

# A new data format for reduced reflectometry data

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Everybody happy with 3-column ASCII file

- $q, l, \Delta l$

But what about spread in  $q$ ?

- $q, \Delta q, l, \Delta l$
- $q, l, \Delta q, \Delta l$
- $q, l, \Delta l, \Delta q$

And what about metadata?

`https://www.reflectometry.org`

- > Working Groups
- > File Formats
- > State of the project
- > Version 0 specification

Combines YAML header (`#` outcommented) with ASCII table

```
# # ORSO reflectivity data file | 0.1 standard | YAML encoding | https://www.reflectometry
# # Interdiffusion in Fe | 2020-12-24 | sample fe-457-2 | R(q_z)
# data_source:
#   owner:
#     name:      Max Mustermann
#     affiliation: Forschungszentrum Jülich, JCNS-MLZ
#     mail:      m.mustermann@fz-juelich.de
#   experiment:
#     title:     Interdiffusion in Fe
#     instrument: MARIA
#     start_data: 2022-03-17
#     ...
#   sample:
#     ...
#   measurement:
#     scheme: angle-dispersive
#     instrument_settings:
#       ...
# reduction:
#   software:
```

```
# reduction:
#   software:
#     ...
#   corrections:
#     ...
# columns:
#   - name:      Qz
#     unit:      1/angstrom
#     description: wavevector transfer
#   - name:      R
#     description: reflectivity
#   - name:      sR
#     description: standard deviation of reflectivity
#   - name:      sQz
#     unit:      1/angstrom
#     description: standard deviation of wavevector transfer resolution
1.0356329600000000e-02 3.88100068000000001e+00 4.3390906800000000e+00 5.1781647800000000e-01
1.0671729400000000e-02 1.1643051099999999e+01 8.8925271899999991e+00 5.3358647100000001e-01
...
```

# Why ASCII?

Google

hdf5 broken



Alle

Bilder

Videos

News

Shopping

Mehr

Suchfilter

Ungefähr 733.000 Ergebnisse (0,51 Sekunden)

```
$ h5totxt /G/int/formats/mlz/toftof/TOFTOF44512.nxs  
h5totxt error: couldn't find data set in HDF5 file
```

## Aren't all file format equivalent?

Yes, we can easily convert ORSO to plain YAML, JSON, XML, hdf5, NeXus.

No, we cannot easily convert NeXus to JSON, YAML, ORSO.

All these formats support hierarchies of arrays (lists) and hashes (dicts).

Additionally, XML, hdf5, NeXus support attributes (represented with prefix @). Bad.