1 ORSO standard for reflectometry data files

1.1 human-readable data file

The header should be formatted using YAML.

1.1.1 Structure of the header

The first line should state what the file is. E.g.
`#reflectivity data file orso file format 0.0`

The header is structured into information on the

- **creator** ownership of the data file
- **data source** ownership and provenience of the raw data
- **reduction** software and reduction steps
- **misc** non-orso content
- **data** column description and units

using key words and structure as listed in the dictionary.

And finaly a one-line column description refering to the data section of the type
```
#     1 Qz    2 RQz   3 sRQz    4 sQz        5 ...
```
or just
```
#        1        2        3        4        5 ...
```

1.1.2 Dictionary of the key words used in the header

creator (required)

This section referes to the creation of this *file*, not the data.

name (required) NX_CHAR
Name of the person who created this file
affiliation (optional) NX_CHAR
Affiliation of the person who created this file
time (optional) NX_DATE_TIME
Date and time of the creation of this file
system (optional) NX_CHAR
Computer and user who created this file

data source (required)

This section deals with the source of the data used for generating this file.

origin (required)

This referes to the legal ownership of the raw data.

owner NX_CHAR
Name of the owner of the raw data facility
Name of the facility where the measurement has been berformed.

experiment ID (required, if applicable) NX_CHAR
The proposal number or experiment ID under which the data were cllected.

experiment date (optional) NX_DATE_TIME
Dates when the experiement was performed (the whole period rather than the individual measurement).

title Title of the experiment / the measurement campain.

experiment (required)

instrument Name and if applicable type of the instrument used.

probe (required)

Radiation used during the experiemnt. Either `neutrons` or `x-rays`.

polarisation (optional)
For neutrons the polarisation might be given as *+1* for fully spin up polarised, *-1* for fully spin down polarised and *0* for unpolarised.
Partial polarisation can be expressed as ....

measurement (required)

How and parameters

scheme (optional) NX_FLOAT

Measurement scheme / geometry. This might be
`angle dispersive`
`erergy dispersive`
or `angle and erergy dispersive`

wavelength range (optional) NX_FLOAT, NX_WAVELENGTH

Value and unit for angle dispersive scheme

Format `<value> # <unit>`

or `{<value>, <unit>}`

Value range and unit for wavelength dispersive scheme.

Format `[<lower limit>, <upper limit>] # <unit>`

or `{<lower limit>, <upper limit>, <unit>}`

wavelength (optional) NX_FLOAT

value or range of values

wavelength unit (required if wavelength is given) NX_WAVELENGTH

possible values: `nm` (recommended), `Aa`

angular range (optional) NX_FLOAT

Value and unit for wavelength dispersive scheme

Format `<value> # <unit>`

Value range and unit for angle dispersive scheme.

Format `[<lower limit>, <upper limit>] # <unit>`

sample (required)

Description of the measured sample.

name (required)
A name uniquely identifying the sample
description (optional)
Nominal composition of the sample if known.
Format suggestion following GenX nomenclature

```
- amb: air
- layer: {material: Ni, thickness: 100 nm}
- subs: Si
```

links (optional)

List of links to related data, publications, instruments and so on. Free format, e.g.

```
related extensive file : fulldatafile.hdf
doi                    : orso2020.123456.789
instrument reference   : doi:10.1016/j.nima.2016.03.007
```

reduction (required)

Information on the reduction steps performed to obtain the data below from the raw data set(s) listed here.

software (required)

Name and version of the software.

call (required)

Echo of the call of the software or soemthing similar which allows to reproduce the data content of this file.

comments (optional)

Plain text with comments about the data reduction. This allows to explain details of the reduction algorithm or what assumptions have been made.

corrections (optional)

List of reduction steps that have been performed. Probably with reference to a standadised procedure (orso repository) or to a publication.

binning (optional)

Description of the binning applied to the data.

several ranges require a repetition of the block.

Qz range [:0.01] # Aaˆ-1
type linear
delta Qz 0.001 # Aaˆ-1

input files (required)

Data files used for creating the data below.

references (required if applicable)

List of files used for normalisation of the data.

file File name
created Date of creation (measurement?) of the raw file
Format YYYY/MM/DD:hh:mm:ss

datafiles (required)

List of files containing the raw data.

file File name
created Date of creation (measurement?) of the raw file
Format YYYY/MM/DD:hh:mm:ss

data state (optional)

key word like summary of the reduction steps

Format ‘ :

misc (optional)

Optional section to be used with non-orso-standard key words.

data (required)

Column description and data array containing the reduced data and related quantities.

The content of columns 1 to 4 is defined. Further columns may contain whatever the creator wants - as long as it is clearly stated what it is and what the units are.

column 1 (required)
Must be one of `Qz`, `alpha_i` or `lambda`.
Together with the unit, i.e. `nm^-1`, `Aa^-1`, `deg`, `rad`, `nm` or `Aa`.

column 2 (required)
Must be the reflectivity or intensity as a function column 1.
If applicable with unit.

column 3 (required)
Must be the uncertainty of the quantity in column 2.
This might be the standard deviation (sigma), FWHM, or the like.
Including appropriate units.

column 4 (optional, but defined if present)
If available the uncertainty of the quantity in column 1.
This might be the standard deviation (sigma), FWHM, or the like.
Including appropriate units.

column 5 (optional)
...

1.2 dictionaries:

1.2.1 definition of vocabulary

proposals/examples:

reflectivity (to be discussed!)
Normalised intensity reflected from a sample surface. The *reflectivity* is dimensionless, but might still contain experimental influences and is thus not identical to the sample property reflectivity, solely based on the laterally averaged density depth profile.

angle of incidence bla bla bla

bin, binning bla bla bla

resolution bla bla bla

1.2.2 dictionary of data reduction steps

proposals/examples:

footprint correction based on geometry The incident intensity on the sample I^0_{sample} is calculated from the total incident intensity I^0_{total}, the beam

width d_{beam}, the sample length l_{sample} and the angle of incidence α_i.

$$I^0_{\text{sample}} = I^0_{\text{total}} \cdot \frac{l_{\text{sample}} \sin \alpha_i}{d_{\text{beam}}} \quad \text{for } \alpha_i < \arcsin \frac{d_{\text{beam}}}{l_{\text{sample}}} \tag{1}$$

$$= I^0_{\text{total}} \quad \text{for } \alpha_i \geq \arcsin \frac{d_{\text{beam}}}{l_{\text{sample}}} \tag{2}$$

(missing: non-flat intensity distribution, convolution with geometrical resolution)

footprint correction using reference sample The footprint is intrinsically corrected by normalisation using a reference measurement: reflected intensity of a supermirror sample $I^r_{\text{reference}}$ with known reflectivity $R_{\text{reference}}(q_z)$ and the same surface shape as the sample.

$$R_{\text{sample}} = \frac{I^r_{\text{sample}}}{I^r_{\text{reference}}} R_{\text{reference}} \tag{3}$$

(incomplete! high angles)