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Processing trails: beyond n-transport only

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Exploring the fusion fuel landscape –
Nuclear data for materials science, component engineering

Preliminary comments

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Nuclear observables, data forms for digital twin needed by **engineer, practitioner** are not always similar, equivalent to the one **evaluated by evaluator**

Processed forms **useful for application(s)** are not **anymore** ENDF-102, ENDF-6 format forms compliant, **similar maybe, derived certainly**

It is subtle to **differentiate** between: **format, formalism, nuclear data forms**

Processed nuclear data forms are **numerous, rich, abundant, diverse**. Some are observable other not; all have a specific importance for at least one application

Processing enhances, enriches, deepens the evaluated nuclear data forms

Lexical semantics

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- **H**ybrid **END** File
- **P**ointwise **END F**ile
- **G**roupwise **END F**ile
- **ANISO**tropy
- **A C**ompact **E**ndf
- **P**robability **T**ables
- PDF and CDF
- …

Nuclear data forms

Formalisms

- **M**ulti-**L**evel-**B**reit-**W**igner, **R**eich-**M**oore, **R**-**M**atrix **L**imited, Legendre, Blatt and Biedenharn, Kalbach-Mann, Froehner, Watt,..

Lexical semantics

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Pre-processing steps: convert the ENDF-6 nuclear data into **simple forms** that can be interpreted

Processing steps: processes the ENDF-6 nuclear data into **complex forms** useful for applications: **particles transport, reactor analysis codes, inventory, source terms, etc.**

Post-processing steps: verify either of the above steps

The **lexical is ancient**, as the ‘tape’ the above usually modular and sequential steps I/O uses. It belongs to the dawn of the computer age, does sound a bit odd now a day, however it does works – just about

if it ain't broke, don't fix it

Processing codes & steps & practices

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ENDF file

- **NJOY-2016.78**
  - reconr
  - broadr
  - unresr
  - **thermr**
  - **heatr**
  - **gaspr**
  - **mixr**
  - **purr**
  - **acer**
  - **groupr**

PENDF file

ACE file

cross-check

- **PREPRO-2023**
  - linear
  - recent
  - sigma1
  - **legend**
  - **sixpack**
  - **spectra**
  - **activate**
  - **merger**
  - **fixup**
  - **dictin**

cross-check

- **CALENDF**
- **FRENDY**
- **AMPX**
- **GALILEE**
- **FUDGE**
- **NECP-Atlas**
- **NDEX**
- **…**

Single shell script, many steps for an entire library

bold = unique to..

Hybrid file

NJOY Processing scripts

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1 basics & isotopic

```
cat>in$isma[$c1] <<EOF
moder
20 -21/  -- moder check &  mode
reconr
-21 -22
'pendf $isma[$c1] ENDF/B-VIII.1 '/
$isma[$c2]/
.001/
0/
moder
-22 36/  -- pendf OK
broadr
-21 -22 -23
$isma[$c2] 1/
.001/
293.6/
0/
unresr
-21 -23 -24
$isma[$c2] 1 1 0/
293.6/
1.e+10/
0/
moder
-24 32/  -- pendf 293.6K sig-0 & T4XS
heatr
-21 -24 -26 30
$isma[$c2] 7 0 0 1 2/   -- heatr gamma heat local & chk print
302 303 304 318 401 403 407/
heatr
-21 -26 -27 33
$isma[$c2] 6 0 0 1 2/
442 443 444 445 446 447/
gaspr
-21 -27 -29
moder
-29 35/  -- pendf 293.6K & gas mt20x, partials mt30x kermas & mt40x damages
viewr
30 31/  -- viewr energy-balance check
```

bold = comments

```
cat>in$isma[$c1] <<EOF
moder
20 -21/  -- moder check & njoy mode
thermr
0 -22 -23
0 $isma[$c2] 20 1 1 0 0 1 221 0/  -- thermr free gas
293.6 /
0.001 10./
purr
-21 -23 -24
$isma[$c2] 1 1 20 64 /   -- purr sig-0 20 bins 64 ladders
293.6 /
1.e+10/
0 /
-- heatr overwrite with gamma transported
heatr
-21 -24 -25 29
$isma[$c2] 7 0 0 0 2/
302 303 304 318 401 442 443/
heatr
-21 -25 -26 30
$isma[$c2] 4 0 0 0 2/
444 445 446 447/
--
-- 1st acer fast
acer
-21 -26 0 32 33/
1 1 1 0.81 0/
'Ace $isma[$c1] ENDF/B-VIII.1'
$isma[$c2] 293.6/
1 1/
/
```

2 ACE & other

```
--
-- 2nd acer check/plot/correc
acer
0 32 34 35 36/
7 1 1 -1/
'Ace $isma[$c1] ENDF/B-VIII.1 - check 1'/
-- tape35 ACE file, tape36 xsdir
--         pendf for Ace 293.6K &
--         mt152  bondarenko unresolved
--         mt153  probability tables unresolved
--         mt221  free gas thermal scattering
--         mt20x  gaz production
--         mt30x  partials kermas
--         mt40x  partials damages
viewr
30 31/ -- heatr gamma heat nonlocal & chk print
viewr
34 37/ -- acer plots check 1
moder
-26 38/ -- pendf ace
stop
```

Loop over entire libraries

NJOY modules Print options: 0, 1, 2

A **plethora of usually untapped information**, intermediary and final forms, **numerical** and **graphical** outputs: **Verification** processes

broadr, heatr, acer, purr, groupr,….

thermal quantities at **293.6 K = 0.0253 eV**

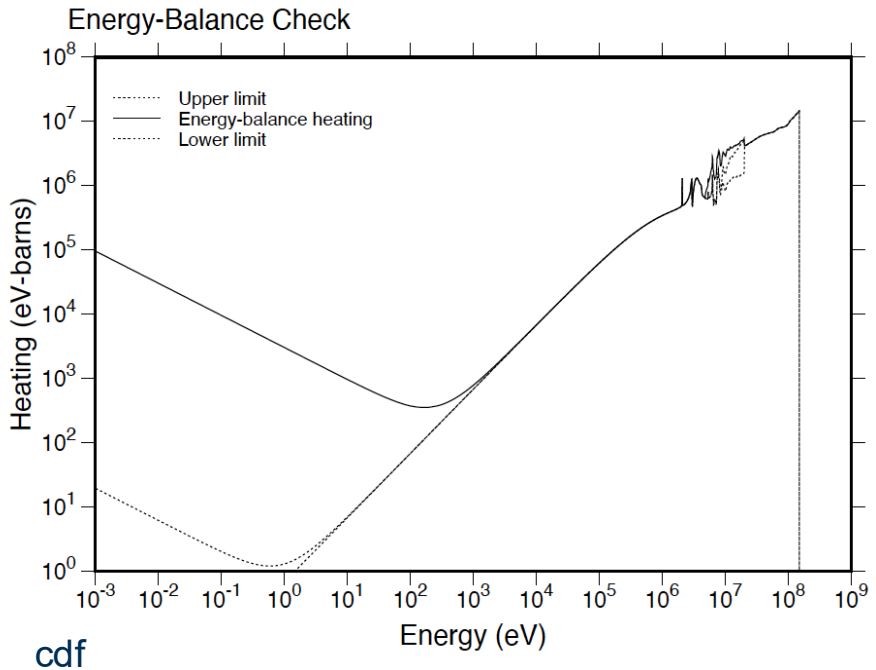
---

thermal capture xsec: 3.8620E-03
thermal capture integral: 3.4230E-03
capture resonance integral: 2.0556E-03

*****

angular distributions for …..
incident particle energy = 2.000000E+00 int = 2 np = 18

cosine	pdf	cdf	**cosine**	pdf	cdf
-1.000000E+00	6.333382E-01	0.000000E+00	-9.210000E-01	5.802944E-01	4.793849E-02
-8.430000E-01	5.368052E-01	9.150538E-02	-7.650000E-01	5.014318E-01	1.319966E-01
-6.870000E-01	4.734805E-01	1.700182E-01	-6.090000E-01	4.522744E-01	2.061226E-01
-5.310000E-01	4.371543E-01	2.408103E-01	-4.520000E-01	4.273886E-01	2.749597E-01
-3.590000E-01	4.221798E-01	3.144646E-01	-2.810000E-01	4.223566E-01	3.474015E-01
-1.870000E-01	4.272212E-01	3.873317E-01	-6.250000E-02	4.399583E-01	4.413136E-01
6.250000E-02	4.580496E-01	4.974392E-01	3.130000E-01	5.026719E-01	6.177696E-01
5.630000E-01	5.472430E-01	7.490090E-01	7.500000E-01	5.738266E-01	8.538290E-01
9.070000E-01	5.884447E-01	9.450673E-01	1.000000E+00	5.929042E-01	1.000000E+00



Look at the output

NJOY output file

Thanks Bob !

Processing script for natural element

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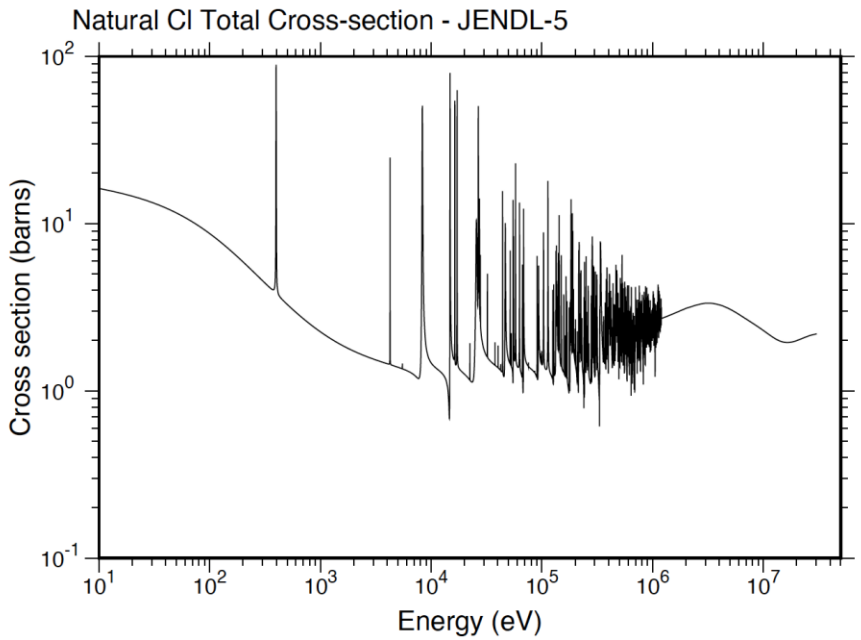
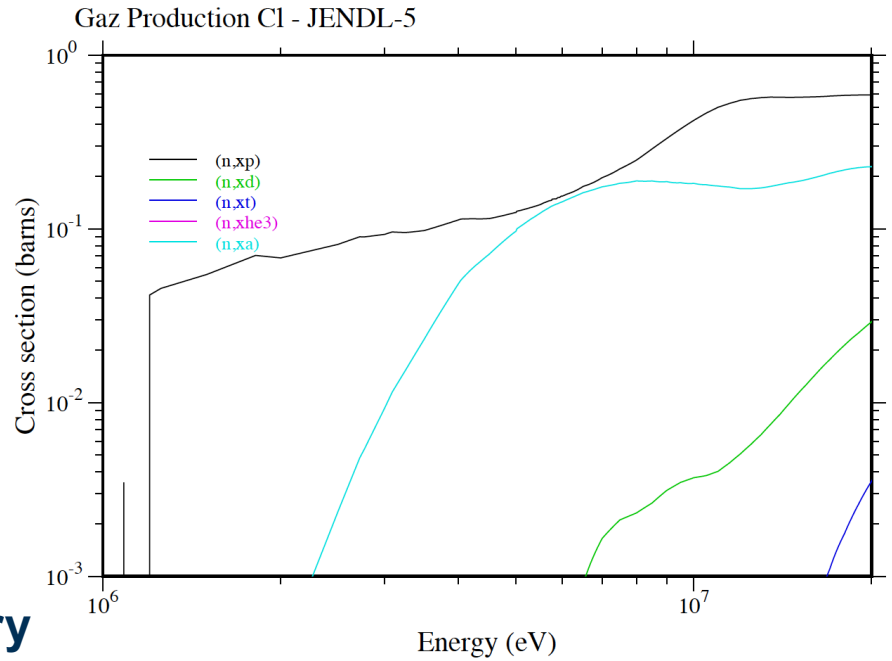
NJOY2016 **mixr & plotr & viewr**

- Any MF=1,3 MT's + derived mts
- DPCS mts= 444 - 447
- KERMA mts= 301- 450
- GAZ production mts= 203 - 205

```
cat>in$zant[$c1] <<EOF
mixr
30 $tx/
1 203 204 205 206 207 301 442 443 444 445 446 447/
$mx/
293.6/
$zant[$c2] $zant[$c5] $zant[$c3]/
' $zant[$c4]-$zant[$c1]-  0   IAEA       TENDL-2025 $zant[$c1] Natural'/
plotr
31/
/
1/
'Natural $zant[$c1] Total Cross-section - TENDL-2025'/
/
4/
1e+1 3.e7/
/
/
/
6 30 $zant[$c2] 3 1 293.6/
0 0 0 0 1/
99/
viewr
31 32
stop
```



Loop over entire library



Format delicacy: ENDF-6 sum rules

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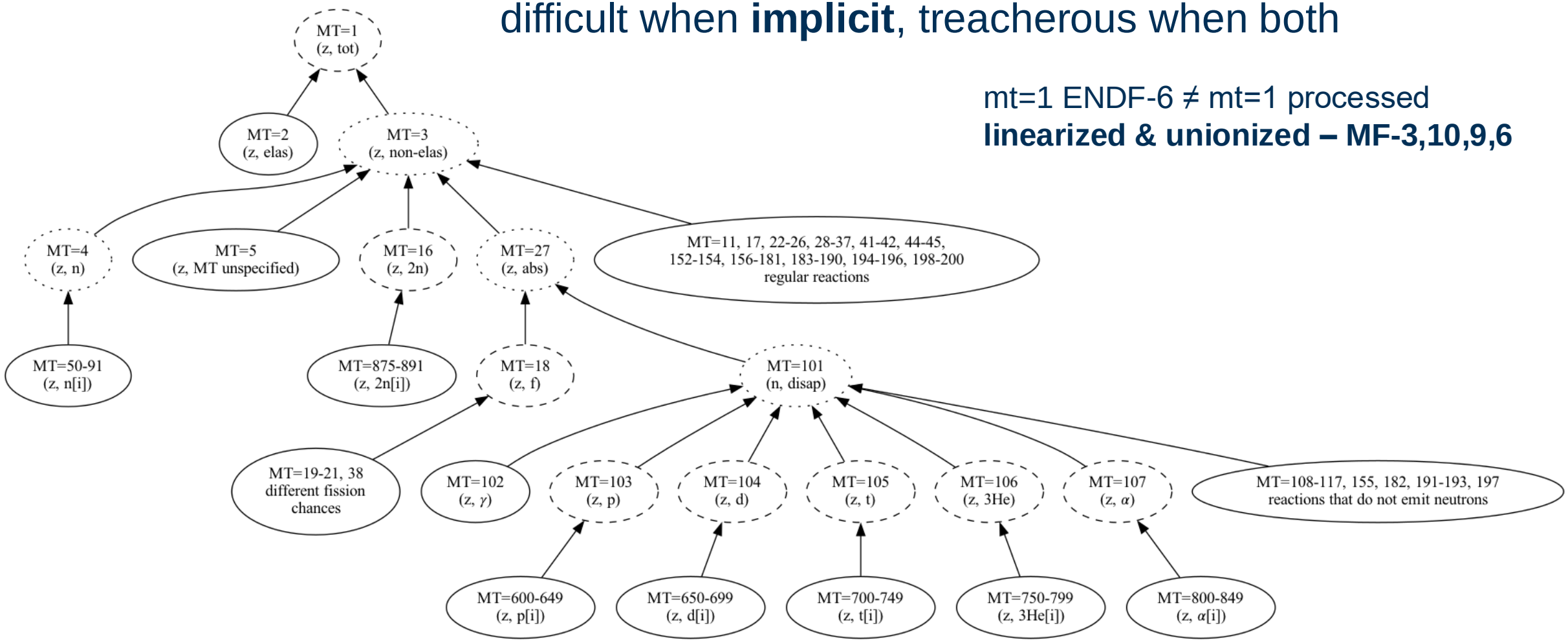
Incomplete when **explicit**, with **grey areas**: TSL, MF-2 open channels, MF-6,…

difficult when **implicit**, treacherous when both

mt=1 ENDF-6 ≠ mt=1 processed
linearized & unionized – MF-3,10,9,6



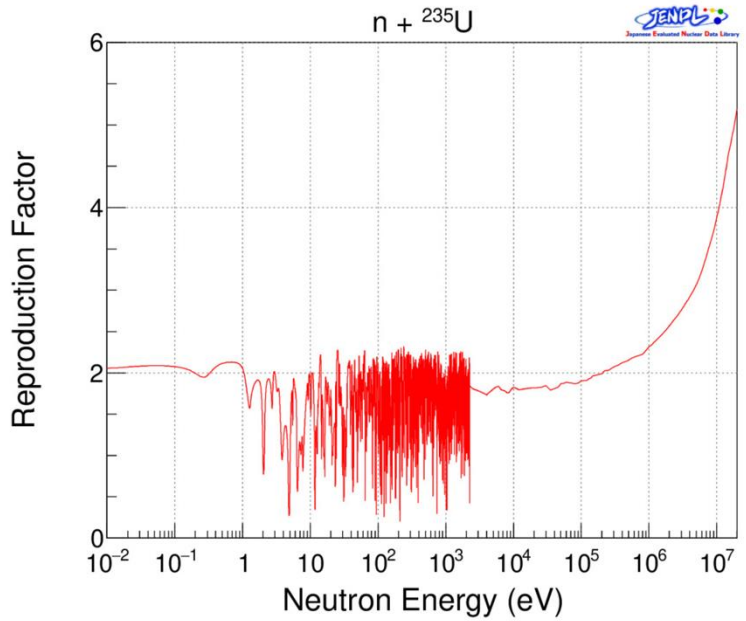
Processing scripts - PREPRO fixup

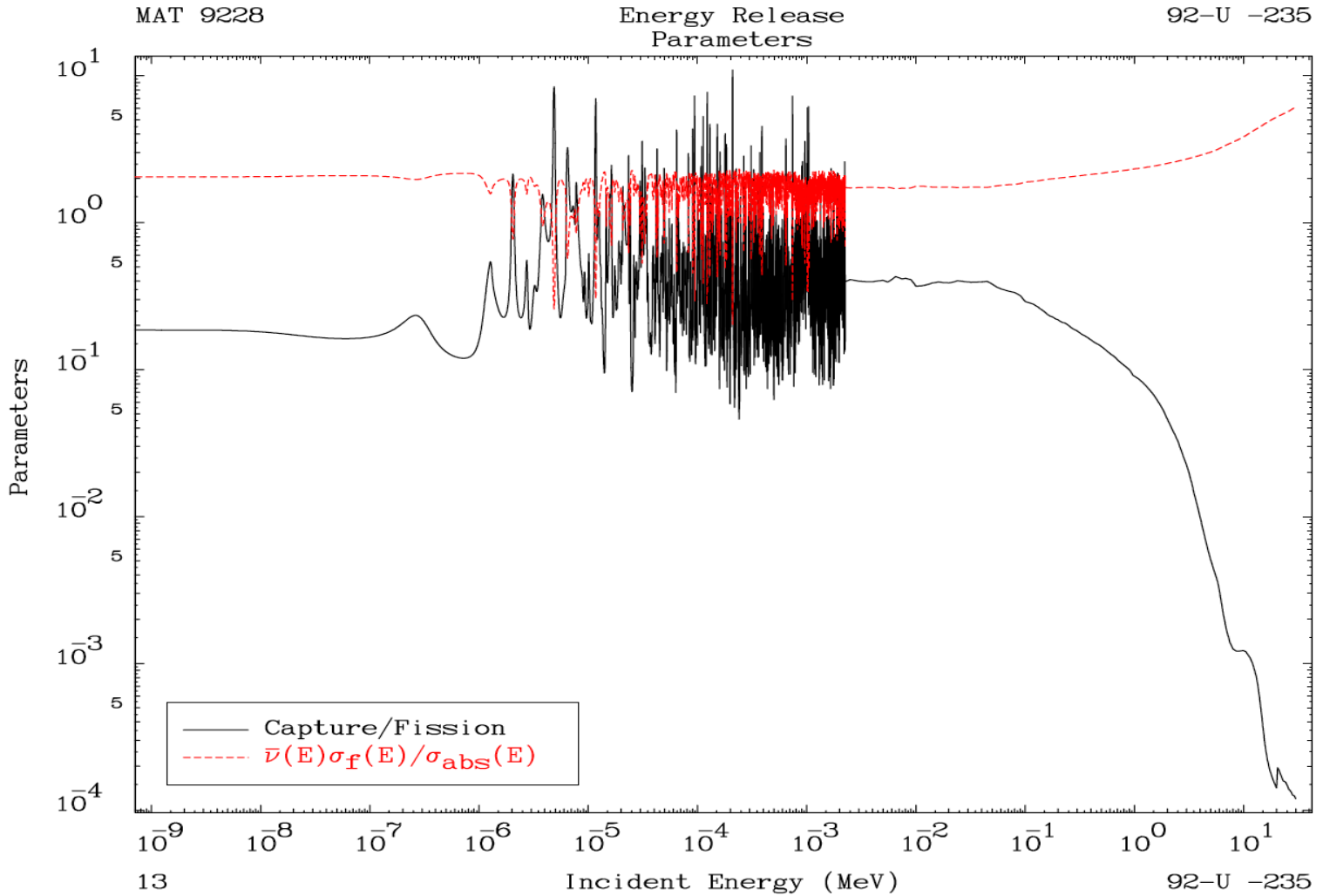
PREPRO fixup can fix many things !! has to

Alpha, Xi, Mu, Nu,…

```
cat>FIXUP.INP <<EOF
10001111111000
../pendf/$isma[$c1]p.asc
FIXUP.OUT
  27=( 18, 18)+(102,117)
*333=(452* 18)
R255=(333/ 27)
R254=(102/ 18)
*****

EOF
```

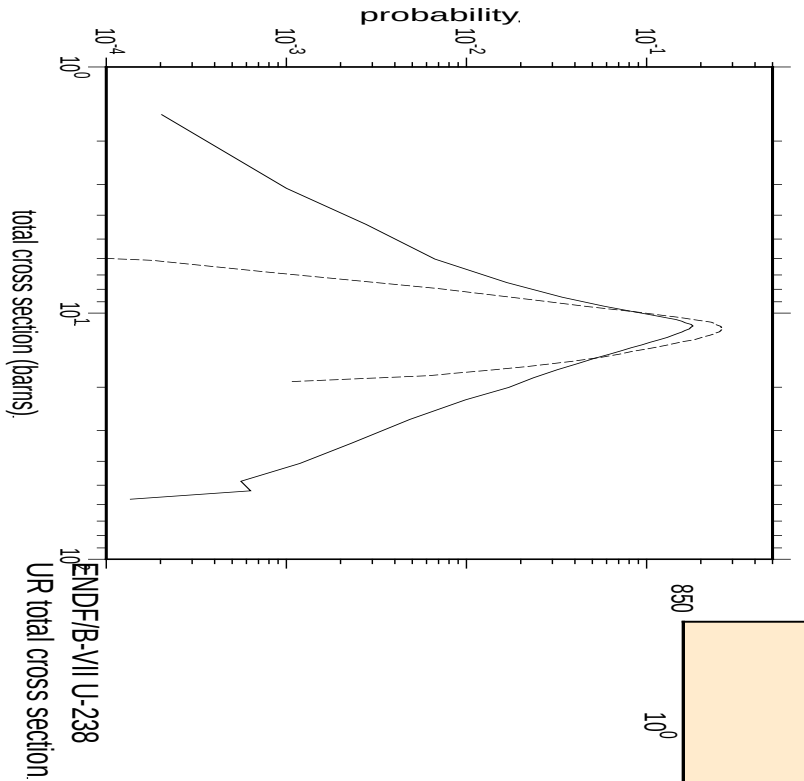




Hidden in the URR, PURR PT's SSF

PDFs @ 20 keV,

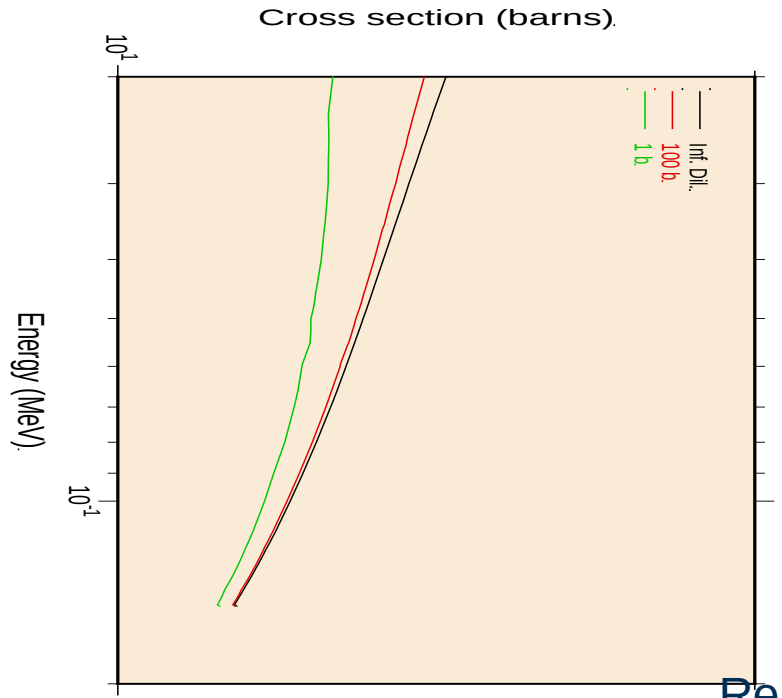
dashed @ 140 keV

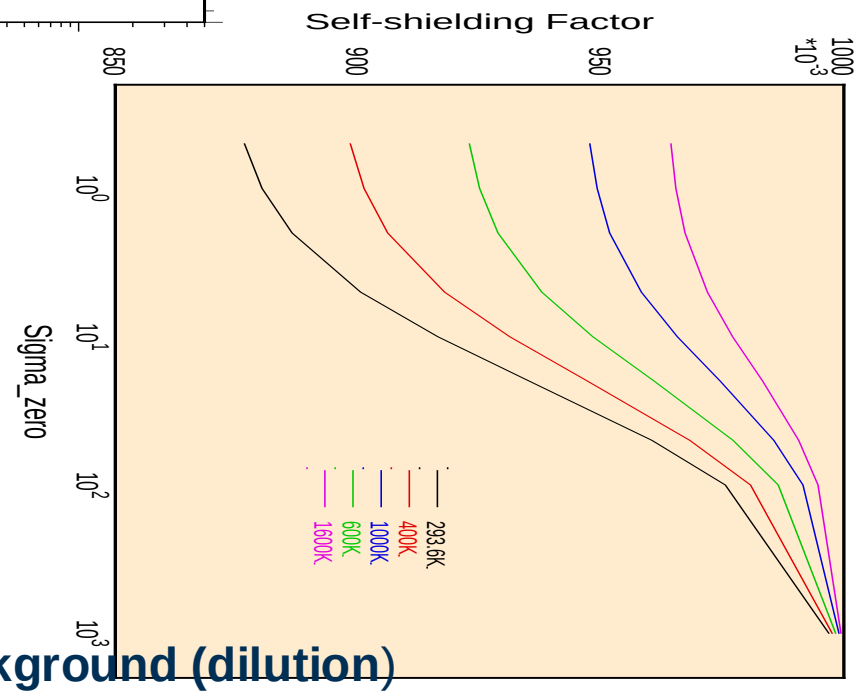


R. E. MacFarlane NJOY

SSF's, without them no robust simulation

300 pcm on Bigten





Reactor physics lexical : **background (dilution)**

Groupwise forms and dilution, Bondarenko

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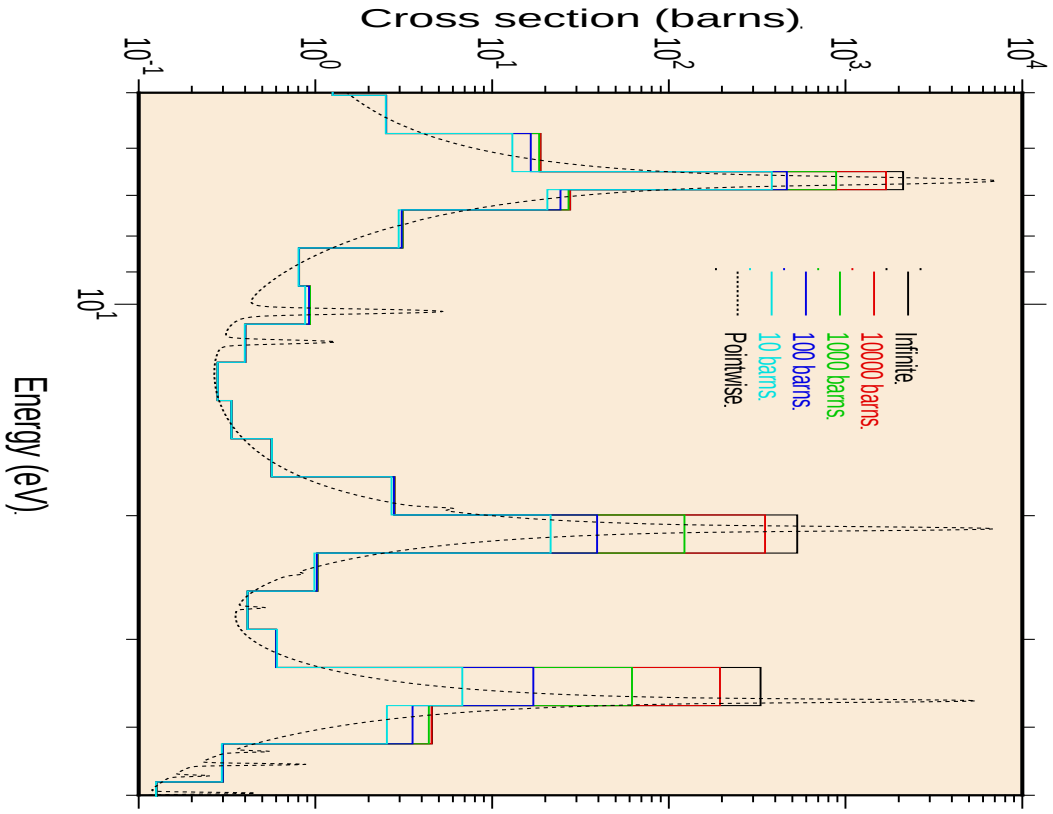
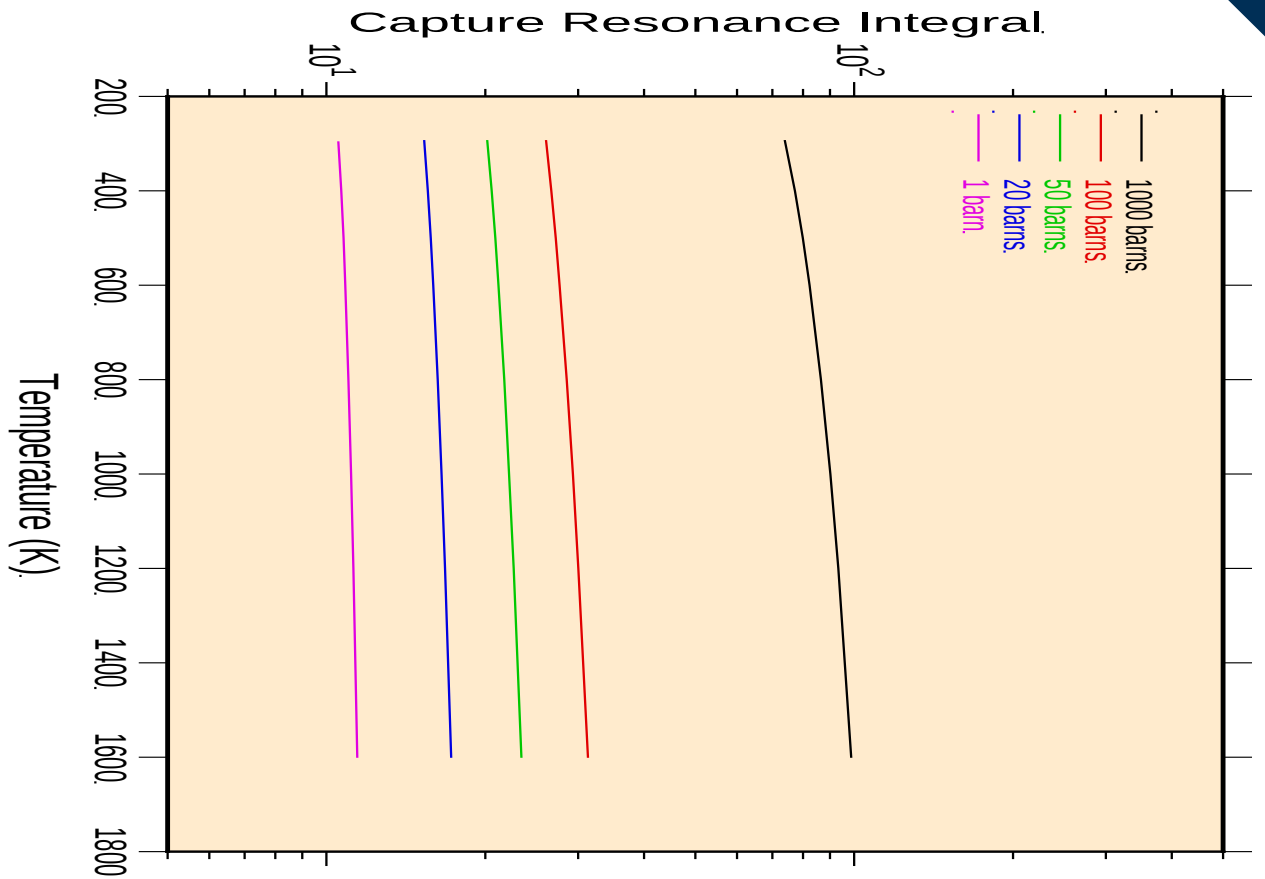
Self Shielding Factor **SSF** on U^{238} first 3 resonances





RI slope with Temperature = **negative temperature coefficient**

Partials and Legendre coefficients

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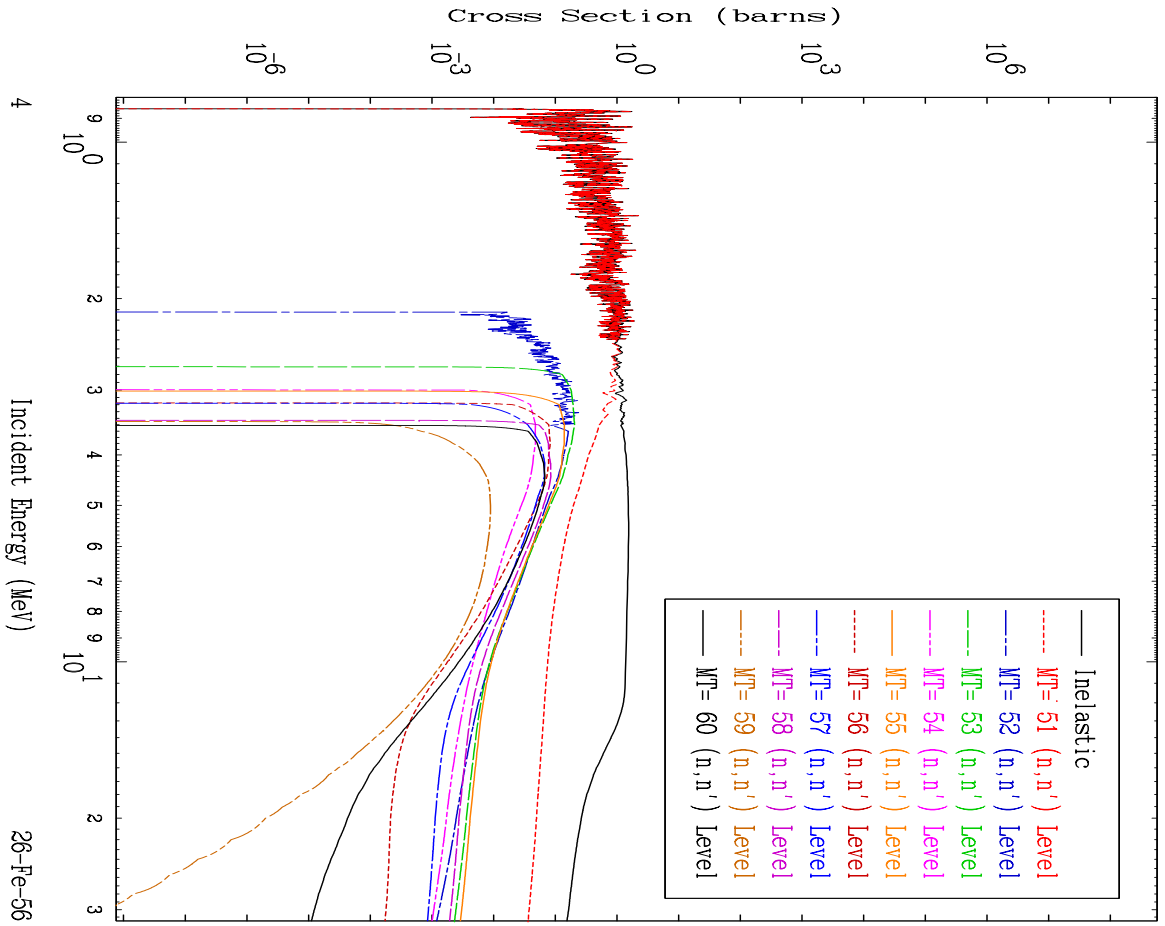
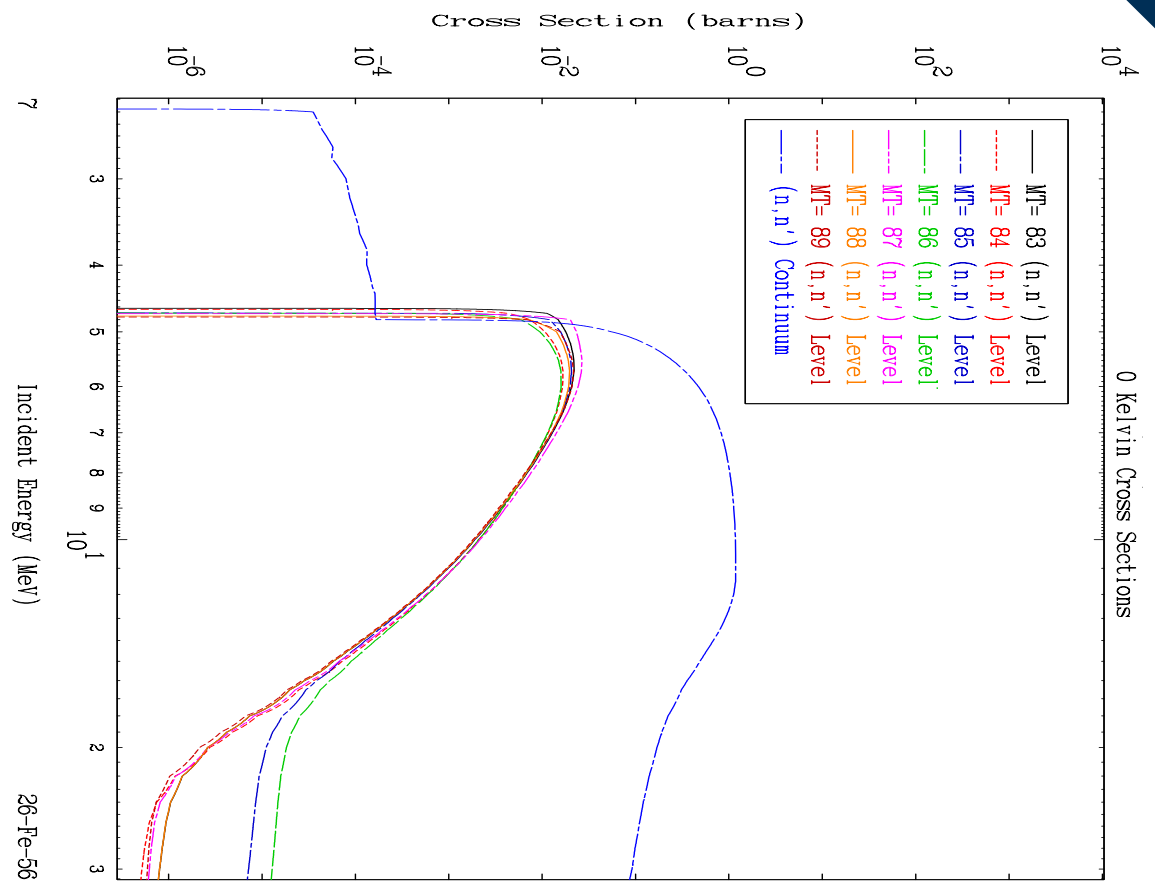


Red Cullen PREPRO



Fluctuations in the MF-3 -
not from resonance parameters MF-2 !!

0K = every K - no broadening

Partials and Legendre coefficients

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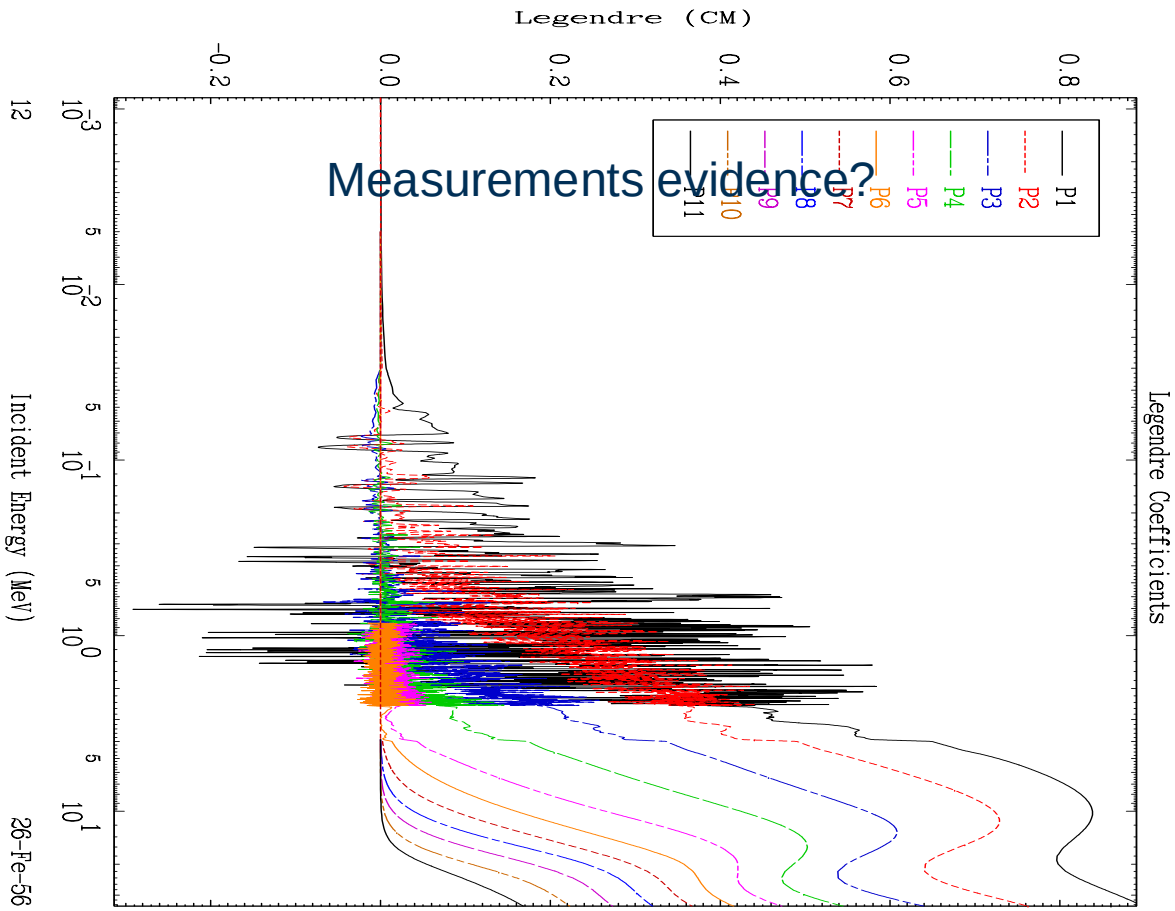
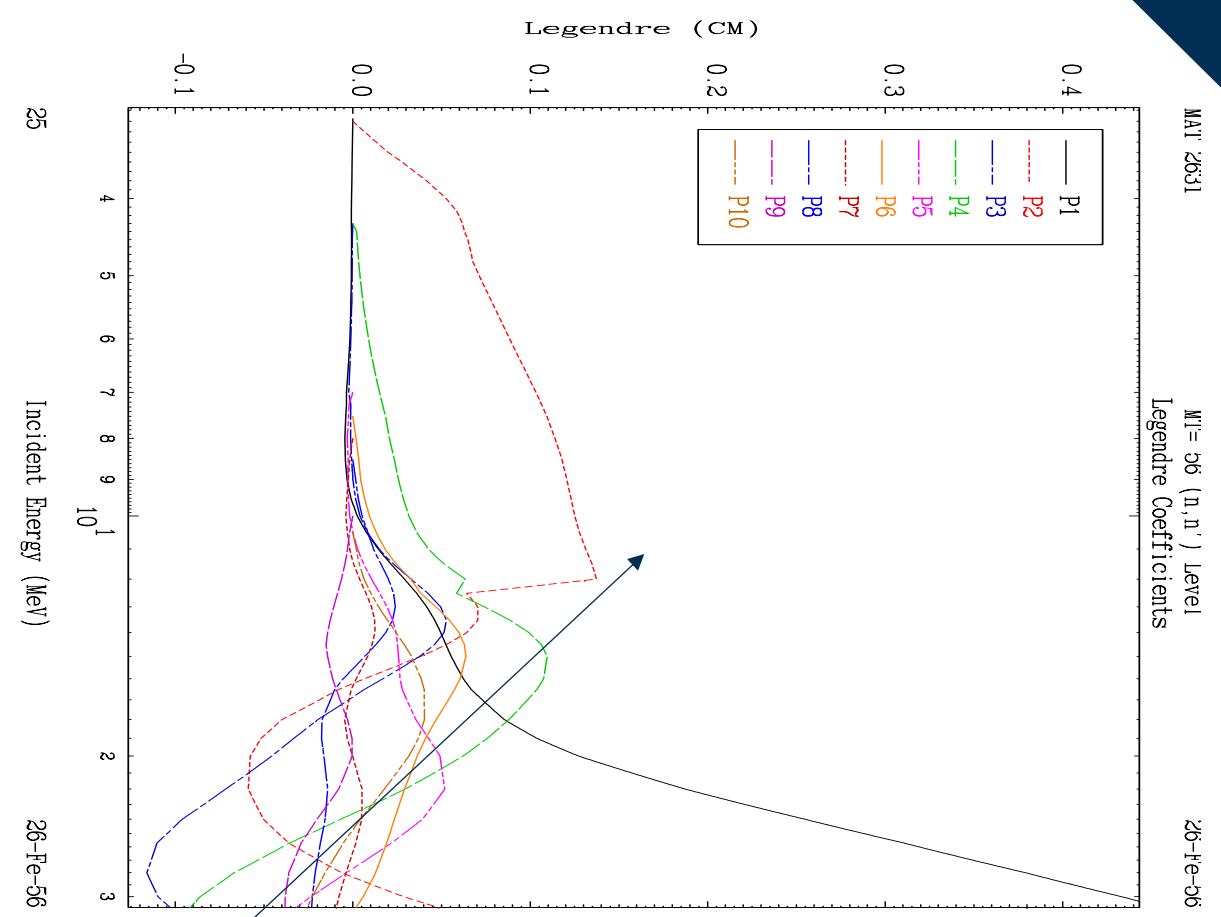
Red Cullen PREPRO



Measurements evidence?



Overdone !! Definitely – really ??

Implicit MF3-MT5*MF6 – prod. yields & A < 4 production

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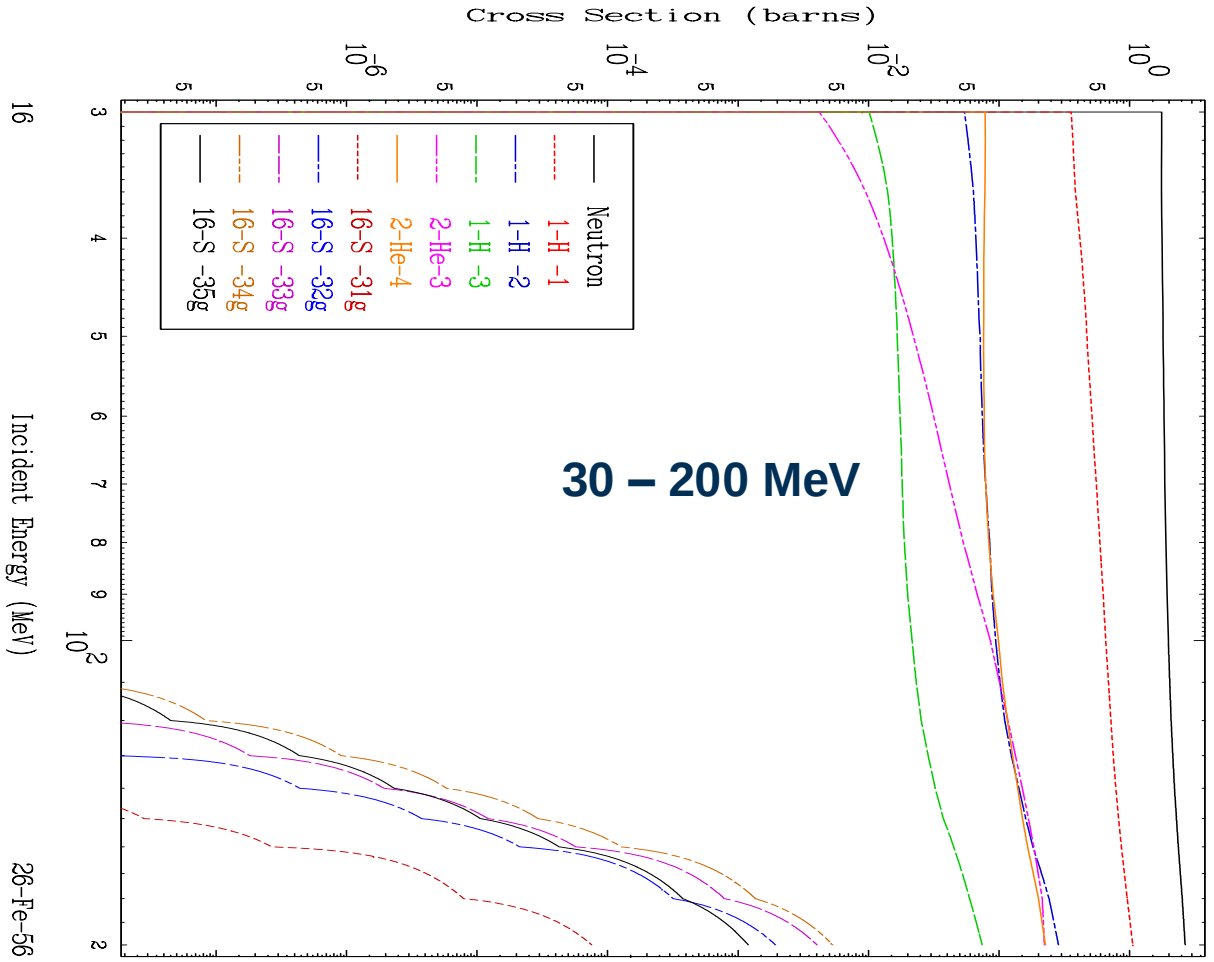
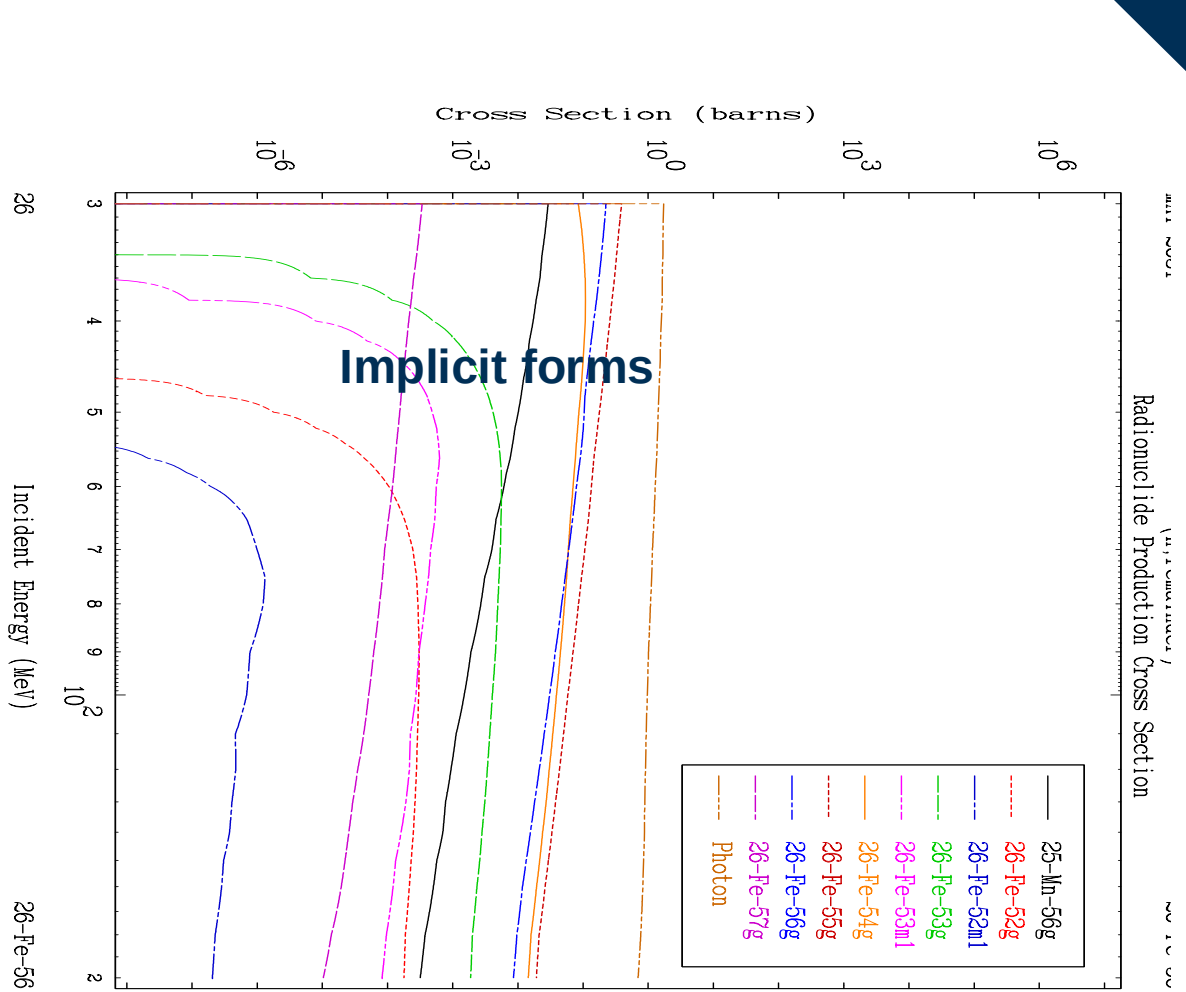
Hundreds of isotopic production yields, A < 4 production - MF-8 dictionary – MT-5*MF-6 using **sixpack - to 200 MeV**





Derived quantities: capture/fission and alpha

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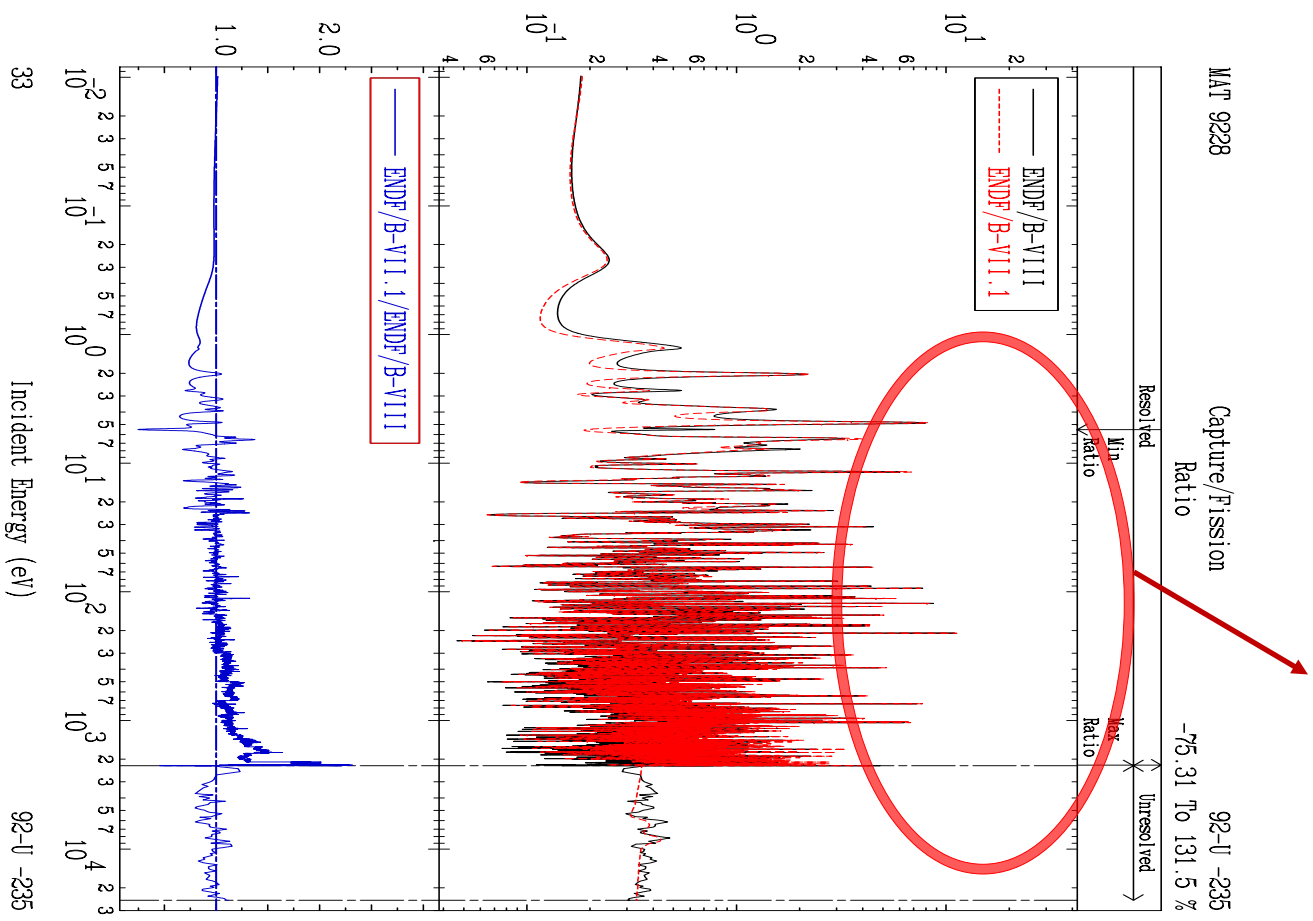
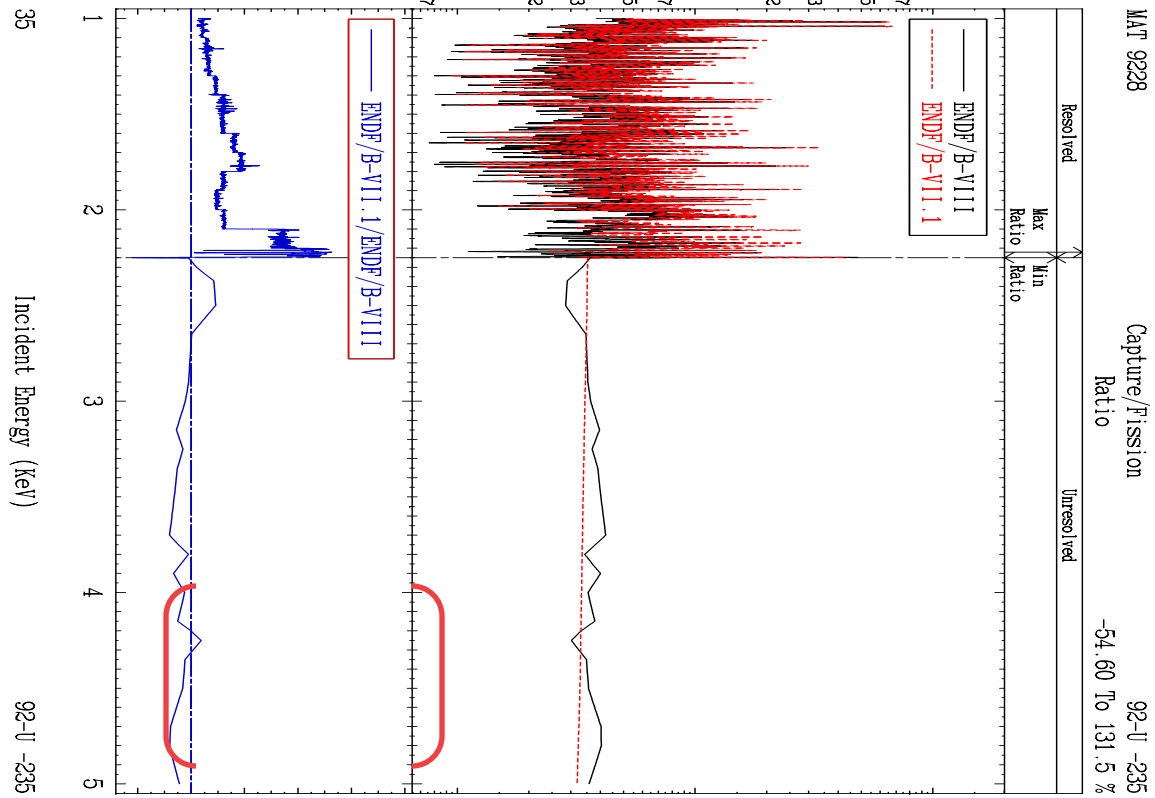
Steps show evaluator **tweaks !!**
to fit Keff C/E – ICSBEP – small, large leakage



Library differences



Below 2.25 KeV

Derived quantities: capture/fission and alpha

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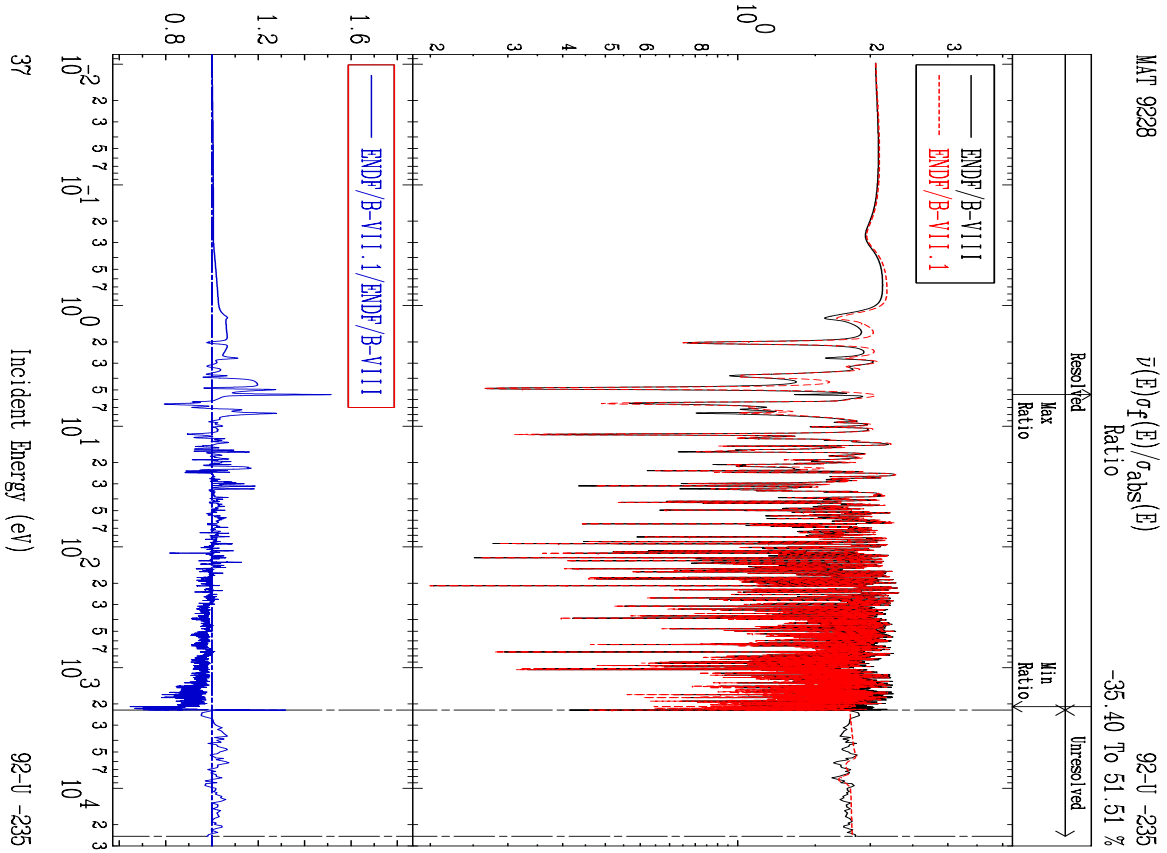
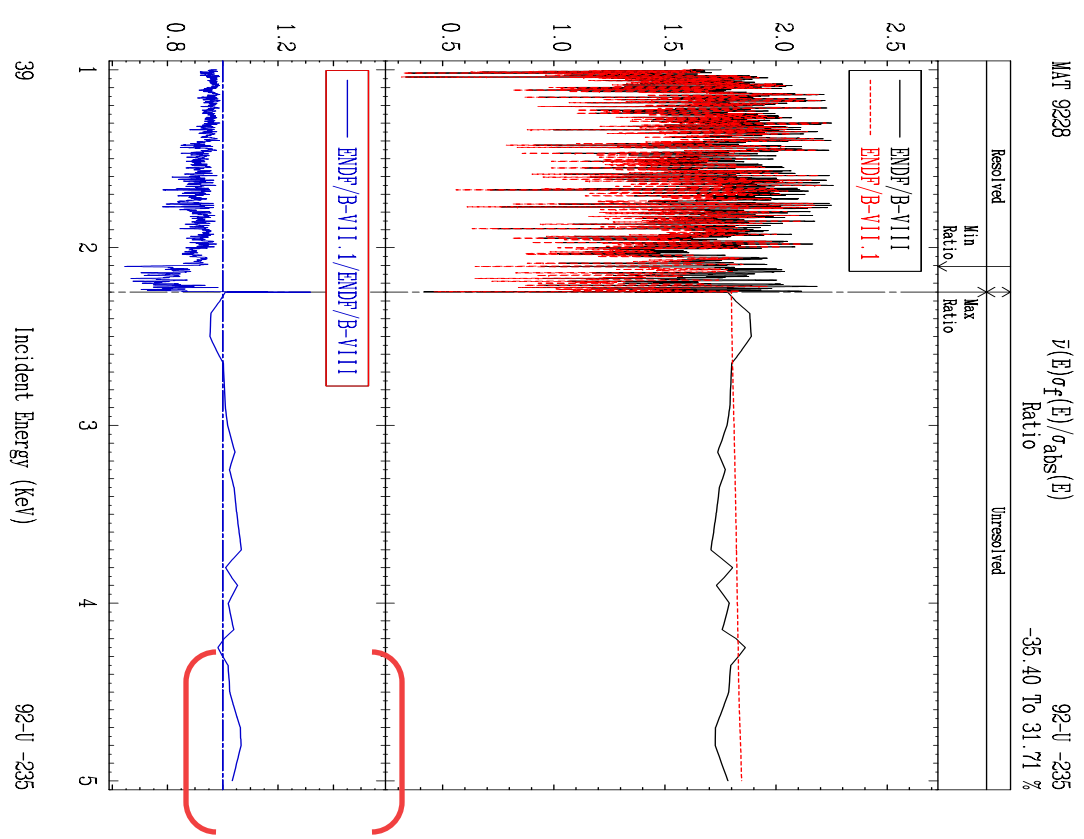


Library differences

Steps influence on **Civilian LWR**

- **big core, small leakage**
- **Keff in cycle – 18 months cycle**



Below 2.25 KeV

Backend of data forms for data portal

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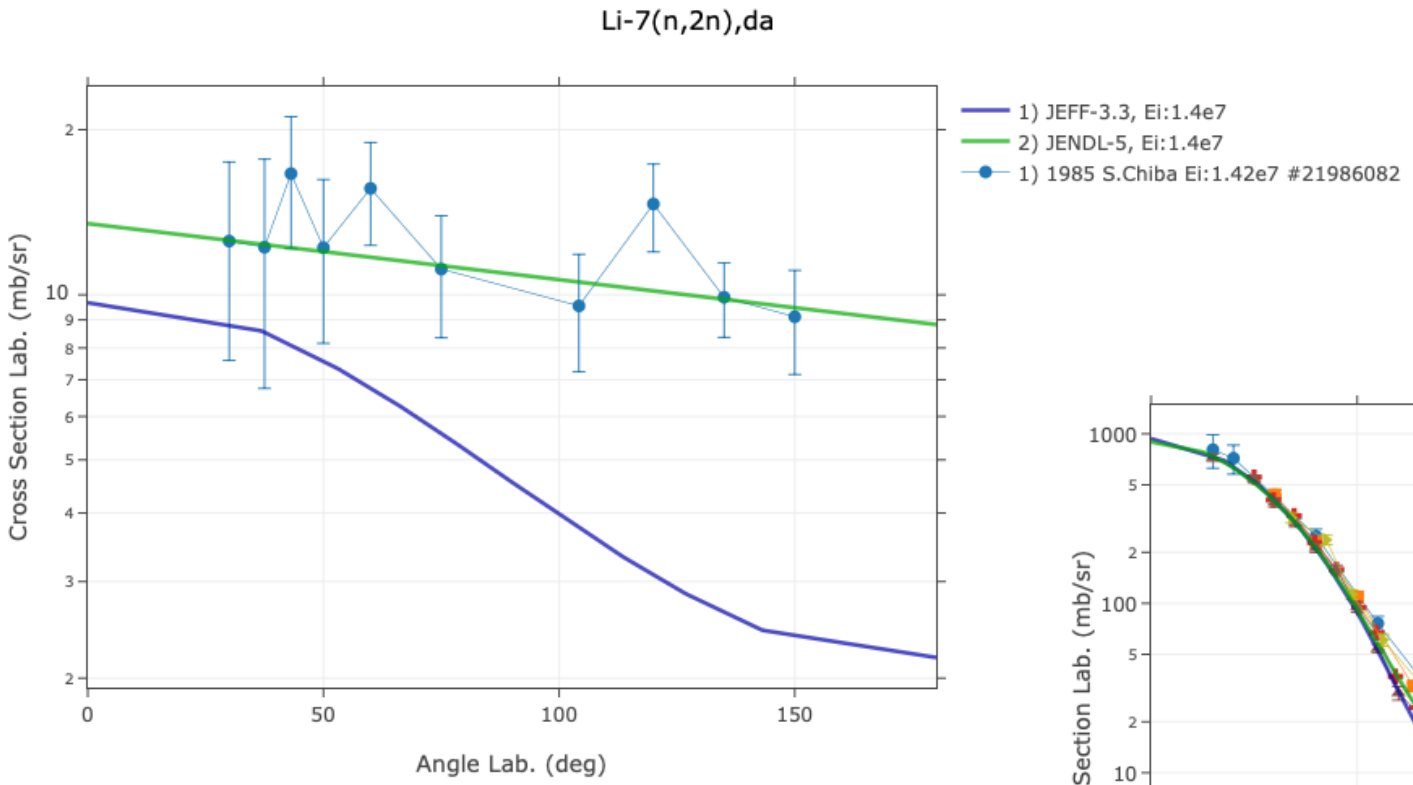
Scripted, automatic, basic and enhanced ENDF-6, GNDS-2.0 **processing steps**, parser and interpreter

Processed data forms are similar, identical to **the ones used by, in application(s)**, not quite what's has been plotted by an evaluator

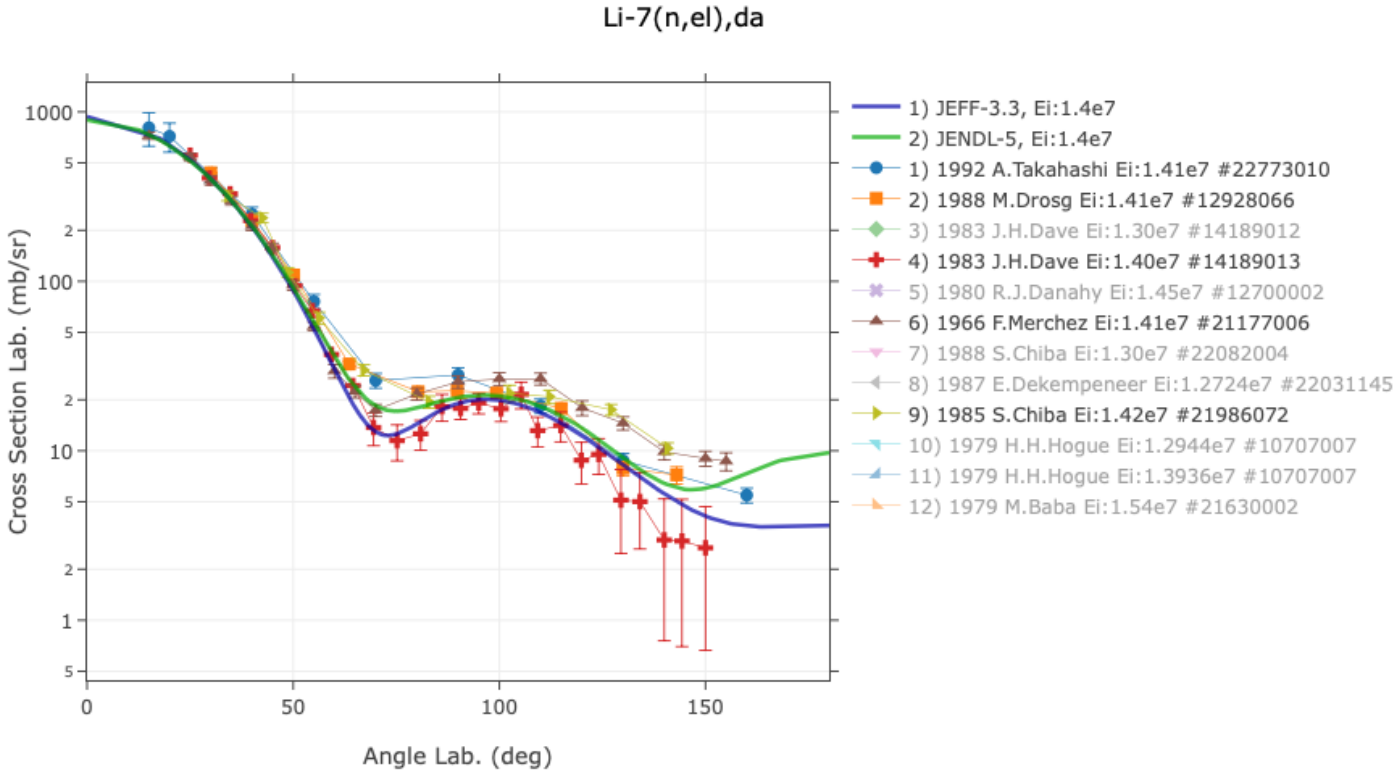
Experimental data and Processed Evaluated data forms may correspond

Check with original NDC https://wwwndc.jaea.go.jp/ENDF_Graph/ 

Processing steps - MF-4 - conversion



PREPRO – LEGEND
only n-outgoing !



EXFOR: DA, μ_{lab} ; evaluated μ_{cm}
0.96 to 1.0 CM cut-off angles
A = mass target/projectile

$$\mu_1 = \frac{(1+A\mu_c)}{\sqrt{A^2+2A\mu_c+1}}$$

Grey EXFOR not plotted !
entrance energies

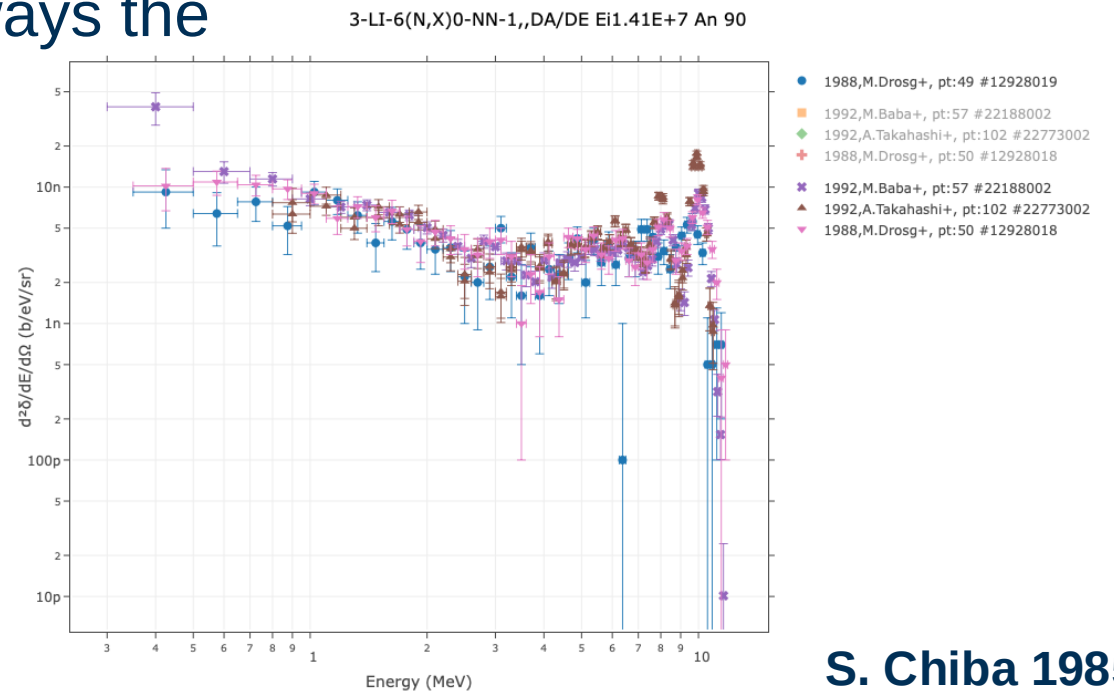
Processing steps - MF-6

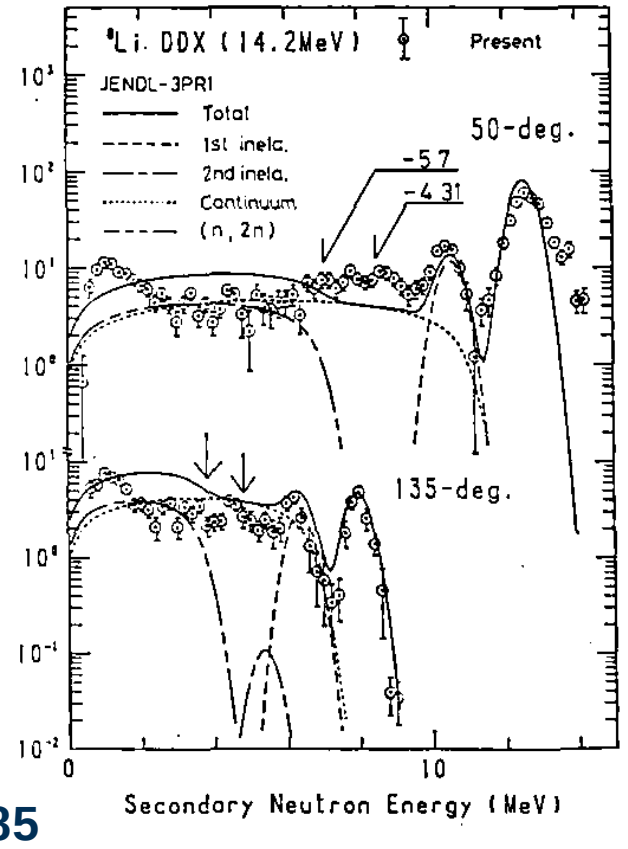
The processing steps for evaluated DA/DE @ E_{in} from MF-6 entries to compare with experimental information mb/sr/MeV (lab) requires:

- **Processing capabilities for all allowed format representations**
- **Accounting for all channels, levels: continuum, 1st, 2nd,.. inelastic, (n,2n), …**
- **Conversion to lab from cm co-ordinate for all observables**

The experimental data forms need to have been properly compiled, not always the case, complex process

Works, **not quite**… for E_{in}= 14.1 MeV





S. Chiba 1985

Processing steps, breakup, LR flags

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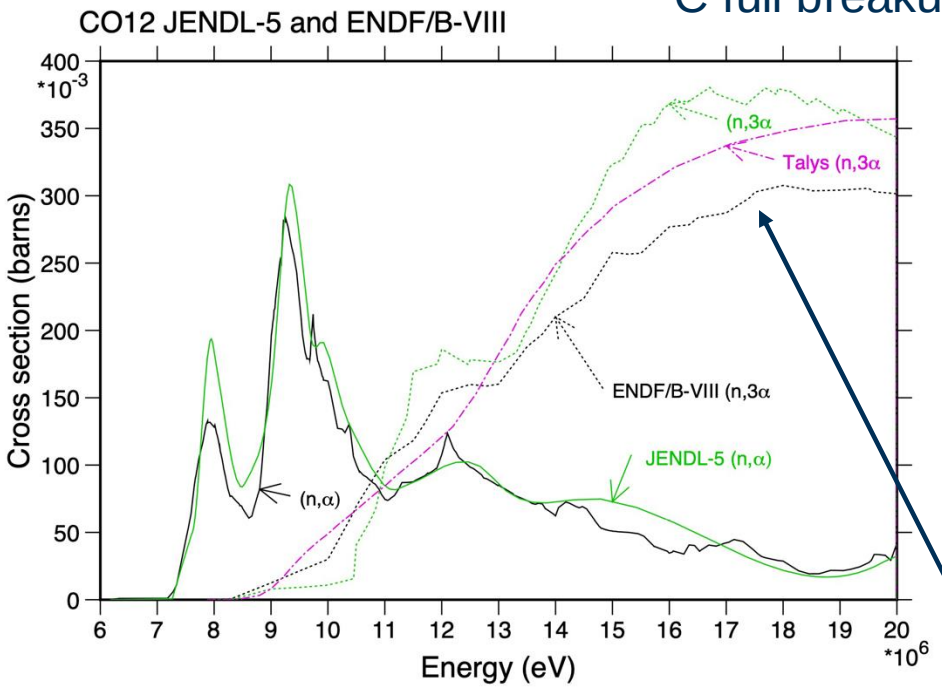
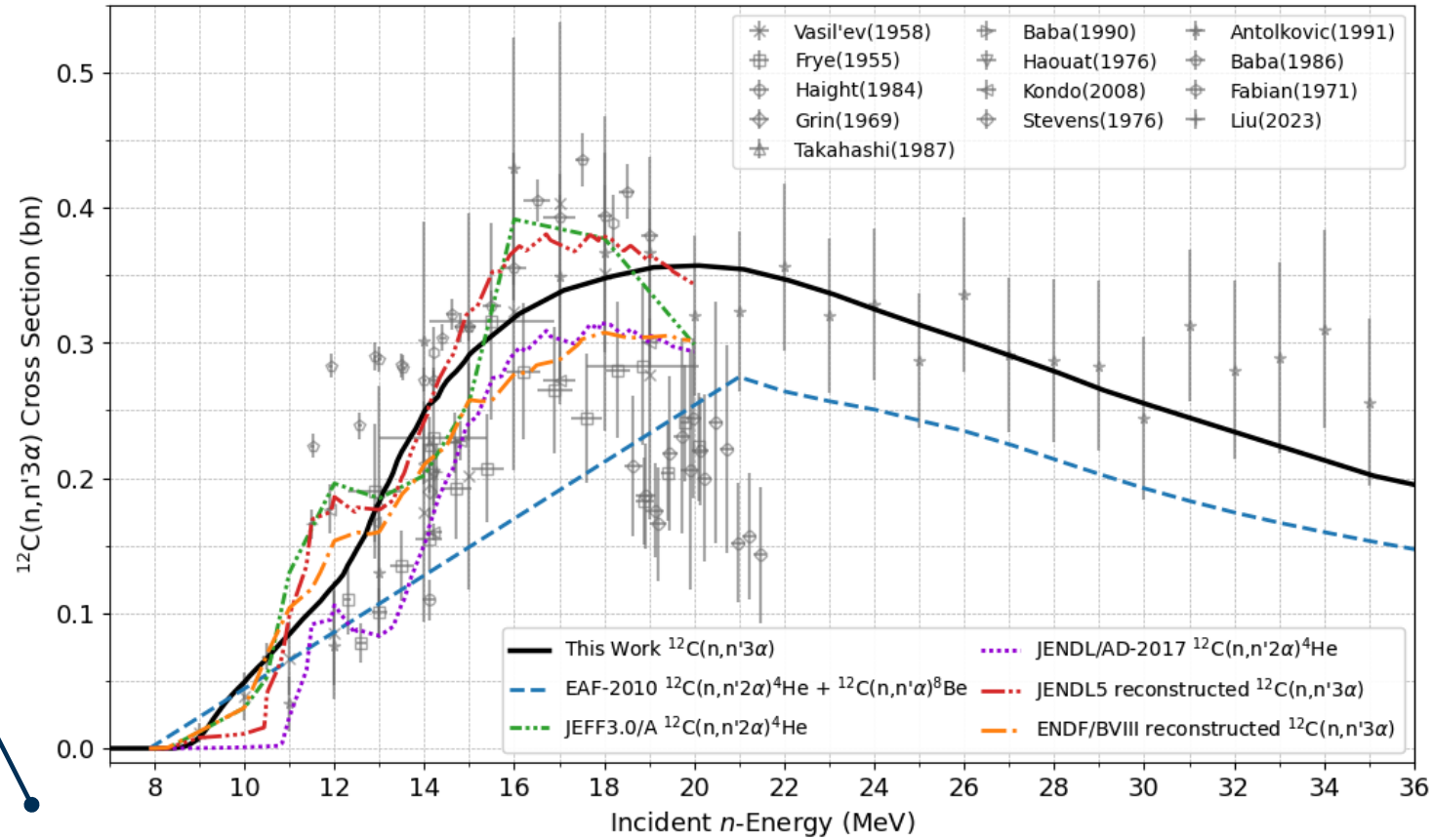
$$n + {}^{12}C \rightarrow n' + {}^{12}C^* \hookrightarrow \alpha + {}^{8}Be \hookrightarrow 2\alpha$$
$$\rightarrow \alpha + {}^{9}Be^* \hookrightarrow \alpha + {}^{5}He \hookrightarrow n + \alpha$$
$$\hookrightarrow n + {}^{8}Be \hookrightarrow 2\alpha$$

Reaction Pathways Considered

EXFOR measured quantity ???
EXFOR $^{12}C(n,2a+n)^4He$ and $^{12}C(n,X)^4He$??
Compiled as MT=29, n2a !!!
EXFOR data, not reliable !!!

^{12}C full breakup





Inelastic LR=23 flag ➔ **derived form MT=23,** constructed during processing

Conclusions

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The **processing steps, practices** that need to be envisaged for modern nuclear data portal forms benefit from:

- Relying on more than **one processing systems**, none are ***complete***
- Target simple **comparable experimental metrics, but not only**
- Use **open-source systems**, preferably the same as the ones use for many application(s)
- Rely on **open-access steps, processes, practices**
- Output simple, **defined**, verifiable data forms, use modern graphics
- Been **externally audited**, **Verified and Validated V&V, shared**
- **Been associated** with model code physics : TALYS, CCONE, CoH3,…