a GUI to load the data found in the XML file. Refer to the WWW site for more details.

5.3 Java JAXB binding

$Revision: 127 $ $Date: 2009-09-30 14:01:08 -0500 (Wed, 30 Sep 2009) $

Documentation for the JAXB binding is spotty at this time. You can check it out with subversion:

```
svn checkout http://svn.smallangles.net/svn/canSAS/1dwg/trunk cansas-1d-standard
```

(where cansas-1d-standard is a local directory name).

5.3.1 JAXB

- Question : What is JAXB?
- Answer : Java Architecture for XML Binding (JAXB): http://java.sun.com/developer/technicalArticles/WebServices/jaxb/
- Wow! : Is it available for other languages?
- Answer : Ask Google. JAXB is for Java. One good advisory page: http://www.devx.com/ibm/Article/20261
- Question : How do I pull out the *I(Q)* data?
- Answer : see fragment below (gets data for desmearing)

5.3.2 JAXB_cansas1d_reader.java: example usage in JAVA

Here is a Java class that shows how to use the JAXB binding.Use this with any of the test data supplied with the cansas-1d-standard directory (above).By default, it shows what is in the *1998spheres.xml* example file: two samples.(You'll have to get the directory paths right until this documentation improves.)

```
/**
 *
 */
package jlake;

import java.io.File;
import java.util.List;

import javax.xml.bind.JAXBContext;
import javax.xml.bind.JAXBElement;
import javax.xml.bind.JAXBException;
import javax.xml.bind.Unmarshaller;
import cansas1d.SASdataType;
import cansas1d.SASentryType;
import cansas1d.SASrootType;
import cansas1d.SASentryType.Run;

/**
 * @author Pete Jemian
 *
 */
public class JAXB_cansas1d_reader {
```

```
  /**
   * @param args
   */
  @SuppressWarnings("unchecked")
  public static void main(String[] args) {
    JAXBContext jc;
    String xmlFile;
//    xmlFile = "cs_af1410.xml";
    xmlFile = "1998spheres.xml";
    try {
      // use the cansas1d/1.0 schema that is bound to a Java structure
      jc = JAXBContext.newInstance("cansas1d");
      Unmarshaller unmarshaller = jc.createUnmarshaller();
      // open the XML into a Java data structure
      JAXBElement<SASrootType> xmlJavaData = (JAXBElement<SASrootType>) unmarshaller
          .unmarshal(new File(xmlFile));
      // canSAS XML file is now loaded in memory
      SASrootType sasRootType = xmlJavaData.getValue();
      int numEntries = sasRootType.getSASentry().size();
      System.out.println("SASentry elements: " + numEntries);
      for( int i = 0; i < numEntries; i++ ) {
        System.out.println("SASentry");
        SASentryType entry = sasRootType.getSASentry().get(i);
        System.out.printf("Title:\t%s\n", entry.getTitle());
        List<SASentryType.Run> runs = entry.getRun();
        System.out.printf("#Runs:\t%d\n", runs.size());
        for( int j = 0; j < runs.size(); j++ ) {
          Run run = (Run) runs.get(j);
          System.out.printf("Run@name:\t%s\n", run.getName());
          System.out.printf("Run:\t%s\n", run.getValue());
        }
        List<SASdataType> datasets = entry.getSASdata();
        System.out.printf("#SASdata:\t%d\n", entry.getSASdata().size());
        for( int j = 0; j < runs.size(); j++ ) {
          SASdataType sdt = (SASdataType) datasets.get(j);
          System.out.printf("SASdata@name:\t%s\n", sdt.getName());
          System.out.printf("#points:\t%d\n", sdt.getIdata().size());
        }
        System.out.println();
      }

      System.out.println("the end.");

    } catch (JAXBException e) {
      // TODO Auto-generated catch block
      e.printStackTrace();
      System.out.printf("Could not open (unmarshall) XML file: %s\n", xmlFile);
    }
  }

}
```

5.3.3 example: how to retrieve I(Q)

Look for the line that has **Qsas[i] = sdt.getIdata().get(i).getQ().getValue();** to see the operations to unwind the data into usable double[] vectors. Pretty straightforward.

- sdt : SASdataType object

- getIdata() : /SASdata/Idata
- get(i) : /SASdata/Idata[i]
- getQ() : /SASdata/Idata/Q
- getValue() : /SASdata/Idata/Q (value, not the unit)

5.3.3.1 GetSASdata.java

```
/**
 *
 */
package jlake;

import java.io.File;
import java.util.List;

import javax.xml.bind.JAXBContext;
import javax.xml.bind.JAXBElement;
import javax.xml.bind.JAXBException;
import javax.xml.bind.Unmarshaller;

import cansas1d.SASdataType;
import cansas1d.SASdetectorType;
import cansas1d.SASentryType;
import cansas1d.SASinstrumentType;
import cansas1d.SASrootType;
import cansas1d.SASentryType.Run;


/**
 * @author Pete Jemian
 *
 */
public class GetSASdata {


  private static SASrootType sasRoot;   // SAS data (from cansas1d/1.0 XML file)
  private static double[] Qsas;     // input Q
  private static double[] Isas;     // input I (slit-smeared)
  private static double[] Idev;     // input Idev (slit-smeared)
  private static double[] Ismr;     // calculated I slit-smeared
  private static double[] Idsm;     // calculated I desmeared
  private static double[] IdsmDev;    // calculated Idev desmeared
  private static double   slit_length;


  /**
   * @param xmlPropertyFile
   */
  public GetSASdata(String xmlDataFile)
  {
    // load SAS data into memory
    try {
      sasRoot = (SASrootType) loadXML("cansas1d", xmlDataFile);
    } catch (JAXBException e) {
      e.printStackTrace();
      System.out.println("ERROR: Cannot find or interpret SAS XML data file:\t" +  ↩
          xmlDataFile);
      return;
```

```
  }

  // SAS data are loaded
  // grab the SAS data to be desmeared
  int entryIndex = 0; // /SASentry[1] : unit base in XML, 0 base in Java
  int dataIndex = 0;  // SASdata[1]
  int detectorIndex = 0;  // SASdetector[1]
  SASentryType entry = (SASentryType) sasRoot.getSASentry().get(entryIndex);
  SASdataType sdt = (SASdataType) entry.getSASdata().get(dataIndex);
  if (sdt.getName().trim().compareTo("slit-smeared") != 0) {
    System.out.println("selected SASdata element must start: <SASdata name=\"slit-smeared ↩
        \">");
    // throw something (an exception) here?
    return;
  }
  int numPoints = sdt.getIdata().size();
  Qsas = new double[numPoints]; // input Q
  Isas = new double[numPoints]; // input I (slit-smeared)
  Idev = new double[numPoints]; // input Idev (slit-smeared)
  for (int i = 0; i < numPoints; i++) {
    Qsas[i] = sdt.getIdata().get(i).getQ().getValue();
    Isas[i] = sdt.getIdata().get(i).getI().getValue();
    Idev[i] = sdt.getIdata().get(i).getIdev().getValue();
  }
  Ismr = new double[numPoints];   // calculated I slit-smeared
  Idsm = new double[numPoints];   // calculated I desmeared
  IdsmDev = new double[numPoints];  // calculated Idev desmeared
  SASinstrumentType instrument = (SASinstrumentType) entry.getSASinstrument();
  SASdetectorType detector = (SASdetectorType) instrument.getSASdetector().get( ↩
      detectorIndex);
  slit_length = detector.getSlitLength().getValue();
}


/**
 * @param (String) pkg Java package containing XML Schema bound to Java data structures
 * @param (String) xmlFile XML file to be opened
 * @return (Object) root object of Java data structure from XML file
 * @throws JAXBException
 */
@SuppressWarnings("unchecked")
private static Object loadXML(String pkg, String xmlFile) throws JAXBException {
  // use the $(pkg) schema that is bound to a Java structure
  JAXBContext jc = JAXBContext.newInstance(pkg);
  Unmarshaller unmarshaller = jc.createUnmarshaller();
  // open the XML file into a Java data structure
  Object obj = (Object) ((JAXBElement<Object>) unmarshaller
      .unmarshal(new File(xmlFile))).getValue();
  return obj;
}


/**
 * @param dt (DesmearingType) Desmearing properties
 * @param sasRoot (SASrootType) SAS data from XML file
 */
public void inputReporter()
{
  System.out.println("dataFile:\t" + dt.getDataFile().trim());
  System.out.printf("dataset selected:\t/SASroot/SASentry[%d]/SASdata[%d]\n",
      dt.getEntryIndex(), dt.getDataIndex());
```

```
    System.out.printf("detector selected:\t/SASroot/SASentry[%d]/SASinstrument/SASdetector ↩
        [%d]\n",
        dt.getEntryIndex(), dt.getDataIndex(), dt.getDetectorIndex());
    System.out.println("extrapolation_form:\t" + dt.getExtrapolationForm().trim());
    System.out.println("x_start_extrapolation_evaluation:\t" + dt. ↩
        getXStartExtrapolationEvaluation().getValue());
    System.out.println("x_start_extrapolation_evaluation unit:\t" + dt. ↩
        getXStartExtrapolationEvaluation().getUnit());
    System.out.println("iterations:\t" + dt.getIterations());
    System.out.println("iterative_weight_method:\t" + dt.getIterativeWeightMethod().trim()) ↩
        ;

    System.out.println("#---------------------------------------");

    int numEntries = sasRoot.getSASentry().size();
    System.out.println("SASentry elements: " + numEntries);
    for( int i = 0; i < numEntries; i++ ) {
      System.out.println("SASentry");
      SASentryType entry = sasRoot.getSASentry().get(i);
      System.out.printf("Title:\t%s\n", entry.getTitle());
      List<SASentryType.Run> runs = entry.getRun();
      System.out.printf("#Runs:\t%d\n", runs.size());
      for( int j = 0; j < runs.size(); j++ ) {
        Run run = (Run) runs.get(j);
        System.out.printf("Run@name:\t%s\n", run.getName());
        System.out.printf("Run:\t%s\n", run.getValue());
      }
      List<SASdataType> datasets = entry.getSASdata();
      System.out.printf("#SASdata:\t%d\n", datasets.size());
      for( int j = 0; j < datasets.size(); j++ ) {
        SASdataType sdt = (SASdataType) datasets.get(j);
        System.out.printf("SASdata@name:\t%s\n", sdt.getName());
        System.out.printf("#points:\t%d\n", sdt.getIdata().size());
      }
      List<SASdetectorType> detectors = entry.getSASinstrument().getSASdetector();
      System.out.printf("#SASdetector:\t%d\n", detectors.size());
      for( int j = 0; j < detectors.size(); j++ ) {
        SASdetectorType det = (SASdetectorType) detectors.get(j);
        System.out.printf("SASdata@name:\t%s\n", det.getName());
        try {
          System.out.printf("SDD:\t%g\t(%s)\n", det.getSDD()
              .getValue(), det.getSDD().getUnit());
        } catch (Exception e) {
          System.out.println("SDD:\tundefined");
        }
        try {
          System.out.printf("slit_length:\t%g\t(%s)\n", det
              .getSlitLength().getValue(), det.getSlitLength()
              .getUnit());
        } catch (Exception e) {
          System.out.println("slit_length:\tundefined");
        }
      }
      System.out.println();
    }
  }

  /**
   * @param args
   */
  public static void main(String[] args) {
    // load test desmearing properties and data into memory
```

```
    GetSASdata sas = new GetSASdata("test.xml");
    sas.inputReporter();
    System.out.println("the end.");
  }


  /**
   * @return the sasRoot
   */
  public SASrootType getSasRoot() {
    return sasRoot;
  }

  /**
   * @param sasRoot the sasRoot to set
   */
  public void setSasRoot(SASrootType sasRoot) {
    GetDesmearingInfo.sasRoot = sasRoot;
  }

  /**
   * @return the qsas
   */
  public double[] getQsas() {
    return Qsas;
  }

  /**
   * @param qsas the qsas to set
   */
  public void setQsas(double[] qsas) {
    Qsas = qsas;
  }

  /**
   * @return the isas
   */
  public double[] getIsas() {
    return Isas;
  }

  /**
   * @param isas the isas to set
   */
  public void setIsas(double[] isas) {
    Isas = isas;
  }

  /**
   * @return the idev
   */
  public double[] getIdev() {
    return Idev;
  }

  /**
   * @param idev the idev to set
   */
  public void setIdev(double[] idev) {
    Idev = idev;
  }
```

```
  /**
   * @return the ismr
   */
  public double[] getIsmr() {
    return Ismr;
  }

  /**
   * @param ismr the ismr to set
   */
  public void setIsmr(double[] ismr) {
    Ismr = ismr;
  }

  /**
   * @return the idsm
   */
  public double[] getIdsm() {
    return Idsm;
  }

  /**
   * @param idsm the idsm to set
   */
  public void setIdsm(double[] idsm) {
    Idsm = idsm;
  }

  /**
   * @return the idsmDev
   */
  public double[] getIdsmDev() {
    return IdsmDev;
  }

  /**
   * @param idsmDev the idsmDev to set
   */
  public void setIdsmDev(double[] idsmDev) {
    IdsmDev = idsmDev;
  }

  /**
   * @return
   */
  public double getSlitLength() {
    return slit_length;
  }

}
```

5.3.3.2 test.xml

Ok, better to use SVN/TRAC for these files. This example will be improved but it proves the point.

```
<?xml version="1.0"?>
<?xml-stylesheet type="text/xsl" href="example.xsl" ?>
<SASroot version="1.0"
    xmlns="cansas1d/1.0"
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
```

```
    xsi:schemaLocation="cansas1d/1.0 http://svn.smallangles.net/svn/canSAS/1dwg/trunk/ ↩
        cansas1d.xsd"
    >
  <SASentry>
    <Title>standard test dataset for Lake desmearing routine</Title>
    <Run>Run</Run>
    <SASdata name="slit-smeared">
      <Idata><Q unit="1/A">0.000371484</Q><I unit="1/cm">211554</I><Idev unit="1/cm ↩
          ">1874.86</Idev></Idata>
      <Idata><Q unit="1/A">0.000386255</Q><I unit="1/cm">201603</I><Idev unit="1/cm ↩
          ">1721.35</Idev></Idata>
      <Idata><Q unit="1/A">0.000392446</Q><I unit="1/cm">193423</I><Idev unit="1/cm ↩
          ">4250.66</Idev></Idata>
      <Idata><Q unit="1/A">0.000400937</Q><I unit="1/cm">205280</I><Idev unit="1/cm ↩
          ">1563.25</Idev></Idata>
      <Idata><Q unit="1/A">0.000415708</Q><I unit="1/cm">198569</I><Idev unit="1/cm ↩
          ">1446.58</Idev></Idata>
      <Idata><Q unit="1/A">0.000430391</Q><I unit="1/cm">198201</I><Idev unit="1/cm ↩
          ">1334.48</Idev></Idata>
      <Idata><Q unit="1/A">0.000445162</Q><I unit="1/cm">191430</I><Idev unit="1/cm ↩
          ">624.224</Idev></Idata>
      <Idata><Q unit="1/A">0.000451353</Q><I unit="1/cm">188171</I><Idev unit="1/cm ↩
          ">605.955</Idev></Idata>
      <Idata><Q unit="1/A">0.000459932</Q><I unit="1/cm">192450</I><Idev unit="1/cm ↩
          ">592.662</Idev></Idata>
      <Idata><Q unit="1/A">0.000474703</Q><I unit="1/cm">186589</I><Idev unit="1/cm ↩
          ">566.562</Idev></Idata>
      <Idata><Q unit="1/A">0.000489386</Q><I unit="1/cm">184247</I><Idev unit="1/cm ↩
          ">541.442</Idev></Idata>
      <Idata><Q unit="1/A">0.000504157</Q><I unit="1/cm">179316</I><Idev unit="1/cm ↩
          ">519.719</Idev></Idata>
      <Idata><Q unit="1/A">0.000510348</Q><I unit="1/cm">172441</I><Idev unit="1/cm ↩
          ">505.368</Idev></Idata>
      <Idata><Q unit="1/A">0.000518928</Q><I unit="1/cm">175473</I><Idev unit="1/cm ↩
          ">497.727</Idev></Idata>
      <Idata><Q unit="1/A">0.000533699</Q><I unit="1/cm">171012</I><Idev unit="1/cm ↩
          ">479.382</Idev></Idata>
      <Idata><Q unit="1/A">0.000548381</Q><I unit="1/cm">167081</I><Idev unit="1/cm ↩
          ">461.221</Idev></Idata>
      <Idata><Q unit="1/A">0.000563063</Q><I unit="1/cm">162303</I><Idev unit="1/cm ↩
          ">446.693</Idev></Idata>
      <Idata><Q unit="1/A">0.000569255</Q><I unit="1/cm">158623</I><Idev unit="1/cm ↩
          ">439.165</Idev></Idata>
      <Idata><Q unit="1/A">0.000577834</Q><I unit="1/cm">160015</I><Idev unit="1/cm ↩
          ">434.267</Idev></Idata>
      <Idata><Q unit="1/A">0.000592605</Q><I unit="1/cm">155494</I><Idev unit="1/cm ↩
          ">421.757</Idev></Idata>
      <Idata><Q unit="1/A">0.000607376</Q><I unit="1/cm">151073</I><Idev unit="1/cm ↩
          ">407.866</Idev></Idata>
      <Idata><Q unit="1/A">0.000622059</Q><I unit="1/cm">146555</I><Idev unit="1/cm ↩
          ">396.055</Idev></Idata>
      <Idata><Q unit="1/A">0.00062825</Q><I unit="1/cm">143885</I><Idev unit="1/cm ↩
          ">390.636</Idev></Idata>
      <Idata><Q unit="1/A">0.00063683</Q><I unit="1/cm">143034</I><Idev unit="1/cm ↩
          ">384.251</Idev></Idata>
      <Idata><Q unit="1/A">0.0006516</Q><I unit="1/cm">139041</I><Idev unit="1/cm ↩
          ">373.826</Idev></Idata>
      <Idata><Q unit="1/A">0.000666371</Q><I unit="1/cm">136947</I><Idev unit="1/cm ↩
          ">365.092</Idev></Idata>
      <Idata><Q unit="1/A">0.000681054</Q><I unit="1/cm">134324</I><Idev unit="1/cm ↩
          ">357.809</Idev></Idata>
      <Idata><Q unit="1/A">0.000687245</Q><I unit="1/cm">131392</I><Idev unit="1/cm ↩
```

```
        ">352.914</Idev></Idata>
      <Idata><Q unit="1/A">0.000695825</Q><I unit="1/cm">131867</I><Idev unit="1/cm ↩
        ">350.159</Idev></Idata>
      <Idata><Q unit="1/A">0.000710507</Q><I unit="1/cm">128250</I><Idev unit="1/cm ↩
        ">342.395</Idev></Idata>
      <Idata><Q unit="1/A">0.000725278</Q><I unit="1/cm">125404</I><Idev unit="1/cm ↩
        ">334.673</Idev></Idata>
      <Idata><Q unit="1/A">0.000739961</Q><I unit="1/cm">122355</I><Idev unit="1/cm ↩
        ">327.753</Idev></Idata>
      <Idata><Q unit="1/A">0.000746152</Q><I unit="1/cm">119544</I><Idev unit="1/cm ↩
        ">323.132</Idev></Idata>
      <Idata><Q unit="1/A">0.000754732</Q><I unit="1/cm">118748</I><Idev unit="1/cm ↩
        ">319.076</Idev></Idata>
      <Idata><Q unit="1/A">0.000769502</Q><I unit="1/cm">115545</I><Idev unit="1/cm ↩
        ">311.966</Idev></Idata>
      <Idata><Q unit="1/A">0.000784273</Q><I unit="1/cm">113124</I><Idev unit="1/cm ↩
        ">305.553</Idev></Idata>
      <Idata><Q unit="1/A">0.000798956</Q><I unit="1/cm">110665</I><Idev unit="1/cm ↩
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        ">289.296</Idev></Idata>
      <Idata><Q unit="1/A">0.000843269</Q><I unit="1/cm">103730</I><Idev unit="1/cm ↩
        ">283.712</Idev></Idata>
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        ">278.13</Idev></Idata>
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      <Idata><Q unit="1/A">0.000872633</Q><I unit="1/cm">98975.8</I><Idev unit="1/cm ↩
        ">272.922</Idev></Idata>
      <Idata><Q unit="1/A">0.000887404</Q><I unit="1/cm">96617</I><Idev unit="1/cm ↩
        ">267.848</Idev></Idata>
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        ">263.148</Idev></Idata>
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        ">258.983</Idev></Idata>
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        ">258.352</Idev></Idata>
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        ">255.102</Idev></Idata>
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        ">251.208</Idev></Idata>
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        ">247.126</Idev></Idata>
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        ">243.068</Idev></Idata>
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        ">242.072</Idev></Idata>
      <Idata><Q unit="1/A">0.000990624</Q><I unit="1/cm">83582.8</I><Idev unit="1/cm ↩
        ">238.943</Idev></Idata>
      <Idata><Q unit="1/A">0.00100539</Q><I unit="1/cm">81637.9</I><Idev unit="1/cm ↩
        ">234.966</Idev></Idata>
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        ">231.251</Idev></Idata>
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        ">228.051</Idev></Idata>
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        ">227.629</Idev></Idata>
      <Idata><Q unit="1/A">0.00104953</Q><I unit="1/cm">76980.6</I><Idev unit="1/cm ↩
```

```
        ">225.019</Idev></Idata>
    <Idata><Q unit="1/A">0.0010643</Q><I unit="1/cm">75445.5</I><Idev unit="1/cm ↩
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    <Idata><Q unit="1/A">0.00107907</Q><I unit="1/cm">73855.7</I><Idev unit="1/cm ↩
        ">218.547</Idev></Idata>
    <Idata><Q unit="1/A">0.00109384</Q><I unit="1/cm">72137.1</I><Idev unit="1/cm ↩
        ">215.031</Idev></Idata>
    <Idata><Q unit="1/A">0.00110003</Q><I unit="1/cm">71587.7</I><Idev unit="1/cm ↩
        ">214.305</Idev></Idata>
    <Idata><Q unit="1/A">0.00110853</Q><I unit="1/cm">70608.1</I><Idev unit="1/cm ↩
        ">211.782</Idev></Idata>
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        ">208.548</Idev></Idata>
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        ">205.543</Idev></Idata>
    <Idata><Q unit="1/A">0.00115284</Q><I unit="1/cm">66343.4</I><Idev unit="1/cm ↩
        ">202.81</Idev></Idata>
    <Idata><Q unit="1/A">0.00115903</Q><I unit="1/cm">65983.2</I><Idev unit="1/cm ↩
        ">202.392</Idev></Idata>
    <Idata><Q unit="1/A">0.00116752</Q><I unit="1/cm">65188.2</I><Idev unit="1/cm ↩
        ">200.268</Idev></Idata>
    <Idata><Q unit="1/A">0.0011822</Q><I unit="1/cm">64072.9</I><Idev unit="1/cm ↩
        ">197.834</Idev></Idata>
    <Idata><Q unit="1/A">0.00119697</Q><I unit="1/cm">62740.3</I><Idev unit="1/cm ↩
        ">195.054</Idev></Idata>
    <Idata><Q unit="1/A">0.00121175</Q><I unit="1/cm">61380.9</I><Idev unit="1/cm ↩
        ">192.227</Idev></Idata>
    <Idata><Q unit="1/A">0.00121794</Q><I unit="1/cm">60799.2</I><Idev unit="1/cm ↩
        ">191.38</Idev></Idata>
    <Idata><Q unit="1/A">0.00122652</Q><I unit="1/cm">60016.7</I><Idev unit="1/cm ↩
        ">189.35</Idev></Idata>
    <Idata><Q unit="1/A">0.0012412</Q><I unit="1/cm">58722.4</I><Idev unit="1/cm ↩
        ">186.613</Idev></Idata>
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        ">184.131</Idev></Idata>
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        ">181.407</Idev></Idata>
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    <Idata><Q unit="1/A">0.00145383</Q><I unit="1/cm">44843.2</I><Idev unit="1/cm ↩
        ">156.44</Idev></Idata>
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        ">149.07</Idev></Idata>
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    <Idata><Q unit="1/A">0.00174863</Q><I unit="1/cm">31319.9</I><Idev unit="1/cm ↩
        ">124.828</Idev></Idata>
    <Idata><Q unit="1/A">0.00180753</Q><I unit="1/cm">29339.2</I><Idev unit="1/cm ↩
        ">119.87</Idev></Idata>
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    <Idata><Q unit="1/A">0.00186653</Q><I unit="1/cm">27449.7</I><Idev unit="1/cm ↩
        ">115.05</Idev></Idata>
    <Idata><Q unit="1/A">0.00192553</Q><I unit="1/cm">25747.7</I><Idev unit="1/cm ↩
```

```
        ">110.669</Idev></Idata>
      <Idata><Q unit="1/A">0.00198443</Q><I unit="1/cm">24113.1</I><Idev unit="1/cm ↩
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        ">100.667</Idev></Idata>
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        ">85.5865</Idev></Idata>
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        ">82.5591</Idev></Idata>
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        ">83.7386</Idev></Idata>
      <Idata><Q unit="1/A">0.00239722</Q><I unit="1/cm">15654</I><Idev unit="1/cm ↩
        ">77.0515</Idev></Idata>
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        ">74.475</Idev></Idata>
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        ">65.3736</Idev></Idata>
      <Idata><Q unit="1/A">0.0027802</Q><I unit="1/cm">11030.1</I><Idev unit="1/cm ↩
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      <Idata><Q unit="1/A">0.0030161</Q><I unit="1/cm">8974.34</I><Idev unit="1/cm ↩
        ">55.8783</Idev></Idata>
      <Idata><Q unit="1/A">0.00325199</Q><I unit="1/cm">7394.04</I><Idev unit="1/cm ↩
        ">50.0284</Idev></Idata>
      <Idata><Q unit="1/A">0.00348788</Q><I unit="1/cm">6118.83</I><Idev unit="1/cm ↩
        ">44.9183</Idev></Idata>
      <Idata><Q unit="1/A">0.00372368</Q><I unit="1/cm">5113.03</I><Idev unit="1/cm ↩
        ">40.5794</Idev></Idata>
      <Idata><Q unit="1/A">0.00395958</Q><I unit="1/cm">4318.86</I><Idev unit="1/cm ↩
        ">7.43972</Idev></Idata>
      <Idata><Q unit="1/A">0.00419538</Q><I unit="1/cm">3658.3</I><Idev unit="1/cm ↩
        ">6.64065</Idev></Idata>
      <Idata><Q unit="1/A">0.00443127</Q><I unit="1/cm">3139.32</I><Idev unit="1/cm ↩
        ">5.99763</Idev></Idata>
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        ">5.45451</Idev></Idata>
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      <SASdetector>
        <name>calculated</name>
        <slit_length unit="1/A">0.08</slit_length>
      </SASdetector>
    </SASinstrument>
    <SASnote/>
  </SASentry>
</SASroot>
```

5.4 Python binding

$Revision: 127 $ $Date: 2009-09-30 14:01:08 -0500 (Wed, 30 Sep 2009) $

Specific *support* for the cansas1d/1.0 data standard in Python is being developed by *NIST/NCNR* as part of their contribution to the *DANSE* project.

Here are some terse instructions to get you started:

```
svn co http://danse.us/trac/sans/browser/trunk/DataLoader DataLoader
cd DataLoader
python setup.py install
```

The *release notes* have a list of the dependencies.

5.4.1 Comments

Other constructive suggestions (that predate the NIST/NCNR support) have been gathered on this page.

5.4.2 gnosis.xml.objectify

The GnosisUtils [1] offer a method to read any XML file into Python data structures. This utility does not validate the XML against a specific XML Schema which can be both good (flexible, especially when XML Foreign Namespace elements are used) and not so good (XML content not guaranteed to be valid *by the rules*).

[1] http://freshmeat.net/projects/gnosisxml/

A quick test of this turned up an acceptable result in that it was able to read several of the canSAS test XML files, including those with foreign namespaces. And ***it was very easy.*** (Especially with some help from http://www.xml.com/pub/a/2003/07/02/py-xml.html)

Here is a quick example.

5.4.2.1 installation

Here is the condensed installation (without all that output) steps. Your system may have gnosis already installed. You may also need sysAdmin privileges. You may need ...

```
cd /tmp
wget http://freshmeat.net/redir/gnosisxml/22028/url_tgz/Gnosis_Utils-1.2.2.tar.gz
tar xzf Gnosis_Utils-1.2.2.tar.gz
cd Gnosis_Utils-1.2.2/
python setup.py install_all
```

5.4.2.2 quick test in Python

Here is the Python code (without all that output) (called *python-test.py*):

```
import gnosis.xml.objectify

sasxml = gnosis.xml.objectify.XML_Objectify('bimodal-test1.xml').make_instance()
print sasxml.SASentry.Title.PCDATA
print sasxml.SASentry.Run.PCDATA
print sasxml.SASentry.SASinstrument.name.PCDATA
print sasxml.SASentry.SASdata.Idata[0].Q.unit,  sasxml.SASentry.SASdata.Idata[0].I.unit
print sasxml.SASentry.SASdata.Idata[0].Q.PCDATA,  sasxml.SASentry.SASdata.Idata[0].I.PCDATA ↩
    ,  sasxml.SASentry.SASdata.Idata[0].Idev.PCDATA
```

5.4.2.3 execution of that Python code

```
[Pete@regitte,2441,cansas1dwg-regitte]$ ./python-test.py
SAS bimodal test1
1992
simulated SAS calculation
1/A 1/cm
0.0040157139 3497.473 90.72816
```

5.4.2.4 full session output

```
[Pete@regitte,2429,/tmp]$ cd /tmp
/tmp
[Pete@regitte,2430,/tmp]$ wget http://freshmeat.net/redir/gnosisxml/22028/url_tgz/ ↩
    Gnosis_Utils-1.2.2.tar.gz
--11:43:16--  http://freshmeat.net/redir/gnosisxml/22028/url_tgz/Gnosis_Utils-1.2.2.tar.gz
           => 'Gnosis_Utils-1.2.2.tar.gz'
Resolving freshmeat.net... 66.35.250.168
Connecting to freshmeat.net|66.35.250.168|:80... connected.
HTTP request sent, awaiting response... 302 Found
Location: http://www.gnosis.cx/download/Gnosis_Utils.More/Gnosis_Utils-1.2.2.tar.gz [ ↩
    following]
--11:43:16--  http://www.gnosis.cx/download/Gnosis_Utils.More/Gnosis_Utils-1.2.2.tar.gz
           => 'Gnosis_Utils-1.2.2.tar.gz'
Resolving www.gnosis.cx... 64.41.64.172
```

```
Connecting to www.gnosis.cx|64.41.64.172|:80... connected.
HTTP request sent, awaiting response... 200 OK
Length: 287,989 (281K) [application/x-tar]

100%[==========================================================================================
     287,989       --.--K/s

11:43:16 (2.47 MB/s) - 'Gnosis_Utils-1.2.2.tar.gz' saved [287989/287989]

[Pete@regitte,2431,/tmp]$ tar xzf Gnosis_Utils-1.2.2.tar.gz
[Pete@regitte,2432,/tmp]$ cd Gnosis_Utils-1.2.2/
/tmp/Gnosis_Utils-1.2.2
[Pete@regitte,2433,Gnosis_Utils-1.2.2]$ python setup.py install_all
[Pete@regitte,2434,Gnosis_Utils-1.2.2]$ cd ~/workspace/cansas1dwg-regitte
[Pete@regitte,2435,cansas1dwg-regitte]$ python
Python 2.5.1 (r251:54863, May 18 2007, 16:56:43)
[GCC 3.4.4 (cygming special, gdc 0.12, using dmd 0.125)] on cygwin
Type "help", "copyright", "credits" or "license" for more information.
>>> import gnosis.xml.objectify
>>> sasxml = gnosis.xml.objectify.XML_Objectify('bimodal-test1.xml').make_instance()
>>> print sasxml.SASentry.Title.PCDATA
SAS bimodal test1
>>> print sasxml.SASentry.Run.PCDATA
1992
>>> print sasxml.SASentry.SASinstrument.name.PCDATA
simulated SAS calculation
>>> print sasxml.SASentry.SASdata.Idata[0].Q.unit
1/A
>>> print sasxml.SASentry.SASdata.Idata[0].I.unit
1/cm
>>> print sasxml.SASentry.SASdata.Idata[0].Q.PCDATA,  sasxml.SASentry.SASdata.Idata[0].I. ↩
    PCDATA,  sasxml.SASentry.SASdata.Idata[0].Idev.PCDATA
0.0040157139 3497.473 90.72816
```

5.4.2.5 Conclusion: OK

This has the promise of being a useful approach to reading this format in Python.Now, how to write back out... ?

5.4.3 generateDS.py

generateDS.py (http://www.rexx.com/~dkuhlman/, http://www.rexx.com/~dkuhlman/generateDS.html) can build a binding (map the structure of the XML file directly into a Python data structure) for Python from an XML Schema. However, the cansas1d/1.0 XML schema (cansas1d.xsd) does not seem to fit the model.It seems, for now, that *generateDS-1.12a* fails on a certain *annotate* line.

```
[Pete@regitte,2402,cansas1dwg-regitte]$ python ~/generateDS-1.12a/generateDS.py -p CS1D_ -o ↩
     cansas1d.py -s cansas1dsubs.py cansas1d.xsd
Traceback (most recent call last):
  File "/home/Pete/generateDS-1.12a/generateDS.py", line 3997, in <module>
    main()
  File "/home/Pete/generateDS-1.12a/generateDS.py", line 3993, in main
    processIncludes, superModule=superModule)
  File "/home/Pete/generateDS-1.12a/generateDS.py", line 3909, in parseAndGenerate
    root.annotate()
AttributeError: 'NoneType' object has no attribute 'annotate'
```

5.4.3.1 Conclusion: not ready yet

Either the canSAS standard (by means of the cansas1d.xsd XML Schema) is not ready or *generateDS.py* does not cover the XML Schema requirements we have at this time.Either way, this is not a viable tool to use now. (2008-05-16)

5.4.4 Other suggestions

- http://www.devx.com/ibm/Article/20261
- http://mail.python.org/pipermail/xml-sig/2002-April/007559.html
- http://pywebsvcs.sourceforge.net/

Chapter 6

Case Studies

6.1 Case Study: Dry Chick Collagen

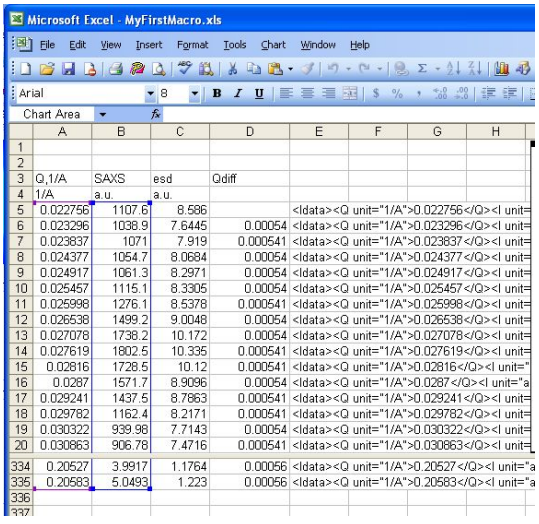
$Revision: 128 $ $Date: 2009-09-30 16:33:30 -0500 (Wed, 30 Sep 2009) $

6.1.1 Overview

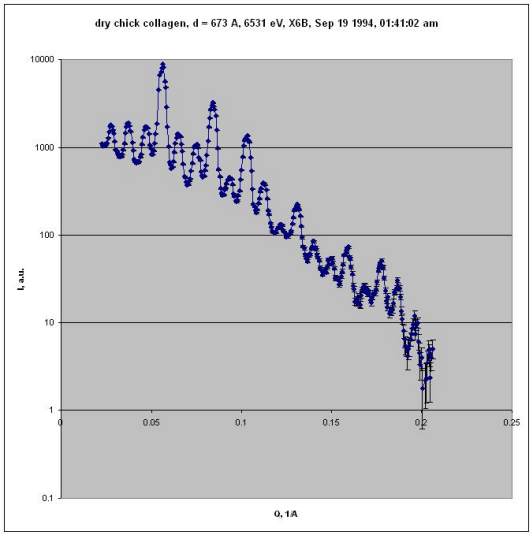
To demonstrate how to get SAS data into the XML standard format, consider this set of SAXS data collected at the National Synchrotron Light Source, Brookhaven National Laboratory, using a SAXS camera set up temporarily at beam line X6B (operated by the Materials Science Division, Argonne National Lab).

The sample was **dry chick collagen.** (Thanks to Malcolm Capel, NSLS beam line X12C for the sample.)

Table 6.1: Figures for dry chick collagen case study



case study: Collagen, SAXS data in Excel table



case study: Collagen, SAXS data in Excel chart

The raw data was collected on a linear position-sensitive detector and reduced to columns of **Q**, **I**, and **Iesd** (estimated standard deviation of **I**).

The only metadata available for this data (without resorting to digging through piles of old notebooks) was obtained from two file headers:

collagen.asc

```
Sep 19 1994     01:41:02 am     Elt: 00090 Seconds
ID: No spectrum identifier defined
Memory Size: 8192 Chls  Conversion Gain: 1024  Adc Offset: 0000 Chls
```

collagen.saxs

```
dry chick collagen, d = 673 A
6531 eV, X6B
```

But, the data can fulfill the minimum requirements of the 1D standard file formatand also make an excellent example of a minimalcanSAS reduced 1-D SAS data file in XML.

6.1.2 Procedure

6.1.2.1 make the basic XML file

It is easiest to copy a template rather than start from an empty file.Copy the *cansas1d.xml* file into your working directory and rename it to **collagen.xml**.

6.1.2.2 modify collagen.xml

It is easier to see the metadata in the XML file before you enter the SAXS data into the file. With the brief metadata available, most lines can be eliminated.This will result in a file that looks like

```
<?xml version="1.0"?>
<?xml-stylesheet type="text/xsl" href="example.xsl" ?>
<SASroot version="1.0"
    xmlns="cansas1d/1.0"
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
    xsi:schemaLocation="cansas1d/1.0 http://svn.smallangles.net/svn/canSAS/1dwg/trunk/ ↩
        cansas1d.xsd"
    >
    <SASentry>
    <Title>dry chick collagen, d = 673 A, 6531 eV, X6B</Title>
        <Run />
        <SASdata>
            <!-- Idata lines will go here -->
        </SASdata>
        <SASsample>
            <ID>dry chick collagen, d = 673 A, 6531 eV, X6B</ID>
        </SASsample>
        <SASinstrument>
            <name>X6B, NSLS, BNL</name>
            <SASsource>
                <radiation>X-ray synchrotron</radiation>
                <wavelength unit="A">
                    1.898
                    <!-- = 12398/6531 -->
                </wavelength>
            </SASsource>
            <SAScollimation />
            <SASdetector>
                <name>X6B PSD</name>
            </SASdetector>
```

```
        </SASinstrument>
        <SASnote>
            Sep 19 1994     01:41:02 am     Elt: 00090 Seconds
            ID: No spectrum identifier defined
            Memory Size: 8192 Chls  Conversion Gain: 1024  Adc Offset: 0000 Chls

            dry chick collagen, d = 673 A
            6531 eV, X6B
        </SASnote>
    </SASentry>
</SASroot>
```

6.1.2.3 prepare the SAXS data

Microsoft Excel is used here to convert the table of SAXS data into therequired lines of XML for the standard. Some may prefer to use a cell formula but here, we develop a bit of Excel Macro code to clarify our procedure.

6.1.2.3.1 Excel macros used

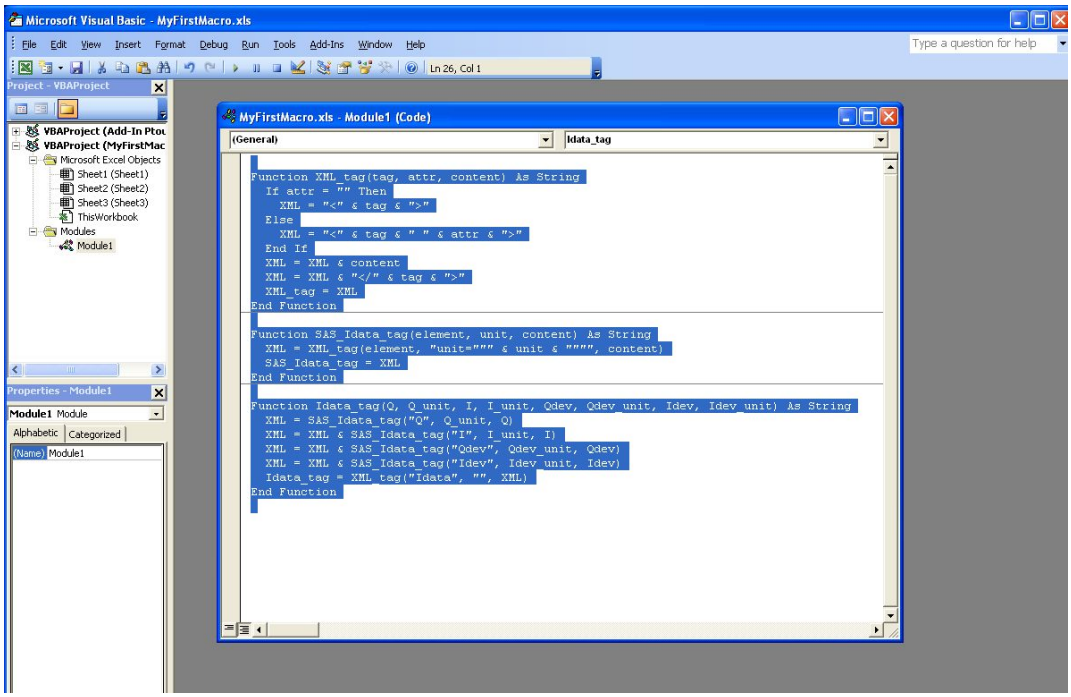
Within Excel, with the SAXS data in columns as shown in the Excel table above, let's define the macros for our use. In Excel, type **<alt><F11>** to open the macro editing window.

```
Function XML_tag(tag, attr, content) As String
  If attr = "" Then
    XML = "<" & tag & ">"
  Else
  XML = "<" & tag & " " & attr & ">"
  End If
  XML = XML & content
  XML = XML & "</" & tag & ">"
  XML_tag = XML
End Function

Function SAS_Idata_tag(element, unit, content) As String
XML = XML_tag(element, "unit=""" & unit & """", content)
  SAS_Idata_tag = XML
End Function

Function Idata_tag(Q, Q_unit, I, I_unit, Idev, Idev_unit) As String
  XML = SAS_Idata_tag("Q", Q_unit, Q)
  XML = XML & SAS_Idata_tag("I", I_unit, I)
  XML = XML & SAS_Idata_tag("Idev", Idev_unit, Idev)
  Idata_tag = XML_tag("Idata", "", XML)
End Function
```

Your window will look similar to this one when you copy/paste the above code: (Yes, my spreadsheet is called MyFirstMacro.xls)



case study: Collagen, SAXS data in Excel chart

Now close the macro editing window and return to the SAXS data in the spreadsheet.

6.1.2.3.2 construct the Idata lines in XML

move to spreadsheet cell **E5** and enter this formula

```
=IDATA_tag(A5,$A$4,B5,$B$4,C5,$C$4)
```

Copy it down all rows in column **E** through cell **E335**

Select cells E5:E335 and copy to clipboard, then paste into **collagen.xml** document inside the **SASdata** element where you see the XML comment .

6.1.3 Final Result

A nicely-formatted display version of the final result can be viewed through the TRAC repository: *http://svn.smallangles.net/-trac/canSAS/browser/1dwg/trunk/cs_collagen_full.xml*

6.1.4 Validate your file

So you think you have an XML file. Let's validate it using the procedure from the documentation.All the instructions are on the documentation page. No sense in repeating them here.

6.1.5 References

All files are available at *http://svn.smallangles.net/trac/canSAS/browser/1dwg/trunk/examples/collagen/*

6.2 Case Study: AF1410 steel

$Revision: 127 $ $Date: 2009-09-30 14:01:08 -0500 (Wed, 30 Sep 2009) $

6.2.1 Overview

Note
This case study has not yet been written up. For now, see the data file (http://svn.smallangles.net/svn/canSAS/1dwg/trunk/-examples/af1410/cs_af1410.xml).
The data file contains multiple SASentry elements that pertain to different samples treated at different conditions in a time series. Each SASentry element contains two SASdata sections that correspond to sector averages from the two-dimensional SANS data. Since the samples had been subjected to a 1.6T magentic field to clear the scattering from magentic domain boundaries in one direction, the sector average for that direction has scattering dominated by purely nuclear scattering moments. The other SASdata section has scattering due to both nuclear and magnetic scattering moments.
Also see the publication: A.J. Allen, D. Gavillet, J.R. Weertman, "Small-Angle Neutron Scattering Studies of Carbide Precipitation in Ultrahigh-Strength Steels," *Acta Metall* **41** (1993) 1869-1884.

Chapter 7

Other matters

Various topics have been considered or presented in considering this standard. Some are described below.

7.1 Definition of Terms

$Revision: 127 $ $Date: 2009-09-30 14:01:08 -0500 (Wed, 30 Sep 2009) $

Note
This Definition of Terms may not be provided in future versions of this manual.

This section provides a glossary defining the details about each specific field (XPath string, XML elements and attributes) in the cansas1d/1.0 standard.

- Each term (element or attribute) is listed by its *XPath* in the XML file. The `cs:` prefix is defined by a `xmlns:cs="cansas1d/1.0"` namespace attribute listed in the XML header.
- Elements are shown below sorted by their XPath. In the XML file, the order of elements is defined by the XML Schema. An example is given in the file: `cansas1d-template.xml`
- Each term in the standard is shown with a comment embedded.
- The comment indicates
  - the name of the element,
  - how many times the element can be used,
    - [0..1] : element is optional but can only appear once within enclosing element
    - [1..1] : element is required and can only appear once within enclosing element
    - [1..inf] : element is required but can appear as many times as needed within enclosing element
    - [0..inf] : element is optional and can appear as many times as needed within enclosing element
    - [] : element is optional, number of appearances within enclosing element is not specified
  - and a short description.
- When shown in the template below with the /@unit XPath, the unit attribute is required.

7.1.1 Glossary

/cs:SASroot

[1..1] The canSAS reduced 1-D SAS data will be in the SASroot database. This is similar to the root element of a NeXus file (`NXroot`).

/cs:SASroot/@version

[1..1] version="1.0" Required attribute to indicate the version of the standard to which this XML document is encoded.

/cs:SASroot/cs:SASentry

[1..inf] A single SAS scan is reported in a SASentry. This is similar to `NXentry` used by NeXus. A `SASentry` can use an optional `name` attribute to provide a string for this SASentry.

/cs:SASroot/cs:SASentry/@name

[0..1] Optional string attribute to identify this particular `SASentry`. Use of the string associated with the `name` attribute is not defined by this standard.

/cs:SASroot/cs:SASentry/<any>

[0..inf] Provision at this point for any element to be entered that is not part of the canSAS standard. Use a xmlns="some-simple-identification-string" to identify that this is a foreign element.

/cs:SASroot/cs:SASentry/cs:Run

[1..inf] Run identification for this SASentry. For many facilities, this is an integer. Use multiple instances of Run as needed. Note: How to correlate this with SASinstrument configurations has not yet been defined.

/cs:SASroot/cs:SASentry/cs:Run/@name

[0..1] Optional string attribute to identify this particular SASrun. Use this to associate (correlate) multiple SASdata elements with Run elements. (Give them the same name.)

/cs:SASroot/cs:SASentry/cs:SASdata

[1..inf] Reduced 1-D SAS data for this SASentry. Use multiple SASdata elements to represent multiple frames. Use this to associate (correlate) multiple SASdata elements with Run elements. (Give them the same name.)

/cs:SASroot/cs:SASentry/cs:SASdata/@name

[0..1] Optional string attribute to identify this particular SASdata.

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata

[1..inf] Idata describes a single SAS data point.

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:dQl

[0..1] Q resolution perpendicular to the axis of scanning (the low-resolution slit length direction).

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:dQl/@unit

[1..1] Required unit for dQl. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:dQw

[0..1] Q resolution along the axis of scanning (the high-resolution slit width direction).

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:dQw/@unit

[1..1] Required unit for dQw. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:I

[1..1] Intensity of the detected radiation.

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:I/@unit

[1..1] Required unit for I. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:Idev

[0..1] Estimated standard deviation of I. Must specify the unit as an attribute.

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:Idev/@unit

[1..1] Required unit for Idev. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:Q

[1..1] Q = (4 pi / lambda) sin(theta) where lambda is the wavelength of the radiation and 2theta is the angle through which the detected radiation has been scattered.

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:Q/@unit

[1..1] Required unit for Q. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:Qdev

[0..1] Estimated standard deviation of Q. Must specify the unit as an attribute.

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:Qdev/@unit

[1..1] Required unit for Qdev. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:Qmean

[0..1] Mean value of Q for this datum. Must specify the unit as an attribute.

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:Qmean/@unit

[1..1] Required unit for Qmean. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/cs:Shadowfactor

[0..1] Describes the adjustment due to the beam stop penumbra. (This definition needs revision. NIST?) NOTE: There is no "unit" attribute.

/cs:SASroot/cs:SASentry/cs:SASdata/cs:Idata/<any>

[0..inf] Provision at this point for any element to be entered that is not part of the canSAS standard. Use a xmlns="some-simple-identification-string" to identify that this is a foreign element.

/cs:SASroot/cs:SASentry/cs:SASinstrument

[1..1] Description of the instrument.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:name

[1..1] Name of the instrument.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation

[1..inf] Description of the instrument collimation.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/@name

[0..1] Optional text to describe this collimation element.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture

[0..inf] Slit or aperture.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/@name

[0..1] Optional name for this aperture.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/@type

[1..1] Optional text to describe the type aperture (pinhole, 4-blade slit, Soller slit, ...).

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/cs:distance

[0..1] Distance from this collimation element to the sample.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/cs:distance/@unit

[1..1] distance requires a unit to be specified. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/cs:size

[0..1] Opening dimensions of this aperture.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/cs:size/@name

[1..1] Optional attribute to clarify the name of this beam size.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/cs:size/cs:x

[0..1] Dimension of the aperture in X.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/cs:size/cs:x/@unit

[1..1] Required unit for the dimension of x. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/cs:size/cs:y

[0..1] Dimension of the aperture in Y.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/cs:size/cs:y/@unit

[1..1] Required unit for the dimension of y. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/cs:size/cs:z

[0..1] Dimension of the aperture in Z. While this is allowed by the standard, it does not make much sense for small-angle scattering.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:aperture/cs:size/cs:z/@unit

[1..1] Required unit for the dimension of z. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:length

[0..1] Amount/length of collimation inserted (on a SANS instrument).

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SAScollimation/cs:length/@unit

[1..1] length requires a unit to be specified. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector

[1..inf] Description of a single or composite detector.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:beam_center

[0..1] Center of the beam on the detector in X and Y.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:beam_center/@name

Optional attribute to clarify the name of this detector beam center.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:beam_center/cs:x

[0..1] Center of the beam on the detector in X.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:beam_center/cs:x/@unit

[1..1] Required unit for the dimension of x. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:beam_center/cs:y

[0..1] Center of the beam on the detector in Y.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:beam_center/cs:y/@unit

[1..1] Required unit for the dimension of y. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:beam_center/cs:z

[0..1] Center of the beam on the detector in Z. While this is allowed by the standard, it does not make much sense for small-angle scattering.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:beam_center/cs:z/@unit

[1..1] Required unit for the dimension of z. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:name

[1..1] Name of the detector.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:offset

[0..1] Offset of the detector position in X, Y, and Z.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:offset/@name

Optional attribute to clarify the name of this beam size.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:offset/cs:x

[0..1] Offset of the detector position in X.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:offset/cs:x/@unit

[1..1] Required unit for the dimension of x. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:offset/cs:y

[0..1] Offset of the detector position in Y.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:offset/cs:y/@unit

[1..1] Required unit for the dimension of y. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:offset/cs:z

[0..1] Offset of the detector position in Z. While this is allowed by the standard, it does not make much sense for small-angle scattering.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:offset/cs:z/@unit

[1..1] Required unit for the dimension of z. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:orientation

[0..1] Orientation (rotation) of the detector in roll, pitch, and yaw. Must specify the unit as an attribute.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:orientation/@name

Optional attribute to name this orientation.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:orientation/cs:pitch

[0..1] Optional rotation of the detector about the X axis (pitch).

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:orientation/cs:pitch/@unit

[1..1] Required unit for the dimension of pitch. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:orientation/cs:roll

[0..1] Optional rotation of the detector about the Z axis (roll).

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:orientation/cs:roll/@unit

[1..1] Required unit for the dimension of roll. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:orientation/cs:yaw

[0..1] Optional rotation of the detector about the Y axis (yaw).

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:orientation/cs:yaw/@unit

[1..1] Required unit for the dimension of yaw. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:pixel_size

[0..1] Size of detector pixels in X and Y.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:pixel_size/@name

Optional attribute to clarify the name of this detector pixel size.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:pixel_size/cs:x

[0..1] Size of detector pixels in X.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:pixel_size/cs:x/@unit

[1..1] Required unit for the dimension of x. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:pixel_size/cs:y

[0..1] Size of detector pixels in Y.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:pixel_size/cs:y/@unit

[1..1] Required unit for the dimension of y. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:pixel_size/cs:z

[0..1] Size of detector pixels in Z. While this is allowed by the standard, it does not make much sense for small-angle scattering.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:pixel_size/cs:z/@unit

[1..1] Required unit for the dimension of z. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:SDD

[0..1] Distance between sample and detector. Must specify the unit as an attribute.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:SDD/@unit

[1..1] Required unit for SDD. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:slit_length

[0..1] Slit length of the instrument for this detector. This is expressed in the same units as Q (reciprocal space units). Must specify the unit as an attribute.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASdetector/cs:slit_length/@unit

[1..1] Required unit for the slit length. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource

[1..1] Description of the source of the radiation.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/@name

[0..1] Optional text description of the source of the radiation (incident on the sample). This can be different from /cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:radiation.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:beam_shape

[0..1] Text description of the shape of the beam (incident on the sample).

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:beam_size

[0..1] Physical dimension of the beam (incident on the sample). Note: If beam is round, just use X dimension. Note: While Z dimension is allowed by the standard, it does not make sense for small-angle scattering.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:beam_size/@name

Optional attribute to clarify the name of this beam size.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:beam_size/cs:x

[0..1] Dimension of the beam size in X.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:beam_size/cs:x/@unit

[1..1] Required unit for the dimension of x. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:beam_size/cs:y

[0..1] Dimension of the beam size in Y.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:beam_size/cs:y/@unit

[1..1] Required unit for the dimension of y. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:beam_size/cs:z

[0..1] Dimension of the beam size in Z. While this is allowed by the standard, it does not make much sense for small-angle scattering.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:beam_size/cs:z/@unit

[1..1] Required unit for the dimension of z. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:radiation

[1..1] Name of the radiation used (neutron, X-ray, synchrotron X-ray, Cu Ka X-ray tube, ..."

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:wavelength

[0..1] wavelength of radiation incident on the sample.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:wavelength/@unit

[1..1] wavelength of radiation requires a unit to be specified. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:wavelength_max

[0..1] Some facilities specify wavelength using a range. The maximum of such a range is given by wavelength_max.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:wavelength_max/@unit

[1..1] wavelength_max requires a unit to be specified. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:wavelength_min

[0..1] Some facilities specify wavelength using a range. The minimum of such a range is given by wavelength_min.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:wavelength_min/@unit

[1..1] wavelength_min requires a unit to be specified. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:wavelength_spread

[0..1] Some facilities specify the width of the wavelength spectrum. The minimum of such a range is given by wavelength_spread.

/cs:SASroot/cs:SASentry/cs:SASinstrument/cs:SASsource/cs:wavelength_spread/@unit

[1..1] wavelength_spread requires a unit to be specified. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASnote

[1..inf] Free form description of anything not covered by other elements.

/cs:SASroot/cs:SASentry/cs:SASprocess

[0..inf] Description of a processing or analysis step.

/cs:SASroot/cs:SASentry/cs:SASprocess/@name

[0..1] Optional attribute to provide a name for this SASprocess.

Note
It is redundant with /cs:SASroot/cs:SASentry/cs:SASprocess/cs:name but it is not the same. It should probably be removed.

/cs:SASroot/cs:SASentry/cs:SASprocess/cs:date

[0..1] Optional date for this data processing or analysis step.

Note
SHOULD WE SPECIFY THE FORMAT FOR THE DATE?

/cs:SASroot/cs:SASentry/cs:SASprocess/cs:description

[0..1] Optional description for this data processing or analysis step.

/cs:SASroot/cs:SASentry/cs:SASprocess/cs:name

[0..1] Optional name for this data processing or analysis step.

/cs:SASroot/cs:SASentry/cs:SASprocess/cs:SASprocessnote

[1..inf] This element is used to describe anything about SASprocess that is not already described.

/cs:SASroot/cs:SASentry/cs:SASprocess/cs:SASprocessnote/<any>

[0..inf] Provision at this point for any element to be entered that is not part of the canSAS standard. Declare a default namespace declaration such as `xmlns="urn:example-namespace:example-context"` to identify that this is a foreign element (where you replace "`example-namespace`" and "`example-context`" with your own terms).

/cs:SASroot/cs:SASentry/cs:SASprocess/cs:term

[0..1] This is used to specify the value of a single variable, parameter, or term related to the SASprocess step.

/cs:SASroot/cs:SASentry/cs:SASsample

[] Description of the sample.

/cs:SASroot/cs:SASentry/cs:SASsample/@name

[0..1] Optional attribute to name this sample. (Should be the same as SASsample/cs:ID)

/cs:SASroot/cs:SASentry/cs:SASsample/<any>

[0..inf] Provision at this point for any element to be entered that is not part of the canSAS standard. Use a xmlns="some-simple-identification-string" to identify that this is a foreign element.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:details

[0..inf] Text string to supply additional sample details.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:ID

[1..1] Text string that identifies this sample.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:orientation

[0..1] Orientation (rotation) of the sample.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:orientation/@name

Optional attribute to name this orientation.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:orientation/cs:pitch

[0..1] Optional rotation of the sample about the X axis (pitch).

/cs:SASroot/cs:SASentry/cs:SASsample/cs:orientation/cs:pitch/@unit

[1..1] Required unit for the dimension of pitch. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASsample/cs:orientation/cs:roll

[0..1] Optional rotation of the sample about the Z axis (roll).

/cs:SASroot/cs:SASentry/cs:SASsample/cs:orientation/cs:roll/@unit

[1..1] Required unit for the dimension of roll. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASsample/cs:orientation/cs:yaw

[0..1] Optional rotation of the sample about the Y axis (yaw).

/cs:SASroot/cs:SASentry/cs:SASsample/cs:orientation/cs:yaw/@unit

[1..1] Required unit for the dimension of yaw. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASsample/cs:position

[0..1] Location in X, Y, and Z of the sample. Must specify the unit as an attribute to each position.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:position/@name

Optional attribute to name this position.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:position/cs:x

[0..1] Location of the sample in X.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:position/cs:x/@unit

[1..1] Required unit for the dimension of x. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASsample/cs:position/cs:y

[0..1] Location of the sample in Y.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:position/cs:y/@unit

[1..1] Required unit for the dimension of y. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASsample/cs:position/cs:z

[0..1] Location of the sample in Z. While this is allowed by the standard, it does not make much sense for small-angle scattering.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:position/cs:z/@unit

[1..1] Required unit for the dimension of z. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASsample/cs:temperature

[0..1] Temperature of this sample. Must specify the unit as an attribute.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:temperature/@unit

[1..1] Required unit for temperature. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASsample/cs:thickness

[0..1] Thickness of this sample. Must specify the unit as an attribute.

/cs:SASroot/cs:SASentry/cs:SASsample/cs:thickness/@unit

[1..1] Required unit for thickness. (See @unit for details.)

/cs:SASroot/cs:SASentry/cs:SASsample/cs:transmission

[0..1] Transmission (1-attenuation) of this sample. Express this as a fraction, not as a percentage. NOTE: there is not "unit" attribute.

/cs:SASroot/cs:SASentry/cs:Title

[1..1] Title of this SASentry.

@unit

Data unit to be given in standard SI abbreviations (e.g., m, cm, mm, nm, K) with the following exceptions: um=micrometres C=celsius A=Angstroms percent=%. fraction a.u.=arbitrary units none=no units are relevant (such as dimensionless)

cs:term

[0..1] This is used to specify the value of a single variable, parameter, or term related to the SASprocess step. This could also be used in a SASnote element to indicate terms not associated with a SASprocess step.

cs:term/@name

[1..1] Name of the term.

cs:term/@unit

[1..1] Unit (string) of the term. (See @unit for details.)

orientation/cs:pitch

[0..1] Rotation about about the X axis. Unit must be specified.

orientation/cs:roll

[0..1] Rotation about about the Z axis. Unit must be specified.

orientation/cs:yaw

[0..1] Rotation about about the Y axis. Unit must be specified.

position/cs:x

[0..1] Translation in the horizontal direction, orthogonal to Y and Z. Positive X direction increases as defined by Y and Z. Unit must be specified.

position/cs:y

[0..1] Translation along the vertical gravitational direction. Positive direction increases upward. Unit must be specified.

position/cs:z

[0..1] Translation along the beam direction. Positive direction increases from source towards detector. Unit must be specified.

roll, pitch, yaw

Coordinates for (roll, pitch, yaw) values representing an orientation or rotation. Unit must be specified for each.

x, y, z

Coordinates for (x, y, z) values representing a position or dimension. Unit must be specified for each.

7.2 XML Help

Listed below are various references useful in learning XML and related topics.

- **XML**: eXtensible Markup Language
  - http://www.w3schools.com/xml/
  - http://www.w3.org/XML/
  - http://en.wikipedia.org/wiki/XML
  - http://www.zvon.org/xxl/XPathTutorial/General/examples.html
- **XSL (or XSLT)**: eXtensible Stylesheet Language (Transformation)

  - http://www.w3schools.com/xsl/
  - http://www.w3.org/Style/XSL/
  - http://en.wikipedia.org/wiki/Extensible_Stylesheet_Language
  - http://en.wikipedia.org/wiki/XSLT
- **XPath**: XPath is a language for finding information in an XML document.
  - http://www.w3schools.com/xpath/
  - http://www.w3.org/Style/XSL/
  - http://en.wikipedia.org/wiki/XPath
- **Schema**: An XML Schema describes the structure of an XML document.
  - http://www.w3schools.com/schema/
  - http://www.w3.org/XML/Schema
  - http://en.wikipedia.org/wiki/XSD
- **XML Namespaces**: XML namespaces are used for providing uniquely named elements and attributes in an XML instance.
  - http://www.zvon.org/xxl/NamespaceTutorial/Output
  - http://en.wikipedia.org/wiki/XML_namespaces
  - http://www.w3schools.com/XML/xml_namespaces.asp
- **XML Foreign Elements**: Inclusion of elements, at select locations, that are not defined by the cansas1d.xsd XML Schema
  - http://books.xmlschemata.org/relaxng/relax-CHP-11-SECT-4.html
  - http://www.w3.org/TR/SVG/extend.html
  - http://www.google.com/search?q=XML+foreign+elements

7.3 The Intensity Problem

The intensity (see SASdata/Idata) is permitted in three different forms:

- **absolute units:** differential cross-section per unit volume per unit solid angle (typical unit: 1/cm)
- **absolute units:** differential cross-section per unit atom per unit solid angle (typical unit: cm^2)
- **arbitrary units:** usually a ratio of two detectors but unit is meaningless (typical unit: a.u.)

This presents a few problems for analysis software to sort out when reading the data. Fortunately, it is possible to analyze the unit attribute to decide 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 three types of intensity indiscriminately.

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

Chapter 8

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