Karlsruhe Institute of Technology

Comments and suggestions related to the use of EXFOR in the preparation of proton activation data file PADF

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Objective

Discussion of proposals for working with EXFOR and data modification

Proton Activation Data File PADF-2007 (FZK, KIT)

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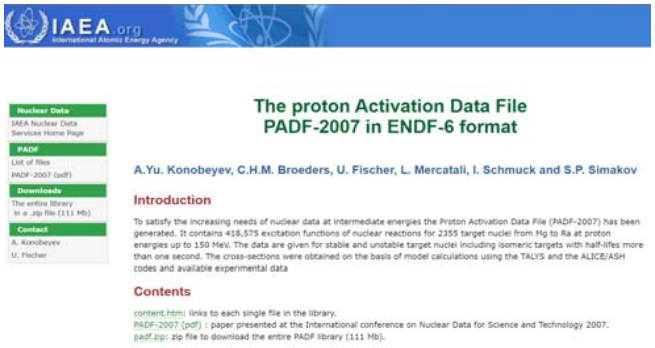
https://www-nds.iaea.org/padf/

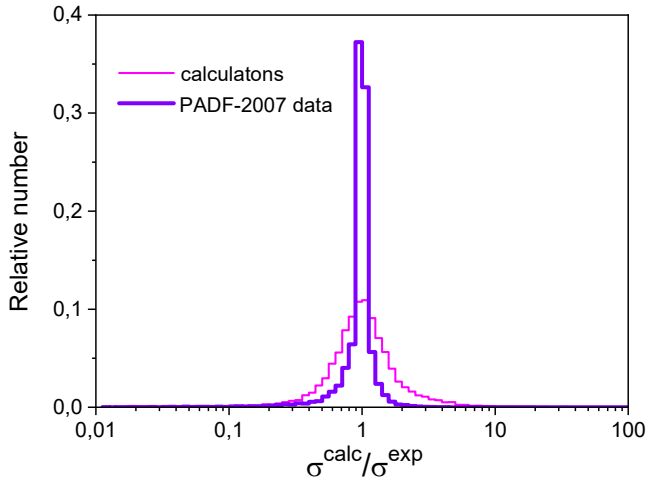


2355 targets nuclei with Z from 12 to 88 and $T_{1/2}$ > 1 sec.
418,575 excitation functions at energies from threshold to 150 MeV

Experimental data:
independent (non-cumulative) residual yields from 1434 EXFOR files

Fitting and correction of calculated excitation functions

Deviation factor	Before evaluation	After evaluation, PADF-2007
$\left(\frac{1}{N}\sum_{i=1}^{N}\left(\frac{\sigma_i^{exp}-\sigma_i^{calc}}{\Delta\sigma_i^{exp}}\right)^2\right)^{1/2}$	122.	4.69
$\frac{1}{N}\sum_{i=1}^{N}\frac{\sigma_i^{calc}}{\sigma_i^{exp}}$	1.71	0.975
$\frac{1}{N}\sum_{i=1}^{N}\left\|\frac{\sigma_i^{exp}-\sigma_i^{calc}}{\sigma_i^{exp}}\right\|$	1.02	0.124
$10^{\left(\frac{1}{N}\sum_{i=1}^{N}\left[\log(\sigma_i^{exp})-\log(\sigma_i^{calc})\right]^2\right)^{1/2}}$	2.15	1.47



Proton Activation Data File PADF-2 (KIT) : in preparation

A.Yu. Konobeyev, D. Leichtle, A. Stankovskiy (SCK CEN)

Ready

C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Ca, V, Cr, Mn, Fe, Co, Ni, Cu, and Nb up to 200 MeV

W up to 3 GeV

Experimental data

- independent and cumulative cross-sections for isotopes
- independent and cumulative data for natural mixtures of isotopes
- partial cross-sections (if possible)
- relative values (if possible)
- S-factors

PADF-2

Report KIT SWP, 204 (2022), https://dx.doi.org/10.5445/IR/1000152627

Report KIT SWP, 227 (2023), https://dx.doi.org/10.5445/IR/1000162040

Report KIT SWP, 252 (2024), https://doi.org/10.5445/IR/1000176301

File download

only cross-sections, MF=10, MT=5 : https://t1p.de/3vzun

part of JEFF-4 general-purpose files : https://www.oecd-nea.org/dbdata/jeff/ (2025)

The following considerations: not a criticism of the current situation

EXFOR is getting better and easier to use

Great progress over the last 15 years: compilation and presentation of reliable data, the ways of using

Comments and (controversial) proposals: resulting from our activity for PADF-2

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Using data for further evaluation

Currently: in most cases, analysis of original publications is necessary

Ideal case: immediate use C4 or C5 data

What are the stumbling blocks?

Problem with user-side perspective

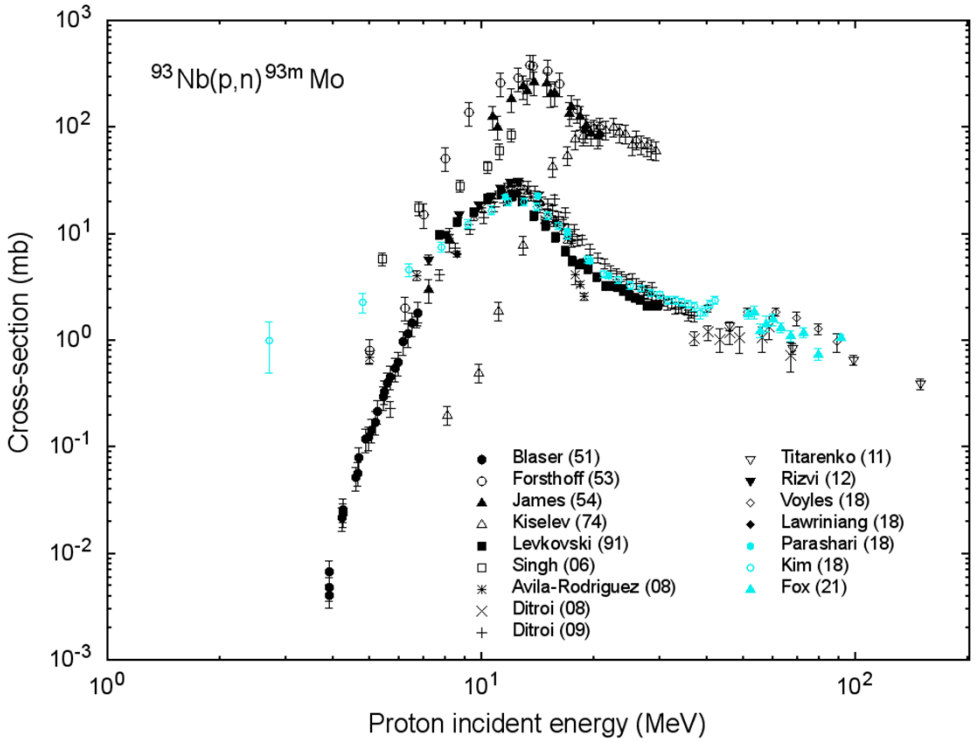
Experimentalist / author : details : not interesting to describe, “self-evident”

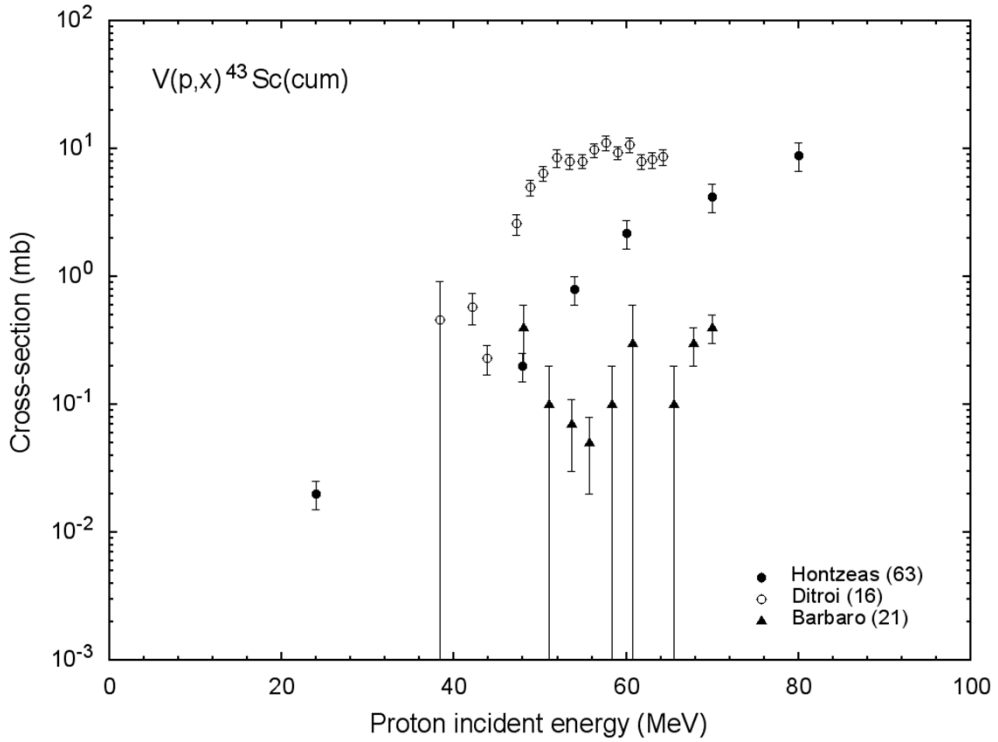
Compiler : uncertain information

Data user : subjective interpretation

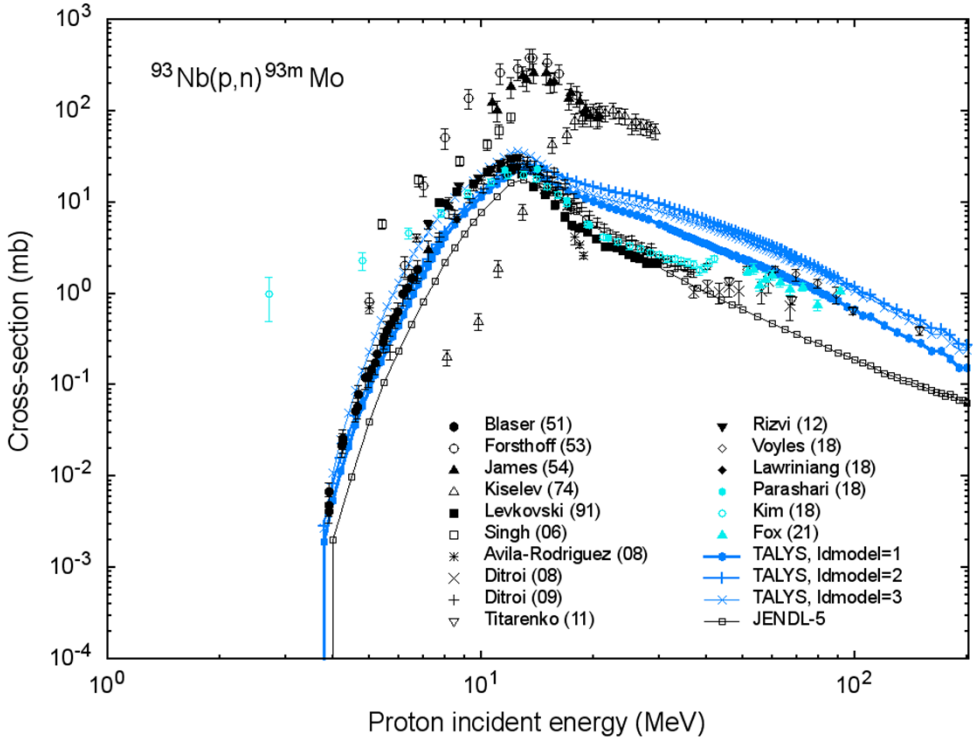
I. Questionable data: *simplified user feedback*

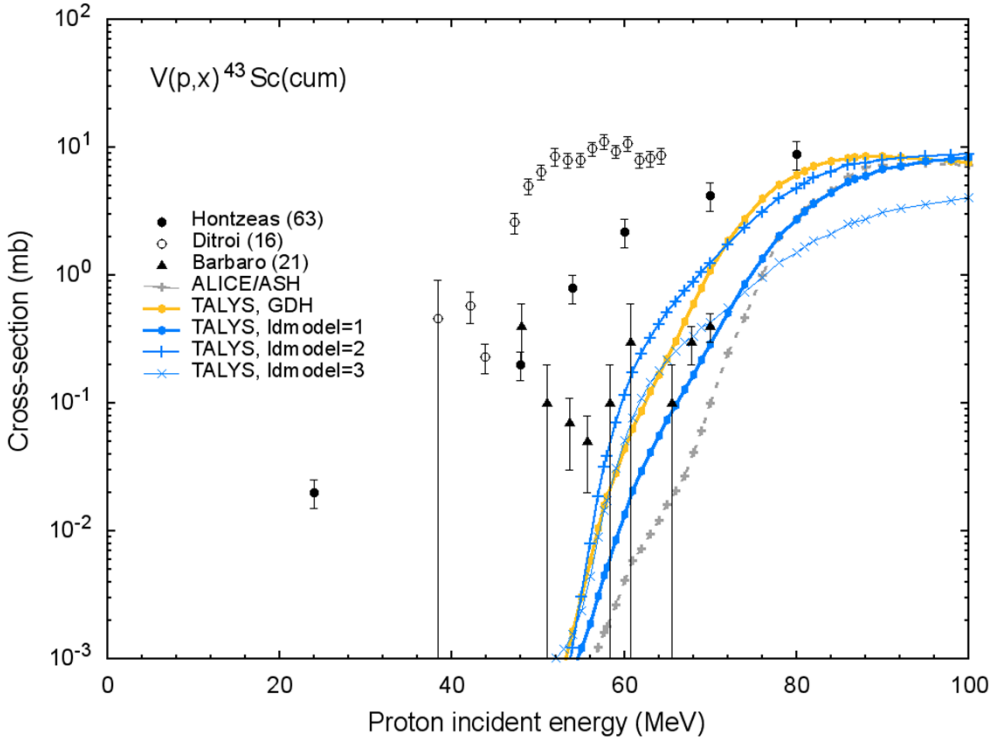
Measured data: analysis of publications does not solve the problem





Measured data and calculations





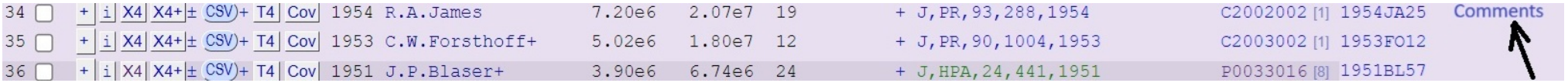
Possible solution

Users' comments: NOT for inclusion in the standard EXFOR file

Easy to change or withdraw

Examples

J. Q. Public (XNL) : Bad data. Significant deviations from approved data
G. Raymond (YNL): Data are probably erroneous. Impurities have an impact on the measured values

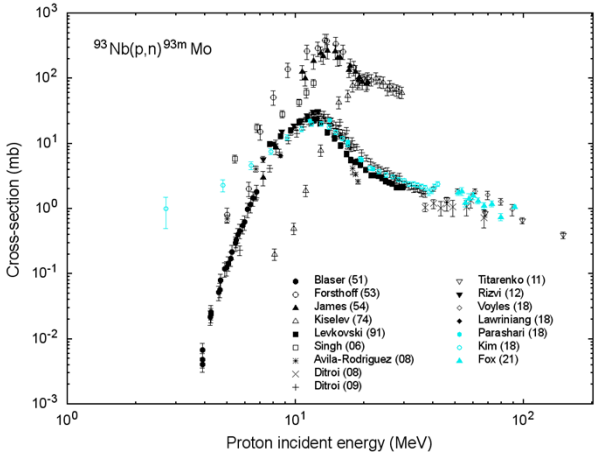


REACTION line: *warning*

C5 format: *warning*, single character in a line with a cross-section for *certain/all* energies

```
#Headers                    EN      dEN     Data    dData
#Units                      EV       EV        B        B
#Proj Targ M MF MT PXC   Energy  dEnergy     Data   dData Cos/LO/ZP dCos/LO/AP LVL/HL dLVL/HL I78
#---><----><-><--><--><-------><-------><-------><-------><-------><-------><-------><-------><-:
 1001 41093   3   4M  5020000.0           8.11E-4
 1001 41093   3   4M  6240000.0           0.00203
 1001 41093   3   4M  7010000.0            0.0152
 1001 41093   3   4M  8000000.0            0.0511
 1001 41093   3   4M  9220000.0             0.138
 1001 41093   3   4M    1.125E7             0.261
 1001 41093   3   4M    1.248E7             0.289
 1001 41093   3   4M    1.344E7             0.383
 1001 41093   3   4M    1.369E7             0.379
 1001 41093   3   4M    1.499E7              0.34
 1001 41093   3   4M    1.618E7             0.258
 1001 41093   3   4M    1.795E7             0.147
```

Extend PXC ?



COMMENT: *explanations if the problem is clear*

II. Data near the reaction threshold: *automatic search*

A. Measured cross-sections (CUM, IND) below the reaction threshold

REACTION line: *warning*

C5 format: *error*, single character in a line with a cross-section for a *certain* energy

B. Measured cross-sections near the reaction threshold

Reactions: (p,xnyp), y ≥1

Residuals: „near“ the target

Energy: E_{th} + ΔE, ΔE = several MeV

σ(TALYS or TENDL) < $\alpha \times \sigma$(measured), α: 0.001 … 0.01

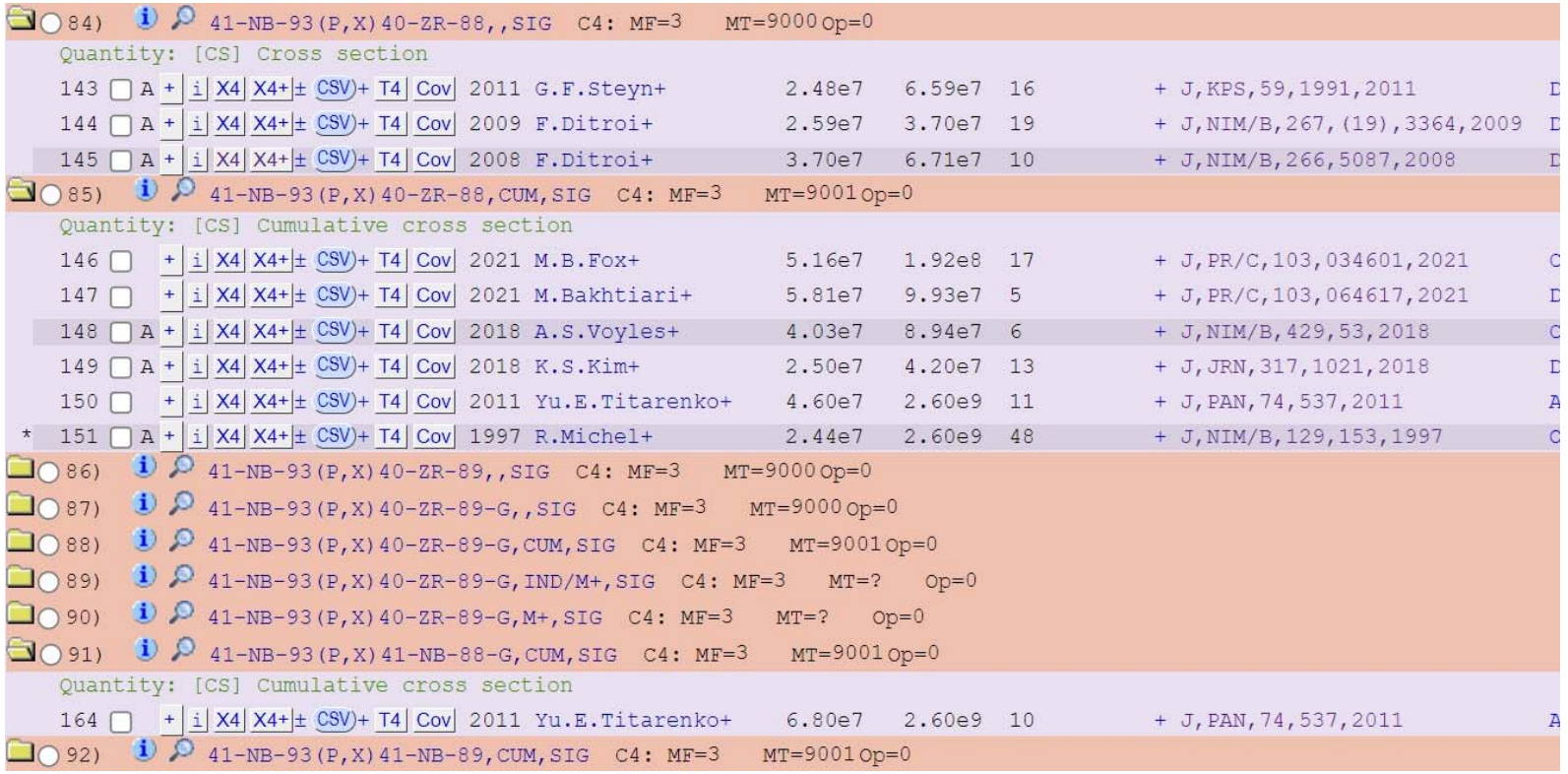
C5 format: *warning* for a *certain* energy

What is achieved:

- simplified decision to use the data or not
- facilitating blind comparison of calculations and measurements

III. Independent and cumulative data

Example: $^{93}Nb(p,x)^{88}Zr$



84) 41-NB-93(P,X)40-ZR-88,,SIG C4: MF=3 MT=9000 Op=0

Quantity: [CS] Cross section

143	A	2011	G.F.Steyn+	2.48e7	6.59e7	16	+	J,KPS,59,1991,2011	D	
144	A	2009	F.Ditroi+	2.59e7	3.70e7	19	+	J,NIM/B,267,(19),3364,2009	D	
145	A	2008	F.Ditroi+	3.70e7	6.71e7	10	+	J,NIM/B,266,5087,2008	D	

85) 41-NB-93(P,X)40-ZR-88,CUM,SIG C4: MF=3 MT=9001 Op=0

Quantity: [CS] Cumulative cross section

146		2021	M.B.Fox+	5.16e7	1.92e8	17	+	J,PR/C,103,034601,2021	C	
147		2021	M.Bakhtiari+	5.81e7	9.93e7	5	+	J,PR/C,103,064617,2021	D	
148	A	2018	A.S.Voyles+	4.03e7	8.94e7	6	+	J,NIM/B,429,53,2018	C	
149	A	2018	K.S.Kim+	2.50e7	4.20e7	13	+	J,JRN,317,1021,2018	D	
150		2011	Yu.E.Titarenko+	4.60e7	2.60e9	11	+	J,PAN,74,537,2011	A	
* 151	A	1997	R.Michel+	2.44e7	2.60e9	48	+	J,NIM/B,129,153,1997	C	

86) 41-NB-93(P,X)40-ZR-89,,SIG C4: MF=3 MT=9000 Op=0

87) 41-NB-93(P,X)40-ZR-89-G,,SIG C4: MF=3 MT=9000 Op=0

88) 41-NB-93(P,X)40-ZR-89-G,CUM,SIG C4: MF=3 MT=9001 Op=0

89) 41-NB-93(P,X)40-ZR-89-G,IND/M+,SIG C4: MF=3 MT=? Op=0

90) 41-NB-93(P,X)40-ZR-89-G,M+,SIG C4: MF=3 MT=? Op=0

91) 41-NB-93(P,X)41-NB-88-G,CUM,SIG C4: MF=3 MT=9001 Op=0

Quantity: [CS] Cumulative cross section

164		2011	Yu.E.Titarenko+	6.80e7	2.60e9	10	+	J,PAN,74,537,2011	A	

92) 41-NB-93(P,X)41-NB-89,CUM,SIG C4: MF=3 MT=9001 Op=0

E_{th} for ^{88}Nb : 43.38 MeV

Easy : REACTION contains comprehensive information

Less easy : the EXFOR file contains important information

Tricky : the original paper (probably) contains necessary information

How to improve the situation?

A. Simplified user feedback

Feedback in the form of special comments to files: opinion of the user

B. Compiling new and modifying existing files

More measurement details

ACTIV method: irradiation time, analysis time, etc.

More compiler comments. Doubts IND or CUM: specify avoiding simple “(CUM)”

Not effective: in case of doubt no SF5 specification: zz-NN-AA,,SIG

C. Analysis with nuclear model calculations

No SF5: IND or CUM ?

Decision: cumulative cross-section

- method ACTIV
- production of precursor is energetically possible
- precursor was not measured. If it was: no IND guarantee - check the text
- precursors are relative short-lived

Calculations: TALYS, PHITS, …

available

TALYS : TENDL

PHITS : (p,x), stable isotopes for 20 elements from C to Nb at E_p < 200 MeV

Measurement energy range [E_1,E_2]

Maximum value of the ratio σ(precursors) / σ(main) < XX % : warning

REACTION line : warning with XX %

Examples: CC1, CC10, CC50, CC: Cumulative Contribution in %

D. Automatic search

a) CUM is given: IND ?

i. No precursors at all

ii. Threshold energy for precursors > E_2, range of measured data: [E_1,E_2]

In case i. or ii. IND or CUM is *not critical*:

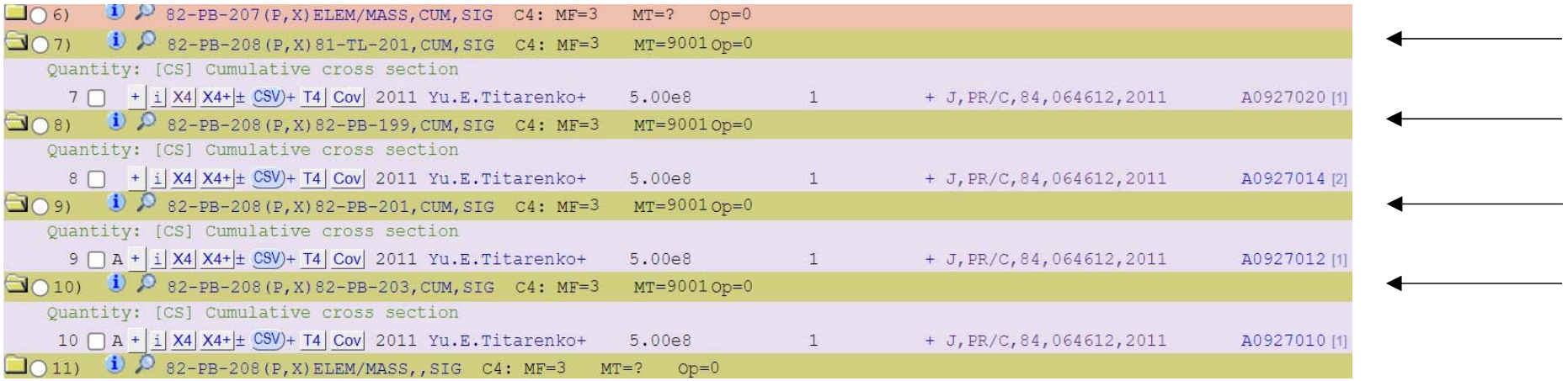
Other cases: CUM instead of IND – *underestimation* of the cross-section

b) *Supracumulative* cross-section

Concept: Titarenko et al, Phys. Rev. C, v.65, p. 064610 (2002)

$$T_{1/2}^{main} \sim T_{1/2}^{precursor}, \qquad \sigma^{supracum} > \sigma^{cum}$$

Problem 1: special symbol. Not a "CUM" cross-section



The same for "ELEM/MASS, CUM, SIG" data

Problem 2: other measurements

Supracumulative values in other measurements besides of Titarenko et al

List of possible products: automatic search

- $T_{1/2}^{precursor} / T_{1/2}^{main} < 5$ (?)
- delay time of measurements after irradiation related to $T_{1/2}^{precursor}$ (?)

Supracumulative cross-sections

- not “DATA-MAX” data
- suitable for cross-section evaluation

IV. Reaction products in ground and metastable state

Problem : no indication of the ground state “G”. Sum of cross-sections $\sigma^g + \sigma^m$ or σ^g ?

Particularly important: the M-state partially decays into the g-state

REACTION … ,,SIG) : no “–G”

REACTION … ELEM/MASS,,SIG) : empty space in ISOMER field

Independent yields

Examples: 25-MN-52,,SIG, 39-Y-83,,SIG, 43-TC-94,,SIG

All isomers decaying to the G-state with br. ratio < 90% : 479

< 80% : 458

Not decaying to the G-state : 297

For most: *no data in EXFOR*

Many measurements: *no exact information about* g-state

Identifying problem cases

Automated check

- nuclide
- measurement method (?)
- “REACTION” line and “ELEM/MASS“ file content

Final decision: analysis of original publications and user feedback

Reading the author's articles: in many cases there is no clear information

The solution: "(M)" ?

IAEA-NDS-206: (M) = uncertain if decay from metastable state included.

IAEA-NDS-208: (M) = Data given are assumed by the compiler to include the formation by partial feeding via isomeric transition, but no definitive statement is given by the author

If “G” is not specified in the article

Problematic

don't specify anything (sum) : the user must analyze the article

(M) : the user must decide about M-contribution or not to use the data

Very useful: experts/compilers/users comments:

a) the cross section probably contains the contribution of M-states (high probability): S1

b) the cross section may contain an M-contribution (medium probability) : S2

c) doubtful, but the cross section can have a contribution from M-states (low probability) : S3

Simplified user feedback: different views and discussion

What's happening now:

- each user has to do the same work to analyze the experiment
- the decision - IND or CUM or -G or SUM is individual and does not benefit from the experience of other users who have made the same analysis
- the experience of users, possibly different opinions, in fact, their discussion, is lost and does not serve as a starting point for further analysis or interpretation of the data

Possible solutions

- automated check
- simplified user feedback : opinions, point of views
- use of nuclear model codes / data libraries
- changes in data presentation

Conclusion

The considerations discussed are based on the natural questions that arise when using EXFOR data to evaluate nuclear reaction cross-sections