HELMHOLTZ
Metadata Collaboration

SECoP@HMC – Data Storage

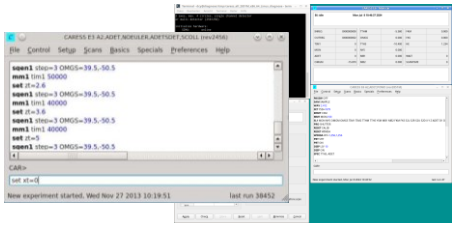
Making sample environment (meta)data understandable

www.helmholtz-metadaten.de

Sample **E**nvironment **Co**mmunication **P**rotocol

HZB

Experiment Control

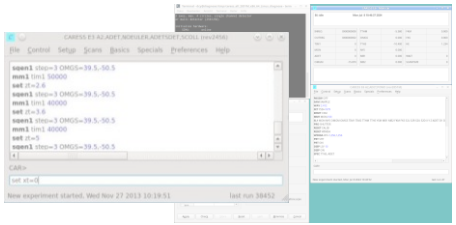


Sample Environment

Sample Environment Communication Protocol

HZB

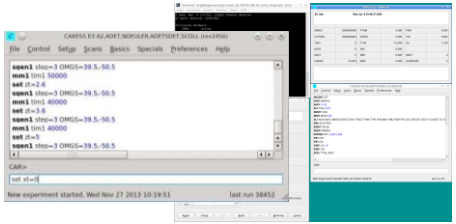
Experiment Control



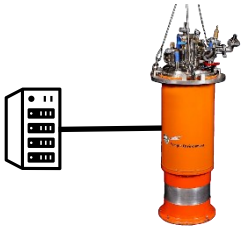
Sample Environment

HZB

Experiment Control
+ SECoP Client



SECoP

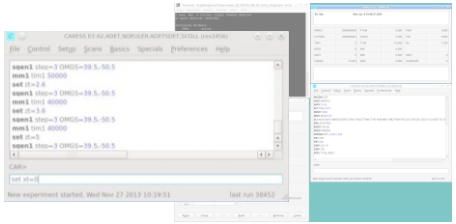


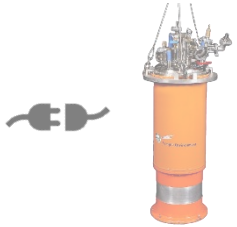
Sample Environment
+ SECoP Server (SECnode)

Sample Environment Communication Protocol

HZB

Experiment Control

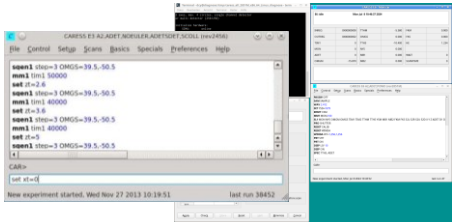




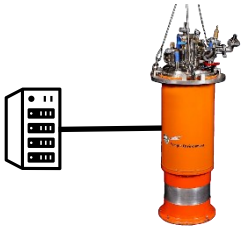
Sample Environment

HZB

Experiment Control
+ SECoP Client



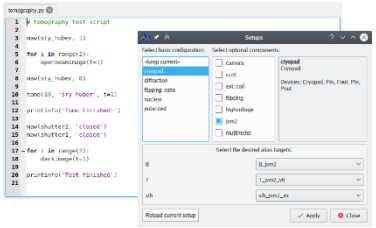
SECoP



Sample Environment
+ SECoP Server (SECnode)

MLZ
Heinz Maier-Leibnitz Zentrum

Experiment Control
+ SECoP Client



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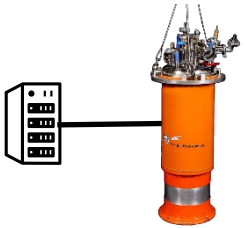


Sample Environment
+ SECoP Server (SECnode)

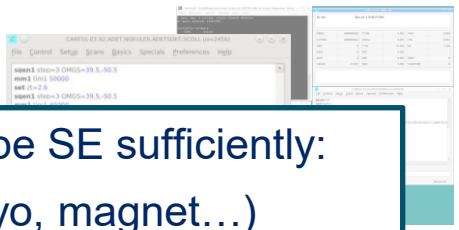
Sample **E**nvironment **Co**mmunication **P**rotocol

Metadata to describe SE sufficiently:

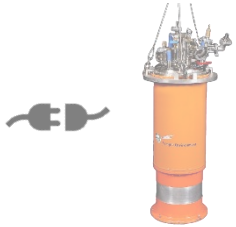
- Model / kind (cryo, magnet…)
- Parameters to read
- Parameters to set (+ limits)
- Units

⇨ Standardised format (schema)

⇨ Standardised storage of (meta)data

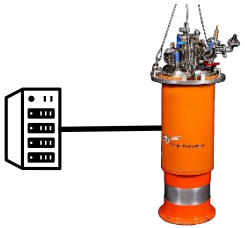


Experiment Control
+ SECoP Client



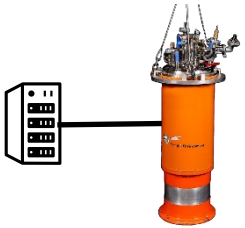
Sample Environment

SECoP



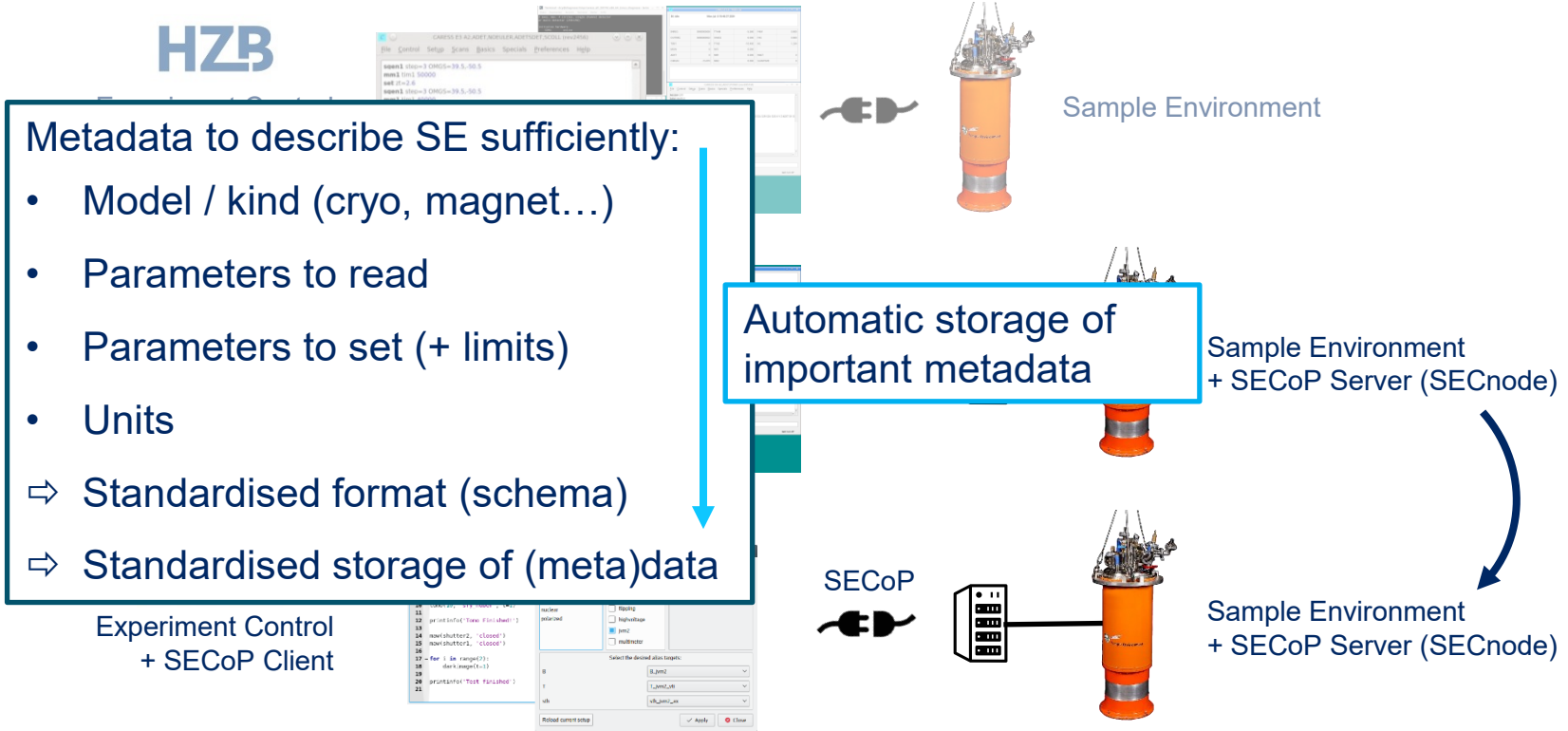
Sample Environment
+ SECoP Server (SECnode)

SECoP



Sample Environment
+ SECoP Server (SECnode)

Sample **E**nvironment **Co**mmunication **P**rotocol



Sample **E**nvironment **Co**mmunication **P**rotocol

```
> describe
< describing .
{
  "description":"TestNode",
  "equipment_id":"HZB_Testnode1",
  "firmware":"SHALL server library (Git 70591a14f66f37b92dcf6386a17159b526fa2913)",
  "modules":
  {
    "temp1":
    {
      "interface_classes":["Writable","Readable"],
      "description":"a meaningful description of the module",
      "accessibles":
      {
        "value":
        {
          "description":"temperature",
          "datainfo":{"type":"double","unit":"K"},
          "readonly":true
        },
        "target":
        {
          "description":"target temperature",
          "datainfo":{"type":"double","unit":"K"},
          "readonly":false
        },
```

General description (static parameters)

List of modules (dynamic parameters) (e.g. a magnet could read/set several temperatures and a magnetic field)

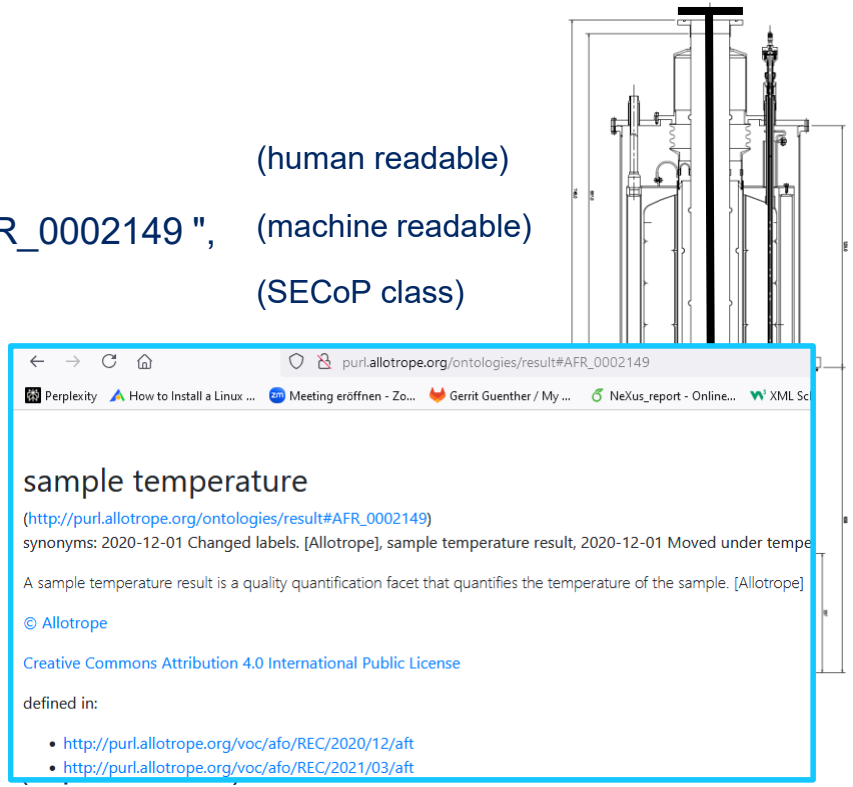
Experiment control can read current temperature

Experiment control can set target temperature

SECoP: Meaning

Each module defines what it does:

```
"meaning": {
    "key": “sample temperature",                                                    (human readable)
    "link": "http://purl.allotrope.org/ontologies/result#AFR_0002149 ",             (machine readable)
    "function": "temperature_regulation",                                           (SECoP class)
    "importance": 20,
    "belongs_to": "sample" }
```



SECoP: Meaning

Each module defines what it does:

"meaning": {

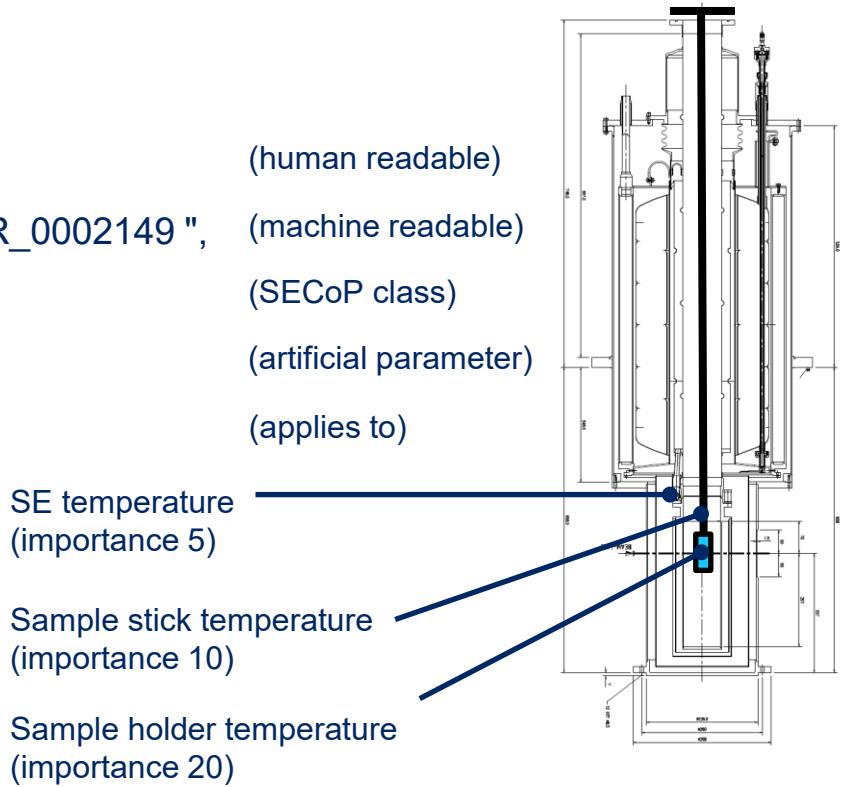
"key": “sample temperature", (human readable)

"link": "http://purl.allotrope.org/ontologies/result#AFR_0002149 ", (machine readable)

"function": "temperature_regulation", (SECoP class)

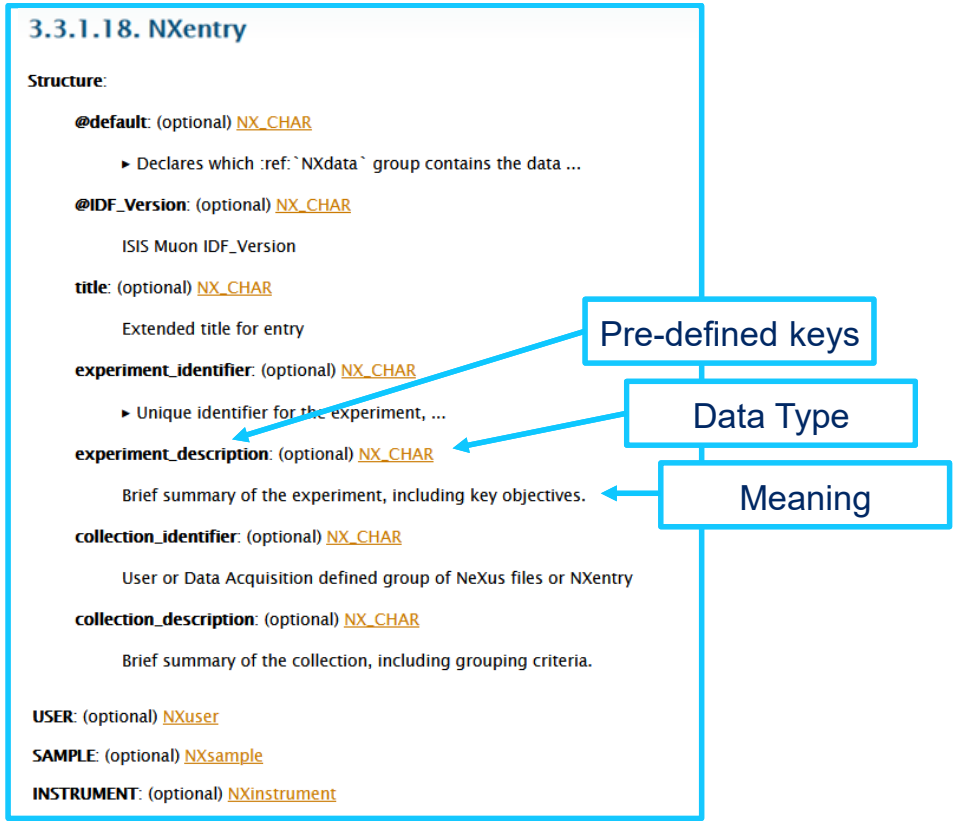
"importance": 20, (artificial parameter)

"belongs_to": "sample" } (applies to)



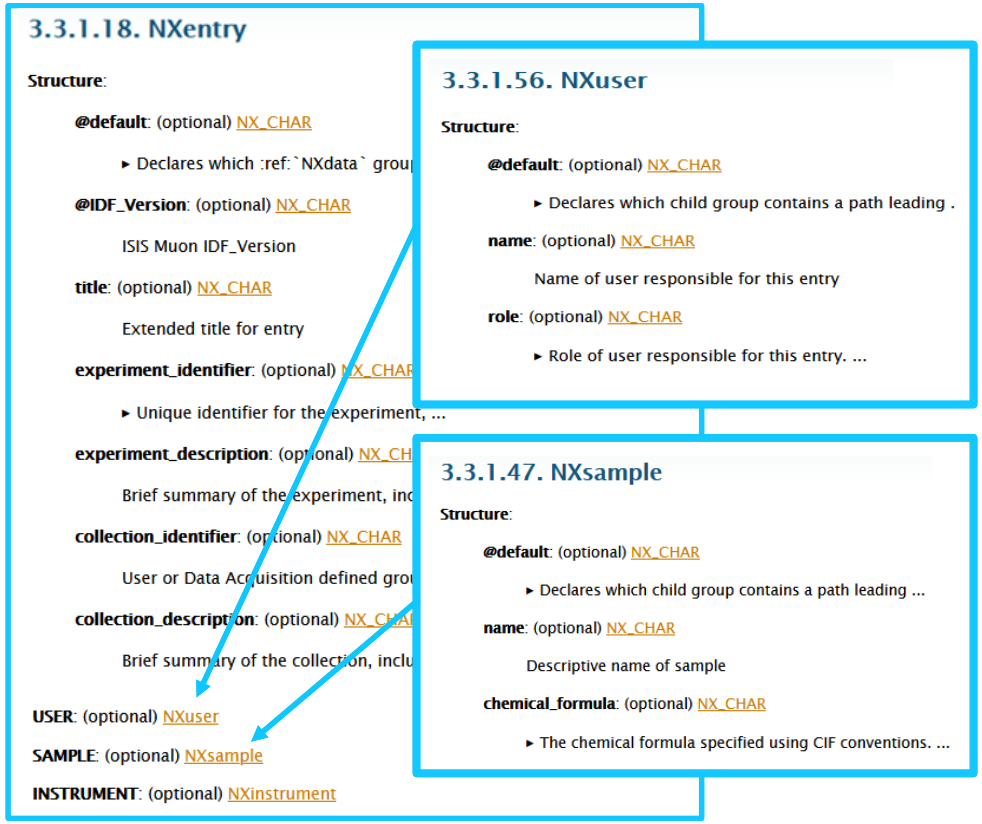
NeXus

- Binary file format (HDF5)
- Hierarchical, defined structure
  - Groups
  - Data Fields
  - @Attributes
- Metadata + data create context
- Persistent web description (URL)
- Modular structure (base classes)
- Metadata schema for experimental data



NeXus

- Binary file format (HDF5)
- Hierarchical, defined structure
  - Groups
  - Data Fields
  - @Attributes
- Metadata + data create context
- Persistent web description (URL)
- Modular structure (base classes)
- Metadata schema for experimental data: logic through structure & semantics



SECoP ⇨ NeXus

```
{
  "description":"TestNode",
  "equipment_id":"HZB_Testnode1",
  "firmware":"SHALL server library (Git 70591a14f6
  "modules":
  {
    "temp1":
    {
      "interface_classes":["Writable","Readable"],
      "description":"a meaningful description of t
      "accessibles":
      {
        "value":
        {
          "description":"temperature",
          "datainfo":{"type":"double","unit":"K"},
          "readonly":true
        },
      "meaning":
      {
          "key": "sample temperature",
          "link": "http://purl.allotrope.org/ontologies/result#AFR_0002149 ",
          "function": "temperature_regulation",
          "importance": 20,
          "belongs_to": "sample"
      },
```

3.3.1.47. NXsample

Structure:

name: (optional) NX_CHAR

Descriptive name of sample

temperature: (optional) NX_FLOAT (Rank: anyRank, Dimensions: [

Sample temperature. This could be a scanned variable

temperature_env: (optional) NXenvironment

Additional sample temperature environment information

magnetic_field: (optional) NXlog

magnetic_field.value is a link to e.g. magnetic_field_env.sensor1.value

chemical_formula: (optional) NX_CHAR

▸ The chemical formula specified using CIF conventions. ...

SECoP ⇨ NeXus

```
{
  "description":"TestNode", SECnode
  "equipment_id":"HZB_Testnode1",
  "firmware":"SHALL server library (Git 70591a14f6
  "modules":
  {
    "temp1":
    {
      "interface_classes":["Writable","Readable"],
      "description":"a meaningful description of t
      "accessibles":
      {
        "value":
        {
          "description":"temperature",
          "datainfo":{"type":"double","unit":"K"},
          "readonly":true
        },
      "meaning":
      {
          "key": "sample temperature",
          "link": "http://purl.allotrope.org/ontologies/result#AFR_0002149 ",
          "function": "temperature_regulation",
          "importance": 20,
          "belongs_to": "sample"
      },
```

3.3.1.47. NXsample

Structure:

name: (optional) NX_CHAR

Descriptive name of sample

temperature: (optional) NX_FLOAT (Rank: anyRank

Sample temperature. This could be a scanne

temperature_env: (optional) NXenvironment

Additional sample temperature environment info

magnetic_field: (optional) NXlog

magnetic_field.value is a link to e.g. magnetic_field_env.sensor1.value

chemical_formula: (optional) NX_CHAR

▸ The chemical formula specified using CIF conventions. ...

3.3.1.19. NXenvironment

Structure:

name: (optional) NX_CHAR

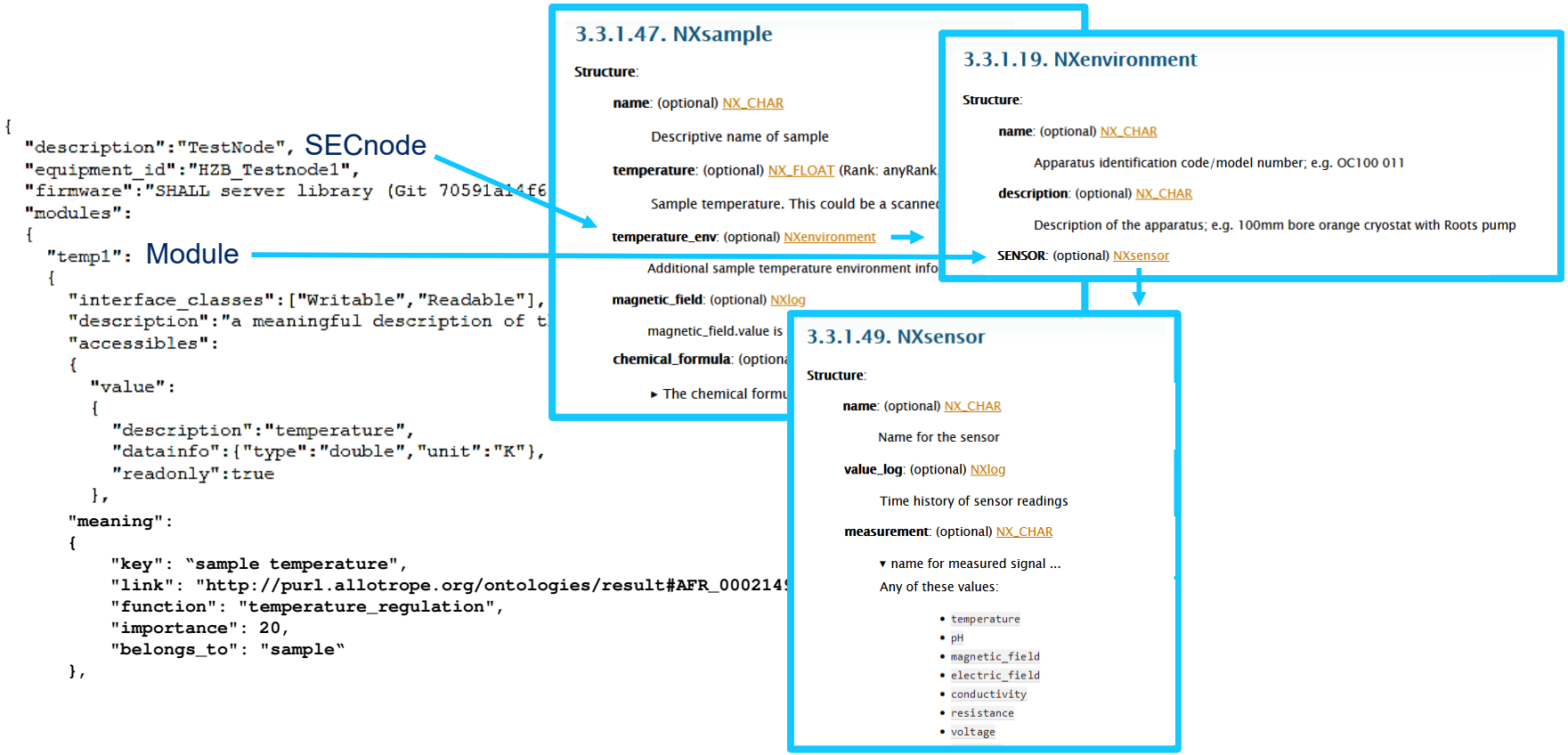
Apparatus identification code/model number; e.g. OC100 011

description: (optional) NX_CHAR

Description of the apparatus; e.g. 100mm bore orange cryostat with Roots pump

SENSOR: (optional) NXsensor

SECoP ⇨ NeXus


{
"description":"TestNode",
"equipment_id":"HZB_Testnode1",
"firmware":"SHALL server library (Git 70591a
"modules":
{
"temp1":
{
"interface_classes":["Writable","Readable"],
"description":"a meaningful description of t
"accessibles":
{
"value":
{
"description":"temperature",
"datainfo":{"type":"double","unit":"K"},
"readonly":true
},
"meaning":
{
"key": "sample temperature",
"link": "http://purl.allotrope.org/ontologies/result#AFR_000214
"function": "temperature_regulation",
"importance": 20,
"belongs_to": "sample"
},
SECnode
Module
3.3.1.47. NXsample
Structure:
name: (optional) NX_CHAR
Descriptive name of sample
temperature: (optional) NX_FLOAT (Rank: anyRank
Sample temperature. This could be a scanne
temperature_env: (optional) NXenvironment
Additional sample temperature environment info
magnetic_field: (optional) NXlog
magnetic_field.value is
chemical_formula: (optiona
▸ The chemical formu
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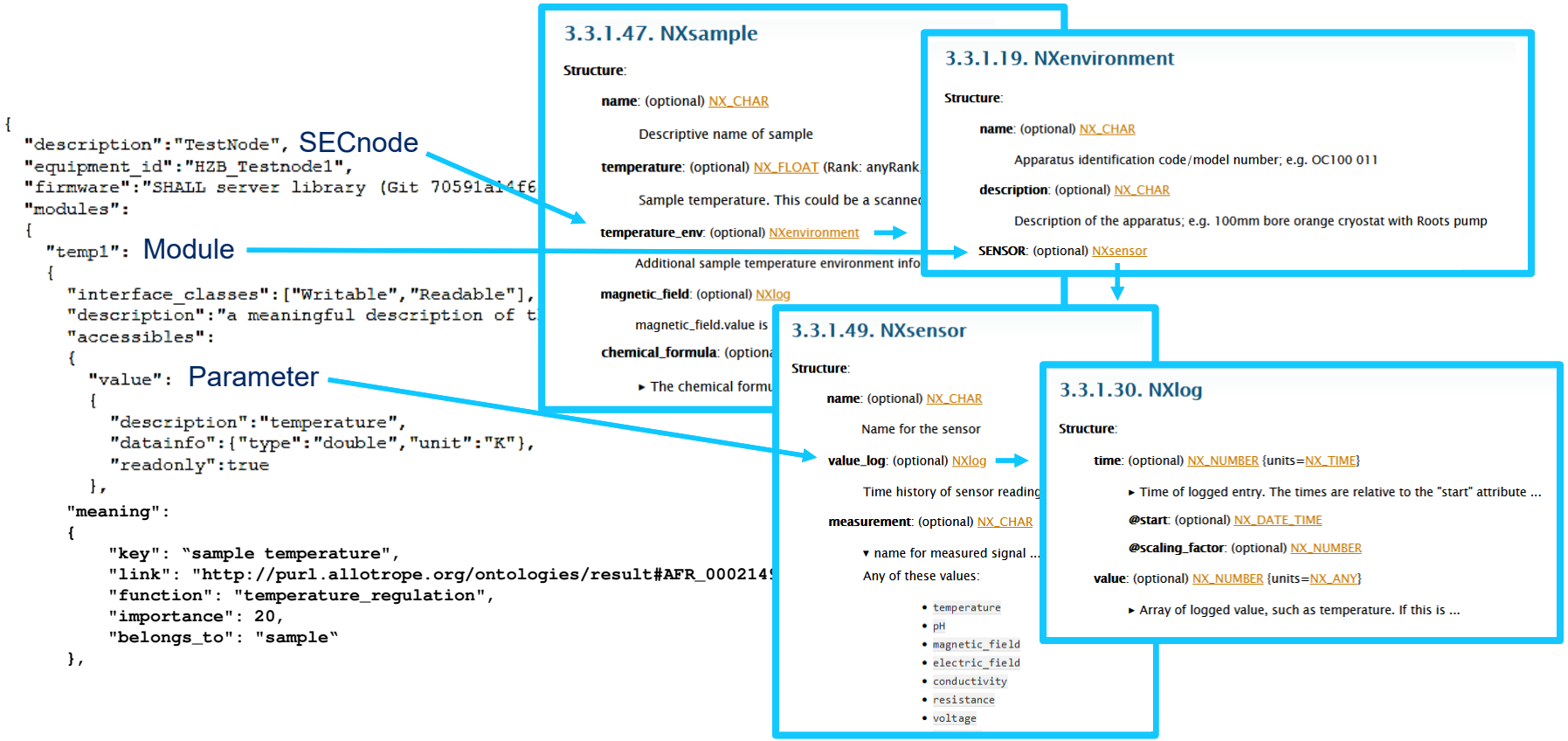
Structure:
name: (optional) NX_CHAR
Apparatus identification code/model number; e.g. OC100 011
description: (optional) NX_CHAR
Description of the apparatus; e.g. 100mm bore orange cryostat with Roots pump
SENSOR: (optional) NXsensor
3.3.1.49. NXsensor
Structure:
name: (optional) NX_CHAR
Name for the sensor
value_log: (optional) NXlog
Time history of sensor readings
measurement: (optional) NX_CHAR
▾ name for measured signal ...
Any of these values:
temperature
pH
magnetic_field
electric_field
conductivity
resistance
voltage

SECoP ⇨ NeXus


{
"description":"TestNode", SECnode
"equipment_id":"HZB_Testnode1",
"firmware":"SHALL server library (Git 70591a
"modules":
{
"temp1": Module
{
"interface_classes":["Writable","Readable"],
"description":"a meaningful description of t
"accessibles":
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"value": Parameter
{
"description":"temperature",
"datainfo":{"type":"double","unit":"K"},
"readonly":true
},
"meaning":
{
"key": "sample temperature",
"link": "http://purl.allotrope.org/ontologies/result#AFR_000214
"function": "temperature_regulation",
"importance": 20,
"belongs_to": "sample"
},
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Structure:
name: (optional) NX_CHAR
Descriptive name of sample
temperature: (optional) NX_FLOAT (Rank: anyRank
Sample temperature. This could be a scanne
temperature_env: (optional) NXenvironment
Additional sample temperature environment info
magnetic_field: (optional) NXlog
magnetic_field.value is
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Structure:
name: (optional) NX_CHAR
Apparatus identification code/model number; e.g. OC100 011
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Description of the apparatus; e.g. 100mm bore orange cryostat with Roots pump
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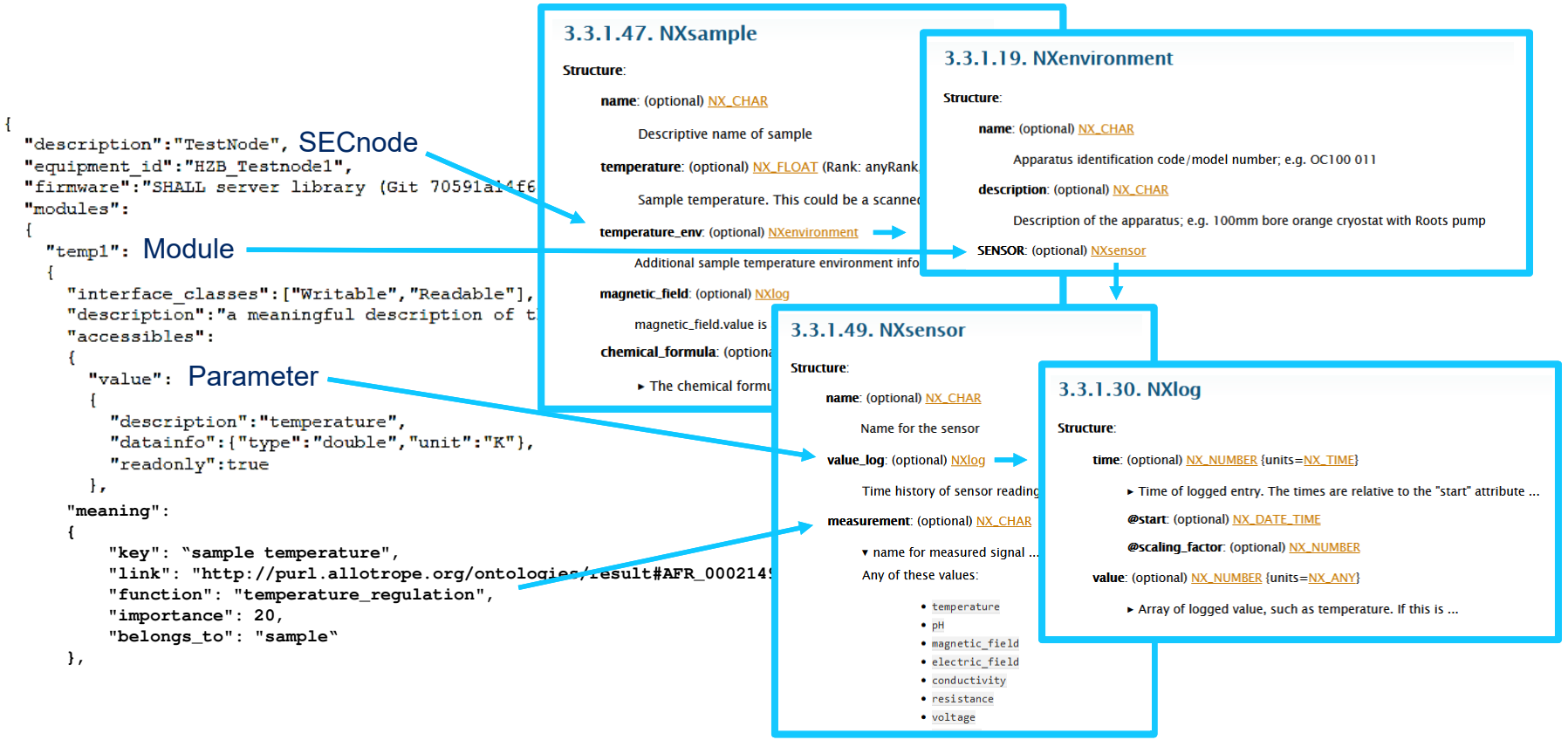
Structure:
name: (optional) NX_CHAR
Name for the sensor
value_log: (optional) NXlog
Time history of sensor reading
measurement: (optional) NX_CHAR
▾ name for measured signal ...
Any of these values:
temperature
pH
magnetic_field
electric_field
conductivity
resistance
voltage
3.3.1.30. NXlog
Structure:
time: (optional) NX_NUMBER {units=NX_TIME}
▸ Time of logged entry. The times are relative to the "start" attribute ...
@start: (optional) NX_DATE_TIME
@scaling_factor: (optional) NX_NUMBER
value: (optional) NX_NUMBER {units=NX_ANY}
▸ Array of logged value, such as temperature. If this is ...

SECoP ⇨ NeXus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"description":"TestNode", SECnode
"equipment_id":"HZB_Testnode1",
"firmware":"SHALL server library (Git 70591a
"modules":
{
"temp1": Module
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"interface_classes":["Writable","Readable"],
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"accessibles":
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"value": Parameter
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"description":"temperature",
"datainfo":{"type":"double","unit":"K"},
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"meaning":
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"key": "sample temperature",
"link": "http://purl.allotrope.org/ontologies/result#AFR_000214
"function": "temperature_regulation",
"importance": 20,
"belongs_to": "sample"
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Structure:
name: (optional) NX_CHAR
Descriptive name of sample
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Sample temperature. This could be a scanne
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▸ Array of logged value, such as temperature. If this is ...

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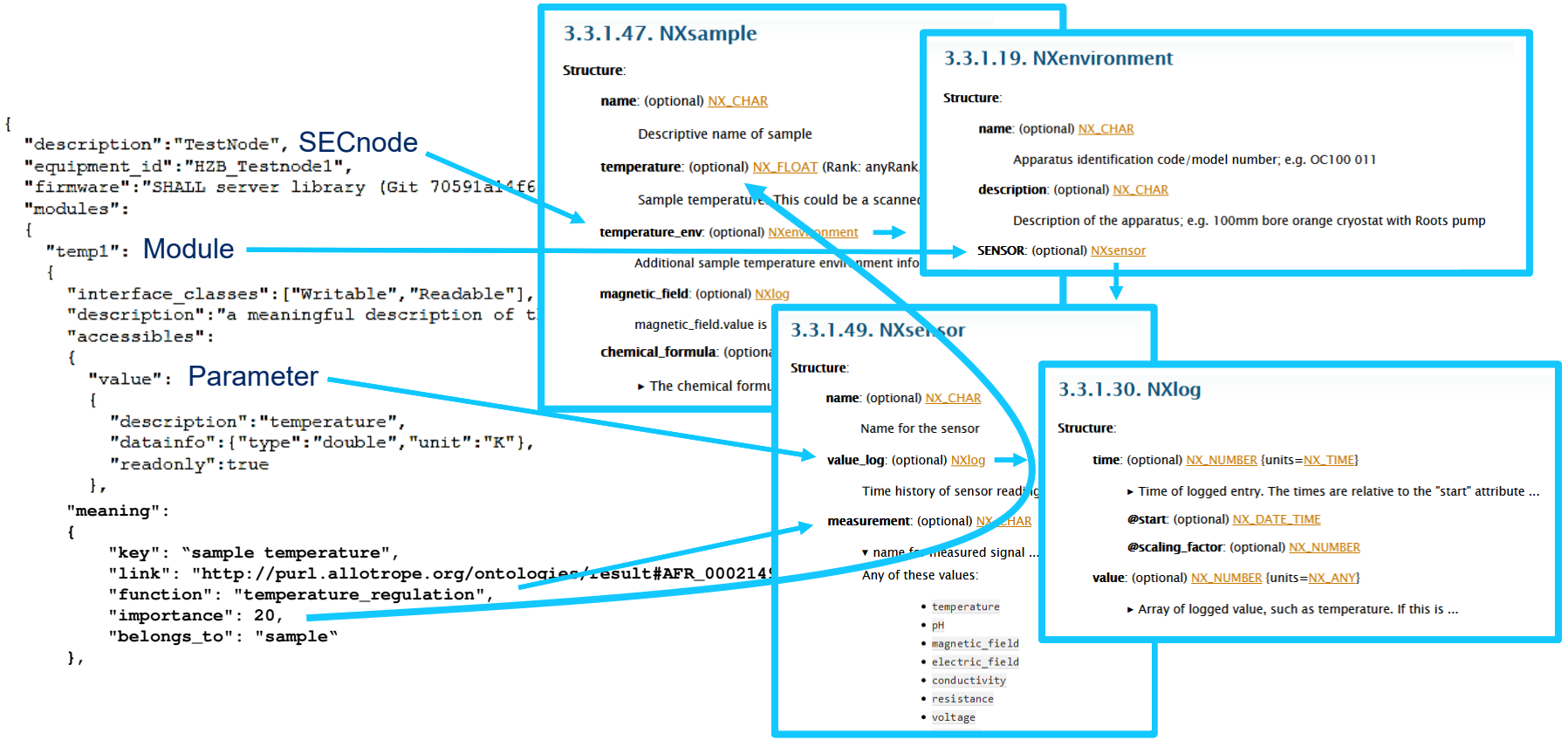
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"description":"temperature",
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"readonly":true
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"meaning":
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"function": "temperature_regulation",
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Apparatus identification code/model number; e.g. OC100 011
description: (optional) NX_CHAR
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Name for the sensor
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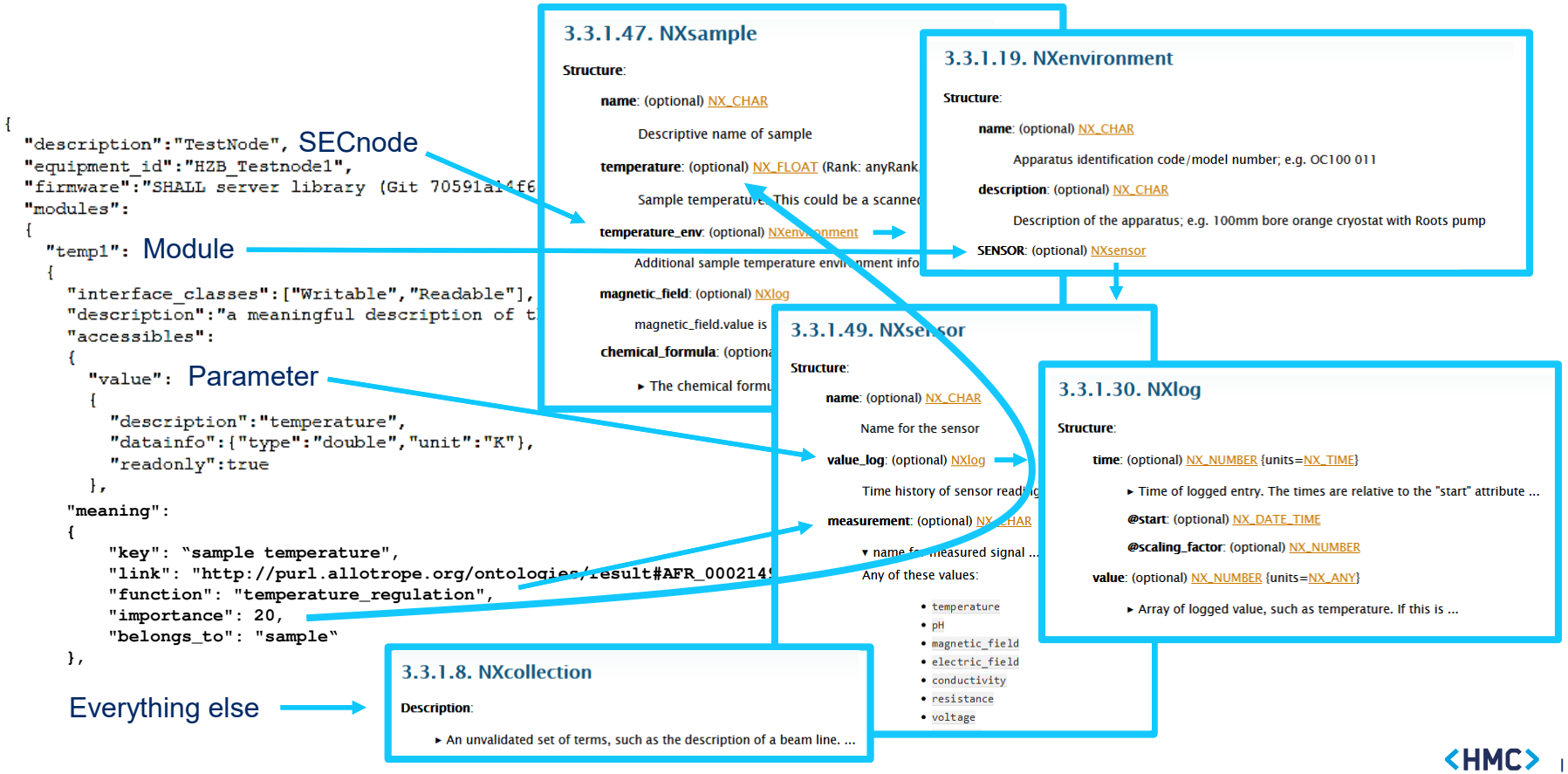
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"description":"temperature",
"datainfo":{"type":"double","unit":"K"},
"readonly":true
},
"meaning":
{
"key": "sample temperature",
"link": "http://purl.allotrope.org/ontologies/result#AFR_000214
"function": "temperature_regulation",
"importance": 20,
"belongs_to": "sample"
},
Everything else
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Descriptive name of sample
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Sample temperature. This could be a scanne
temperature_env: (optional) NXenvironment
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magnetic_field.value is
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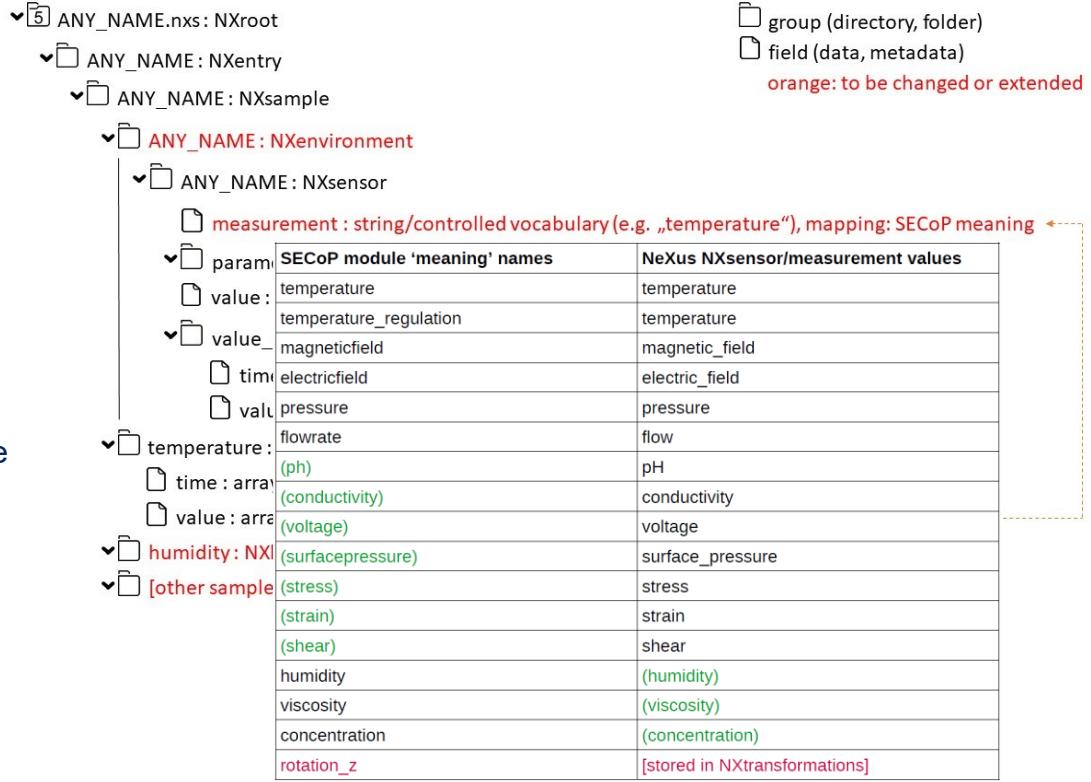
Structure:
name: (optional) NX_CHAR
Apparatus identification code/model number; e.g. OC100 011
description: (optional) NX_CHAR
Description of the apparatus; e.g. 100mm bore orange cryostat with Roots pump
SENSOR: (optional) NXsensor
3.3.1.49. NXsensor
Structure:
name: (optional) NX_CHAR
Name for the sensor
value_log: (optional) NXlog
Time history of sensor readi
measurement: (optional) NX_CHAR
▾ name for measured signal ...
Any of these values:
temperature
pH
magnetic_field
electric_field
conductivity
resistance
voltage
3.3.1.30. NXlog
Structure:
time: (optional) NX_NUMBER {units=NX_TIME}
▸ Time of logged entry. The times are relative to the "start" attribute ...
@start: (optional) NX_DATE_TIME
@scaling_factor: (optional) NX_NUMBER
value: (optional) NX_NUMBER {units=NX_ANY}
▸ Array of logged value, such as temperature. If this is ...
3.3.1.8. NXcollection
Description:
▸ An unvalidated set of terms, such as the description of a beam line. ...

SECoP ⇨ NeXus

Required modifications:

- Extension of ‚measurement' field ('humidity', 'viscosity', and 'concentration')
- Add corresponding fields to NXsample
- Adding ‚NXenvironments' according to ‚measurement' fields (currently only temperature_env and magnetic_field_env are allowed)
- Allow any ‚NXenvironment' (ANY_NAME : NXenvironment)



SECoP module 'meaning' names	NeXus NXsensor/measurement values
temperature	temperature
temperature_regulation	temperature
magneticfield	magnetic_field
electricfield	electric_field
pressure	pressure
flowrate	flow
(ph)	pH
(conductivity)	conductivity
(voltage)	voltage
(surfacepressure)	surface_pressure
(stress)	stress
(strain)	strain
(shear)	shear
humidity	(humidity)
viscosity	(viscosity)
concentration	(concentration)
rotation_z	[stored in NXtransformations]

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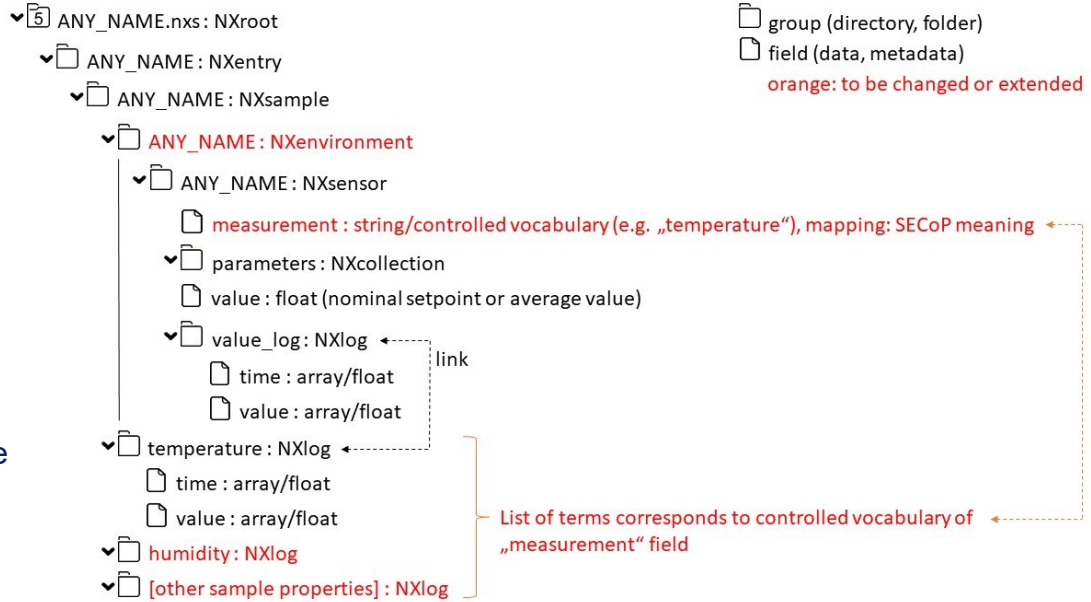
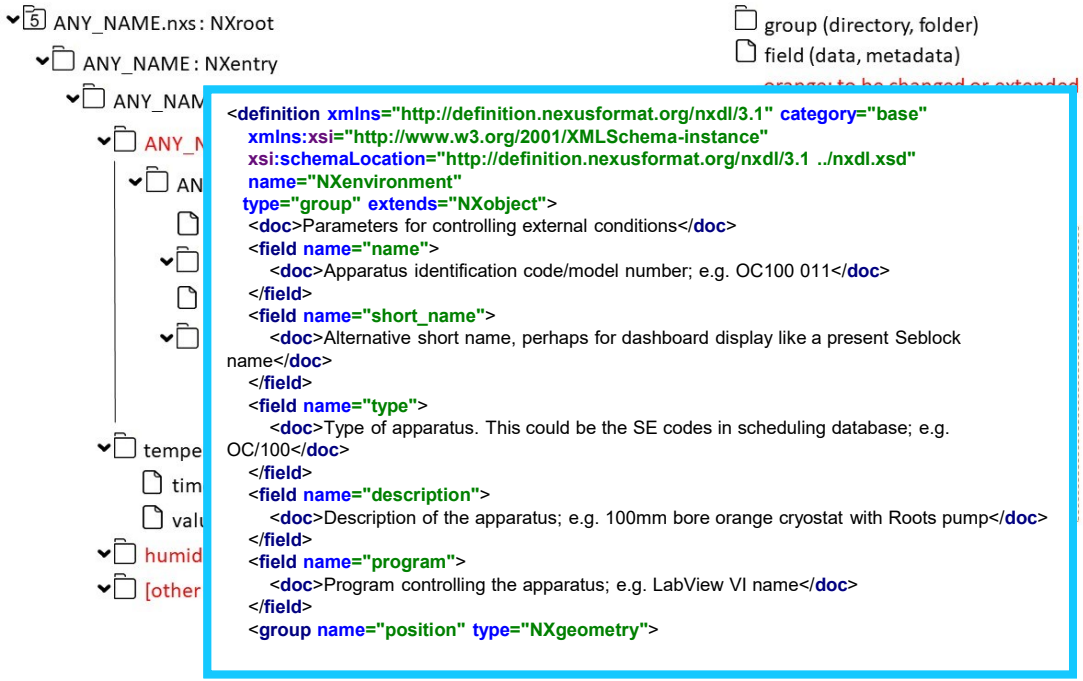


SECoP ⇨ NeXus: Implementation

How to implement changes?

1. Extension of NeXus standard:
   - NXDL description of changes
   - Proposal to NIAC through representatives
2. Meanwhile:
   - Make modified NXDL available via PID (e.g. at Zenodo)
   - Refer from NeXus field ‚definition_local‘ to modified NXDL



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SECoP: Meaning

Each module defines what it does:

"meaning": {

"key": “sample temperature",

"link": "http://purl.allotrope.org/ontologies/result#AFR_0002149 ",

"function": "temperature_regulation",

"importance": 20,

"belongs_to": "sample" }