Developing a New Web Service for Experimental Nuclear Reaction Database (EXFOR) Using RESTful API and JSON Schema

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Scientific database needs

- Toward machine learning-enhanced high-throughput scientific experimentation/developments in chemistry, physics, biology.. etc
  - **Automation**: more automatic, processable, and analysable
  - **Innovation**: materials, drug, chemical substance discovery
  - **Prediction**: predict properties without experiments

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**Automation**

- Fundamental science
- Experiments
- Metadata

**Data**

**Prediction Innovation**

**Modeling**

- Theoretical predictions
- Phenomenological modeling
- Data evaluations

**Discovery**
Experimental databases in various fields

- **High Throughput Experimental Materials Database**
  [https://htem.nrel.gov/](https://htem.nrel.gov/)

- **Cambridge Crystallographic Data Centre**
  [https://www.ccdc.cam.ac.uk/](https://www.ccdc.cam.ac.uk/)

- **Protein Data Bank**
  [https://www.rcsb.org/](https://www.rcsb.org/)

- **High-Energy Physics data**
  [https://www.hepdata.net/](https://www.hepdata.net/)

- **Experimental Nuclear Reaction Database (EXFOR)**
  [https://nds.iaea.org/exfor/](https://nds.iaea.org/exfor/)
EXFOR is compiled by the international collaboration (NRDC)

1. Compile EXFOR data from publications by 13 datacentres worldwide
2. Data check done by NRDC
3. Store (create, update, or delete entries) into the IAEA system
4. Provide interface to end users via https://nds.iaea.org/exfor/
   - X4pro package, C4 or C5 (tabulated) format data for expert users

More diverse users’ requirements to manipulate data in their way
- To compare and plot with model calculation or new measured experimental data,
- To analyze data for the development of a phenomenological model,
- To use data for ML/AI applications ...and so on

S. Okumura/IAEA-NDS @ 16th Varenna Conference on Nuclear Reaction Mechanisms
EXFOR: EXchange FORmat with punch-card legacy

- EXFOR is the document-oriented database in text files
- It is difficult to use directly with plotting software such as Gnuplot
- Many jargons that the users cannot understand

<table>
<thead>
<tr>
<th>ENTRY</th>
<th>13388</th>
<th>891220</th>
<th>20050926</th>
<th>0000</th>
</tr>
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<tbody>
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<td>SUBENT</td>
<td>13388001</td>
<td>891220</td>
<td></td>
<td>0000</td>
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</tbody>
</table>

**BIB**

- INSTITUTE (1USALAS)
- REFERENCE (J,PR,99,730,)
- AUTHOR (A.C.WAHL)
- TITLE FISSION OF U-235 BY 14-MEV NEUTRONS: NUCLEAR CHARGE DISTRIBUTIONS AND YIELD RESULTS
- METHOD (RCHEM)
- DETECTOR (PROPC)
- ERR-ANALYS (DATA-ERR) STANDARD DEVIATION OF THE AVERAGE OF THE RESULTS
- STATUS (RIDER)
- HISTORY (891212C) VM

<table>
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<tr>
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<td>14</td>
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**SUBENTRY: 001**

- REACTION (92-U-235(N,F)ELEM/MASS,IND,FY)
- FACILITY (CCW)
- INC-SOURCE (D-T)
- MONITOR ((MONIT1)92-U-235(N,F)ELEM/MASS,CUM,FY,,SPA)
- (MONIT2)92-U-235(N,F)ELEM/MASS,CUM,FY,,SPA)
- (MONIT3)92-U-235(N,F)ELEM/MASS,CUM,FY,,SPA)
- DECAY-DATA ((1.)53-I-131,8.07D,B-)
- ((2.)53-I-132,2.3HR,B-)  
- ((3.)53-I-133,20.9HR,B-)  
- ((4.)53-I-134,52.5MIN,B-)  
- ((5.)53-I-135,6.7HR,B-)  
- STATUS (DEP,13388002)

<table>
<thead>
<tr>
<th>ENDSUBENT</th>
<th>12</th>
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</thead>
</table>

**COMMON**

- EN EN-NRM MONIT1 MONIT2
- MEV EV PC/FIS PC/FIS
- 14. 0.0253 5.17 6.14

<table>
<thead>
<tr>
<th>ENDCOMMON</th>
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</thead>
</table>

**DATA**

- MASS ELEMENT DATA MONIT3 DECAY-FLAG
- NO-DIM NO-DIM PC/FIS PC/FIS NO-DIM
- 131. 53. 4.47 3.02 1
- 132. 53. 5.03 4.49
- 133. 53. 5.36 6.62
- 134. 53. 5.20 8.00 4
- 135. 53. 4.35 6.31 5

<table>
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<th>ENDDATA</th>
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</table>
Format is the big barrier for newcomers

- Understanding formats (ENDF, ENSDF, and EXFOR) is the first barrier to work in the nuclear data field.

Modern AI/ML tools, including the development and use of Natural Language Processing (NLP) could shorten the time needed for an EXFOR compilation to be completed by automatically processing tables, graphs, and relevant in-text context. The incorporation of these tools, however, will require new skills not currently present in the EXFOR network. **Outdated formats** and compilation rules have also substantially hindered the progress of such modern mechanisms. This has motivated the creation of NEA SG-50, which is working to provide a modern interface to EXFOR as well as a framework for providing corrections, both simple error fixes and more complex ones discovered by evaluators in the course of their work.


Being a specialist ≠ Format understandings
Large scale use cases of EXFOR outside NRDC community

<table>
<thead>
<tr>
<th>Name</th>
<th>Author</th>
<th>Purpose</th>
<th>Language</th>
<th>Data source</th>
<th>Source code/data</th>
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</thead>
<tbody>
<tr>
<td>EXPORTABLES</td>
<td>Arjan Koning</td>
<td>Developing TENDL using experimental data from EXFOR, also used in <a href="https://nds.iaea.org/dataexplorer/">https://nds.iaea.org/dataexplorer/</a></td>
<td>Fortran</td>
<td>C4, C5</td>
<td><a href="https://nds.iaea.org/talys/">https://nds.iaea.org/talys/</a></td>
</tr>
<tr>
<td>EXFOR SQL and NucML</td>
<td>Pedro Jr. Vicente-Valdez</td>
<td>Modernizing the EXFOR Database using Google BigQuery and Python Pipeline for ML-based Nuclear Data Solutions</td>
<td>Python</td>
<td>C4</td>
<td><a href="https://pedrojrv.github.io/projects.html">https://pedrojrv.github.io/projects.html</a></td>
</tr>
<tr>
<td>x4i</td>
<td>David Brown</td>
<td>Parsing EXFOR: For the US evaluation (forked version: x4i3 by Anatoli Fedynitch)</td>
<td>Python</td>
<td>EXFOR master file</td>
<td><a href="https://github.com/brown170/x4i">https://github.com/brown170/x4i</a></td>
</tr>
<tr>
<td>Visualization of nuclear data used in PHITS</td>
<td>Naoya Furutachi</td>
<td>Visualization of nuclear data with ACE format loaded in PHITS Test of a tool to convert EXFOR to PHITS “Frag data” format</td>
<td>Fortran</td>
<td>EXFOR master file</td>
<td><a href="https://conference-indico.kek.jp/event/136/contributions/3032/attachments/2064/2549/P23_Furutachi.pdf">https://conference-indico.kek.jp/event/136/contributions/3032/attachments/2064/2549/P23_Furutachi.pdf</a></td>
</tr>
<tr>
<td>EXFOR_Parser</td>
<td>Shin Okumura</td>
<td>Parsing EXFOR: Convert EXFOR to JSON, tabulated format for the visualization</td>
<td>Python</td>
<td>EXFOR master file</td>
<td><a href="https://github.com/shinokumura/exforparser">https://github.com/shinokumura/exforparser</a></td>
</tr>
</tbody>
</table>

+ more local evaluation systems must exist, and data curation
Development of [https://nds.iaea.org/dataexplorer/](https://nds.iaea.org/dataexplorer/)

- We developed “dataexplorer” in 2021 based on:
  - EXFORTABLES is a directory-structured database from C5 format
  - ENDFTABLES is a pre processed and directory-structured database

* A. Koning, [iaea-nds-0235](https://nds.iaea.org/talys), EXFORTABLES-1.0: An experimental nuclear reaction database based on EXFOR [https://nds.iaea.org/talys/](https://nds.iaea.org/talys/)

** Accessible at [https://nds.iaea.org/dataexplorer/](https://nds.iaea.org/dataexplorer/)

- Increase of access, but the data cannot be updated so frequently (irregularly)
- Need a processing of C4/C5 (by V. Zerkin) and EXFORTABLES production (by A. Koning)

⇒ Require better data pipeline to show latest EXFOR data
Experimental data and FAIR Principles[1]

Research data integrity is crucial because it ensures the transparency and trustworthiness of scientific data. Therefore,

Data should be...

- Findable
- Accessible
- Interoperable
- Reusable

- Easy to find by both human and computer with machine-readable metadata
- Retrievable by the persistent identifier (e.g. DOI)
- Easy to work from different applications, workflows, storage, or processing
- Well-described, self-explanatory

Towards FAIR for EXFOR data

**Findable:** Unified metadata, Query-able by SQL/ORM, graphical frontend

**Accessible:** RESTful API, DOI assignment

**Interoperable:** Open-sourced, transparent data pipeline

**Reusable:** Conversion of EXFOR to JSON, helper for EXFOR jargons, clear JSON schema

Primitives of EXFOR: all remain same
- EXFOR (as a format), EXFOR dictionary
- Compilation
- Data retrieval system (https://nds.iaea.org/exfor)
- Compiled data

Data model
- parsing EXFOR
- json conversion & reversion
- automation (pipeline)

RESTful API, database, data store
- data access APIs
- data management (Licence, DOI)
- data store (text, noSQL, SQL, Git repository)

UX Improvements
- Improvements of UI and API
EXFOR Parser

• A new python program to convert EXFOR text into JSON
  • Python3.x (https://github.com/shinokumura/exforparser)
  • Inspired by “x4i” by David Brown (NNDC, BNL)
  • Convert 25,000 entries into JSON in 30-40 min

• Features
  • EXFOR to JSON
    • Simplify JSON schema
    • Parse blocks (BIB, COMMON, DATA)
    • Parse identifiers (TITLE, AUTHOR, REACTION, METHOD, ERR-ANALYS..etc)
    • Separate EXFOR-code and freetext
    • Separate subentries based on POINTERs
  • Outputs
    1. Pure (best effort) conversion from EXFOR to JSON (noSQL)
    2. Bib info, reaction index, and tabulated data in SQL db
Related repositories

- [https://github.com/IAEA-NDS/exfor_master](https://github.com/IAEA-NDS/exfor_master)
  - Preservation of historical 24,630 EXFOR entries (= 24,630 files)
  - Recovered from more than 430 backup zip files stored in NDS since 2005
  - All updates are merged into main branch
  - Retroactive to any timestamp (commits)

- [https://github.com/IAEA-NDS/exfor_dictionary](https://github.com/IAEA-NDS/exfor_dictionary)
  - Best-effort conversion of EXFOR dictionary to JSON format

- [https://github.com/IAEA-NDS/exfor_json](https://github.com/IAEA-NDS/exfor_json)
  - All entries in JSON format converted by EXFOR_parser
  - (JSON schema is not yet fixed and may will be changed)

- [https://github.com/shinokumura/exfortables_py](https://github.com/shinokumura/exfortables_py)
  - Tabulated data files of datasets from EXFOR entry to the tabulated data like EXFORTABLES* produced by the EXFOR Parser
  - To allow user to download the data file

- [https://github.com/shinokumura/ripl3_json](https://github.com/shinokumura/ripl3_json)
  - Convert RIPL3 into JSON
  - Currently, only discrete level and mass tables

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* A. Koning, iaea-nds-0235, EXFORTABLES-1.0: An experimental nuclear reaction database based on EXFOR
Data pipeline summary

**Experiments**
- **exfor_master**
  - [https://github.com/IAEA-NDS/exfor_master](https://github.com/IAEA-NDS/exfor_master)
  - /exforall/100/100001.x4

- **exfor_json**
  - /json/100/10001.json
  - noSQL

- **exfor_parser**
  - Conversion scripts

- **exfor_dictionary_parser**
  - Conversion scripts

- **ripl3_levels_parser**
  - Conversion scripts

**Database Compilation**
- **exfortables_py**
  - /exfortables/n/Ag107/n,p/xxxx.dat

- **exfortables_py_sql**
  - SQLite database

**Data Evaluation**
- **exfor_dictionary_json**
  - /json/trans.9127.json
  - noSQL

- **ripl3_levels_json**
  - /json/levels/Ag/107Ag.json
  - noSQL

**Processing Validation**
- **dataexplorer_api**
  - [https://nds.iaea.org/dataexplorer/api](https://nds.iaea.org/dataexplorer/api)
  - Flask and Python RESTful API

**Use**
- **dataexplorer**
  - [https://nds.iaea.org/dataexplorer/](https://nds.iaea.org/dataexplorer/)
  - Dash/Plotly modules

**Parser**
- **Parser**
- **Data store**
- **Frontend**
https://github.com/IAEA-NDS/exfor_master

- Clone/download all EXFOR files anytime
  
  
  \[
  \text{git clone https://github.com/IAEA-NDS/exfor_master}
  \]

- Easy access to change logs of entry using Git command
  
  \[
  \text{git log -p exforall/224/22449.x4}
  \]

```bash
commit 0dda483cd04058da0c0dbc4b72a7b07a42c7f56 (tag: Backup-2006-06-16)
Author: shinkoo <s.okumura@iaea.org>
Date:   Sun Oct 2 00:07:10 2022 +0200

  2006-06-16

diff --git a/exforall/224/22449.x4 b/exforall/224/22449.x4
index fbc87f440..a0f5895b7 100644
--- a/exforall/224/22449.x4
+++ b/exforall/224/22449.x4
@@ -1,5 +1,5 @@

 ENTRY  22449  20000202  20010329
-SUBENT  22449001  20000202  20010329
+SUBENT  22449001  20000202  20010329  20050926   0000

 BIB  15  38

 TITLE .The Stellar (N,GAMMA) Cross Section of the Stable Iridium Isotopes
@@ -46,7 +46,7 @@ KEV  NO-DIM  NO-DIM  NO-DIM
     30.  15.7  3.67  12.2
 ENDCOMMON  3
 ENDSUBENT  45
-SUBENT  22449002  20000202  20010329
```

```json
{
  "entry": "22449",
  "last_updated": "2006-07-20",
  "number_of_revisions": "3",
  "histories": [
    {
      "x4_code": "(20000202C)",
      "free_text": [
        "Compiled by S.M."
      ],
    },
    {
      "x4_code": "(20000202U)",
      "free_text": [
        "Last checking has been done."
      ],
    }
  ],
}
```
• Separate information by pointer
• Separate EXFOR Keyword from free text

FACILITY (REAC,2UK HAR) Harwell pile at Atomic Energy Research Establishment.

• Parse folded DATA block

<table>
<thead>
<tr>
<th>EN</th>
<th>EN-RSL</th>
<th>DATA</th>
<th>ERR-T</th>
<th>ERR-S</th>
<th>ERR-1</th>
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<tbody>
<tr>
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<td>ERR-3</td>
<td>ERR-4</td>
<td>ERR-5</td>
<td>ERR-6</td>
<td>ERR-9</td>
</tr>
<tr>
<td>MEV</td>
<td>MEV</td>
<td>MB</td>
<td>PER-CENT</td>
<td>PER-CENT</td>
<td>PER-CENT</td>
</tr>
<tr>
<td>PER-CENT</td>
<td>PER-CENT</td>
<td>PER-CENT</td>
<td>PER-CENT</td>
<td>PER-CENT</td>
<td>PER-CENT</td>
</tr>
<tr>
<td>1.00E-6</td>
<td>4.2E-9</td>
<td>6.38E+5</td>
<td>4.17</td>
<td>0.19</td>
<td>0.48</td>
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<tr>
<td>3.81</td>
<td>0.42</td>
<td>0.02</td>
<td>0.06</td>
<td>0.00</td>
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<tr>
<td>0.27</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.26E-6</td>
<td>5.4E-9</td>
<td>5.37E+5</td>
<td>2.62</td>
<td>0.26</td>
<td>2.03</td>
</tr>
<tr>
<td>0.05</td>
<td>0.43</td>
<td>0.03</td>
<td>0.10</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>0.32</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
EXFOR dictionary in JSON with EXFOR keywords as a JSON key
- Easy to lookup programmatically from JSON friendly computer languages
- Convert abbreviations
  - e.g. "abs." could be "Absolute", "Absorption" does "f." mean fragment, factor, fission, for or final?
- Produce-able without C4/C5
- Best effort to get smallest "dataset" of physical observable and tabulate them

n/Fe-56/n-inl-L1/xs/Fe-56_n-inl-L1_Fe56_Aimen-Ramstrom-20788-008-0-1975.txt

<table>
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<tr>
<th>#</th>
<th>E_in(MeV)</th>
<th>dE_in(MeV)</th>
<th>XS(B)</th>
<th>dXS(B)</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.00000E+00</td>
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<td>1.26000E-01</td>
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<tr>
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<td>1.23000E-01</td>
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</tr>
<tr>
<td>3.29000E+00</td>
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<td>6.12000E-01</td>
<td>9.20000E-02</td>
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<tr>
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<td>5.54000E-01</td>
<td>8.30000E-02</td>
<td></td>
</tr>
<tr>
<td>3.78000E+00</td>
<td>0.00000E+00</td>
<td>4.82000E-01</td>
<td>7.20000E-02</td>
<td></td>
</tr>
<tr>
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<td>0.00000E+00</td>
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<tr>
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<td>3.52000E-01</td>
<td>5.30000E-02</td>
<td></td>
</tr>
<tr>
<td>4.50000E+00</td>
<td>0.00000E+00</td>
<td>3.16000E-01</td>
<td>4.70000E-02</td>
<td></td>
</tr>
</tbody>
</table>
RESTful API

- An architectural style for an application program interface (API) that uses HTTP requests to access and use data - Addressability, Stateless, Uniform Interface
  - **EXFOR entry**: entry, subentry, bib, data, experimental condition, reactions
  - **EXFOR dictionary**: facilities, institutes, methods, detectors
  - **RIPL-3 discrete level**: levels, level records

- API documentation is available

  /dataexplorer/api/exfor/entry/22449

  /dataexplorer/api/ripl3/levels/90Zr
Decay data
"55-Cs-141-00": {
  "Z": "55",
  "ELM": "Cs",
  "MASS": "141",
  "LIS": "00",
  "HL": "2.4910000E+01",
  "LAMBDA": 0.027826,
  "En_beta": "1.5473620E+06",
  "En_gamm": "1.7248140E+06",
  "En_alpha": "7.5359650E+01",
  "DecayInfo": {
    "0": {
      "RTYP": "1.0000000E+00",
      "RFS": "0.0000000E+00",
      "Q": "5.2560000E+06",
      "BR": "9.9965800E-01",
      "DAUGHTER": "56-Ba-141-00"
    },
    "1": {
      "RTYP": "1.5000000E+00",
      "RFS": "0.0000000E+00",
      "Q": "7.2100000E+05",
      "BR": "3.4200000E-04",
      "DAUGHTER": "56-Ba-140-00"
    }
  },
  "daughters": [
    "56-Ba-141-00",
    "56-Ba-140-00"
  ]
},

Decay chain (linearized)
"55-Cs-141-00": {
  "1": {
    "chain": ["56-Ba-141-00", "57-La-141-00", "58-Ce-141-00", "59-Pr-141-00"],
    "branching": [0.999658, 1.0, 1.0, 1.0],
    "rtyp": [1.0, 1.0, 1.0, 1.0],
    "lmbds": [0.027826, 0.0063232, 4.9118e-05, 2.4676e-07, 6.9315e-51],
    "en_betas": ["1.5473620E+06", "9.6628250E+05", "9.8713460E+05", "1.9438810E+05", 0.0],
    "en_gamms": ["1.7248140E+06", "9.0968270E+05", "2.6780420E+04", "7.6901970E+04", 0.0],
  },
  "2": {
    "chain": ["56-Ba-140-00", "57-La-140-00", "58-Ce-140-00"],
  }
},

Decay chain (network diagram plot)
"141Cs"
24.91 sec
99.97% β-
0.03% β + n
"141Ba"
18.27 m
100.00% β-
"141La"
9.80 h
100.00% β-
"141Ce"
32.51 d
100.00% β-
"141Pr"
Long
Renewed interface of https://nds.iaea.org/dataexplorer/

Data plots for:
- Cross Section (XS)
- Residual Production XS
- Fission Yield (FY)
- Angular Distribution (DA)
- Energy Distribution (DE)
- Fission Observables - PFNS, PFGS, $\bar{\nu}$
New UX for EXFOR entry viewer based on API

IAEA Nuclear Data Explorer

Experimental Nuclear Reaction Data (EXFOR) is compiled by the International Network of Nuclear Reaction Data Centres (NRDCC) under the auspices of the International Atomic Energy Agency.

Number of entry: 2448, Number of dataset: 123456

Entry number: 40412: Last updated on 2020-05-15 (Rev. 7) Compilation history EXFOR Git JSON

Title: Measurement of alpha and the 235U and 239Pu fission and capture cross sections for 10-80 keV neutrons


Institute: (RUSFIE)


Reactions: 40412-004-0: (92-U-235(N,G)92-U-236,,SIG,,AV)

History from git log History from (HISTORY)

Bibliographic info

Reactions

EXPERIMENTAL CONDITIONS

CORRECTION

Correction for isotopic impurities, correction for neutron multiplication in the samples, correction for energy dependence nu-bar, correction for multiple neutron scattering and resonance self-shielding.

DETECTOR

Scintillator tank (STANK)

Large (400 cm³) liquid scintillation detector loaded with cadmium

FAGILITY

VDG, 4RUSFIE

Fast ionization chamber with Cf-252. NaI(Tl) Crystal of 150x80 mm size detector.

INC-SOURCE

P-Li7

FEI pulsed Van-de-Graaff accelerator.

METHOD

TOF

Pulse duration 22ns, frequency 300 kHz.

Proton-Lithium-7

Metal lithium targets were used

Proton-tritium, standard tritium-titanium targets were used

Time-of-flight method with resolution 18 nsec/m for neutron energy range from 10 keV to 80 keV. And energy resolution from 10 keV to 30 keV. For neutron energy range from 100 keV to 1 MeV at working on monoenergetic neutrons.

Flight path 1.18 m. (GAMMA-400)

Tooltip from dictionary

Separate code and freetext
If the PRODUCT (SF4) in REACTION is either of MASS, ELEM, or ELEM/MASS, one cannot know real products until reading DATA block.

(89-AC-227(N,F)ELEM/MASS,CUM,FY,,REL/FIS)
New UX to search EXFOR entry

• Search by the reaction or EXFOR subfields
And more...

- **Search by EXFOR taxonomy**

  EXFOR Taxonomy

  - RP
  - SIG: Cross section
  - ARE: Resonance-area
  - D
  - EN: Resonance-energy
  - J: Spin J
  - WID: Resonance width
  - DA: Differential with angle of outgoing particle
  - Others
  - DE: Differential with energy of outgoing particle
  - FY: Fission-product yield
  - KE: Kinetic energy
  - NU: Fission-neutron yield, nu-bar
  - TTY: Thick-target yield of the specified reaction product.
  - DDX
  - EN: Resonance-energy

- **Search by geography**

  Nuclear Reaction Experimental Facilities (From EXFOR BIB)

  - main Facility country=United States of America
count=36
  - lat=35.9311
  - lng=-84.30998
  - name=Oak Ridge National Laboratory, Oak Ridge, TN
  - main Facility institute=1USAORL
  - main Facility type=Cyclotron
Summary

• We are working towards FIAR principle on EXFOR

• Open source/data on GitHub
  • EXFOR Parser: main EXFOR parsing program in Python
  • exfor_master: backup of EXFOR master files
  • exfor_json: JSON converted EXFOR files
  • exfor_dict: JSON converted EXFOR dictionary
  • exfortables_py: tabulated (X-Y table) reaction data

• Future work
  • Deployment, internal test, and security scan toward the production release (w/L. Marian)
  • Automatic update of data pipeline
  • Develop clear JSON schema (w/G. Schnabel)
  • Implementation of FAIR principles for EXFOR and other data stored in IAEA/NDS
    • Findable, Accessible
      • DOI assignment
      • License assignment (CC0/CC BY 4.0) is important
    • Interoperable, Reusable
      • Move on to a research repository
Thank you!