International Atomic Energy Agency

Compilation of Isomeric Ratio for Light-Particles Induced Reactions

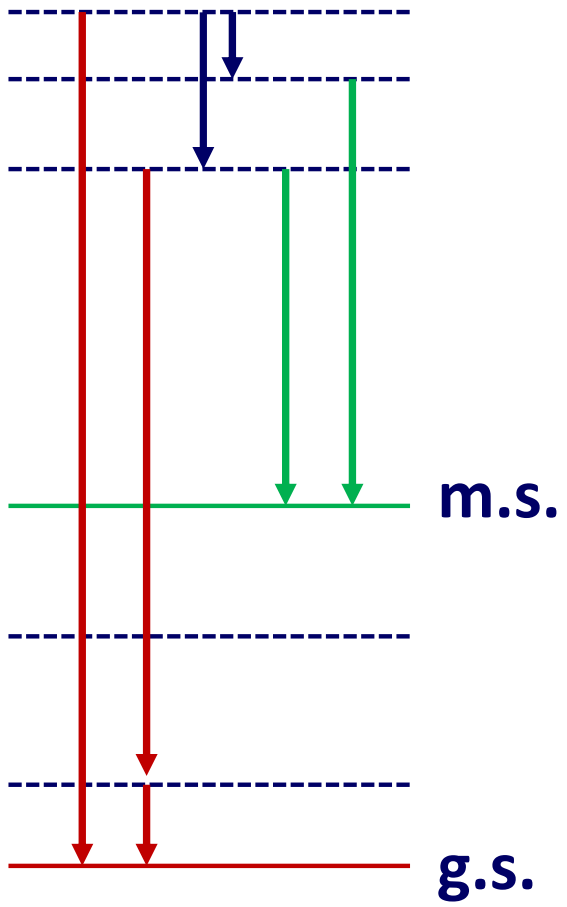
Naohiko Otsuka (IAEA), Alberto Rodrigo (UPM)

NRDC 2023 Action 61 to Takács and Otsuka

"Check presence of the cross sections compiled as total (=ground state plus metastable state) independent production cross sections but deviation of the measured values from the actual total cross sections may be nonnegligible."

Isomeric Ratio (IR)

- Ratio of the products decaying into the g.s. and m.s. by prompt gamma emission
- Important for waste management, radioisotope production etc.
- Modelled with spin cut-off parameter in H.F. calculation etc.



Experimental Determination of IR

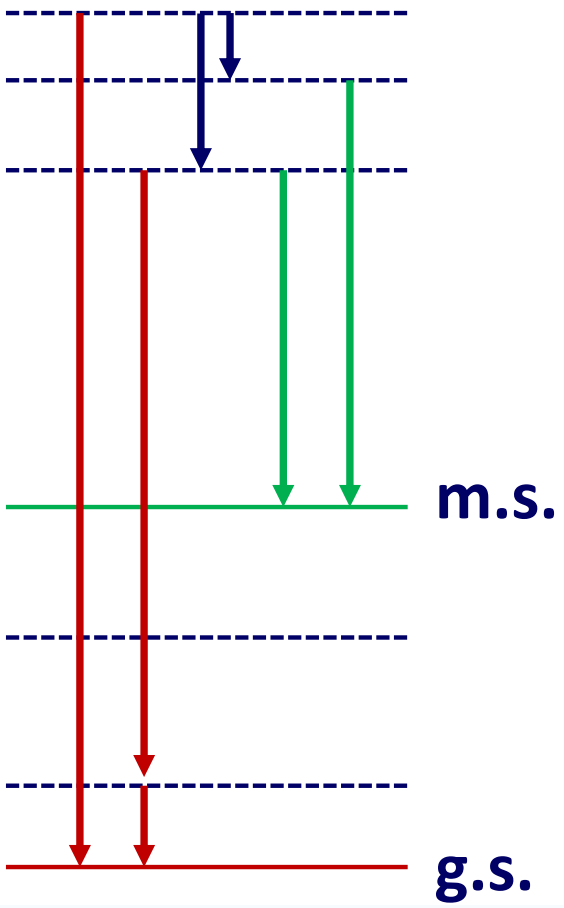
Measurement of IR by measurements of product activities *N*:

$$\frac{\sigma_g}{\sigma_m} = c(t)\left[a\frac{N_g}{N_m} - p\frac{\lambda_g}{\lambda_g - \lambda_m}\right] + p\frac{\lambda_g}{\lambda_g - \lambda_m}$$

N: gamma counts, p: IT probability,

t: irradiation/cooling/counting time

Free from normalization by sample mass, beam flux etc.



Problem in Access to IR information in EXFOR

Extraction of IR from EXFOR is not always straightforward due to variety in the expressions adopted by the author and compiler.

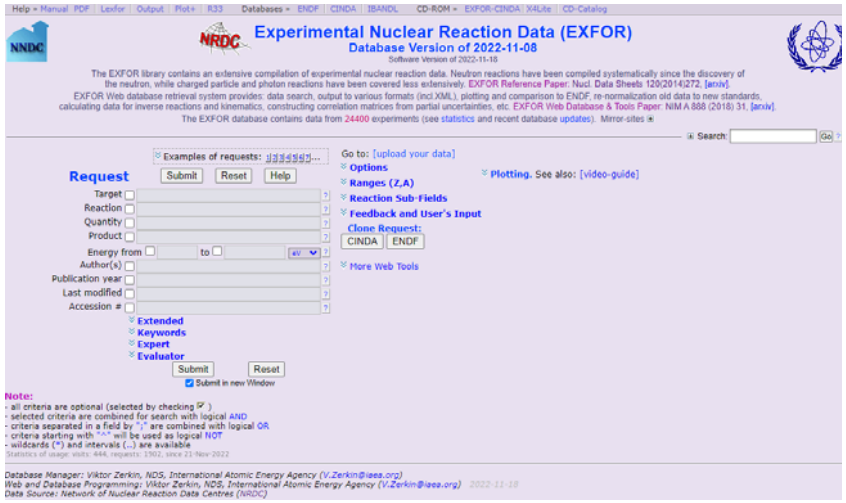
- Varieties in ratio: G/M, M/G, M/T, G/T …
- σ_g and σ_m published/compiled but without IR
- Compilation of σ_g and σ_m with (Z,A) of products as variables in data table (ELEM/MASS in REACTION SF4)
- IR is not in C4/C5 libraries.

Tasks – Alberto's Internship (July-Sept. 2022)

- Extraction of data (cross sections, IR) from EXFOR
- Conversion to unified format and expression (σ_m/σ_t).
- Validation numerically and graphically
- Application

Extraction from EXFOR

NDS web retrieval system



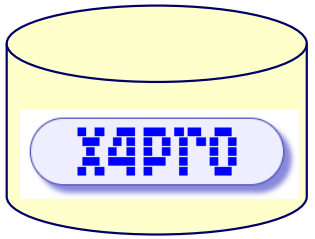
Convenient for quick retrieval and plotting.

Inconvenient for further processing of data downloaded

Good solution to get a large amount of data in computational format.

Retrievable for a part of a dataset.
(e.g., for particular MASS, NUMBER)

X4Pro with SQL commands



SQL Query for X4Pro - $^{16}O(n,\alpha)^{13}C$ Cross Section

Query preparation (x4pro.sql)

```
SELECT
    x4pro_ds.reacode
  ,hdr_x.hdr, hdr_x.units, json_extract(x4.xdat,'$.'||hdr_x.hdr)
  ,hdr_y.hdr, hdr_y.units, json_extract(x4.xdat,'$.'||hdr_y.hdr)
  ,x4pro_ds.DatasetID
FROM
  x4pro_ds
  INNER JOIN x4pro_x4data AS x4     ON x4pro_ds.DatasetID = x4.DatasetID
  INNER JOIN x4pro_hdr    AS hdr_x  ON x4pro_ds.DatasetID = hdr_x.DatasetID   AND hdr_x.hdr  ='EN'
  INNER JOIN x4pro_hdr    AS hdr_y  ON x4pro_ds.DatasetID = hdr_y.DatasetID   AND hdr_y.hdr  ='DATA'
  INNER JOIN REACSTR                ON x4pro_ds.DatasetID = REACSTR.ReacodeID
WHERE
  REACSTR.SF1       = '8-O-16'
  AND REACSTR.SF2   = 'N'
  AND REACSTR.SF3   = 'A'
  AND REACSTR.SF5   = ''
  AND REACSTR.SF6   = 'SIG'
  AND REACSTR.SF7   = ''
  AND REACSTR.SF8   = ''
  AND REACSTR.SF9   = '';
```

SQL Query for X4Pro - $^{16}O(n,\alpha)^{13}C$ Cross Section (Cont)

Query submission on command line

```
[otsukan@NB635819] sqlite3 x4pro.db < x4pro.sql
```

Output

```
...
8-O-16(N,A)6-C-13,,SIG|EN|MEV|4.17|DATA|MB|108.0|21072002
8-O-16(N,A)6-C-13,,SIG|EN|MEV|4.22|DATA|MB|137.0|21072002
8-O-16(N,A)6-C-13,,SIG|EN|MEV|14.8|DATA|MB|328.0|21343010
8-O-16(N,A)6-C-13,,SIG|EN|MEV|12.3|DATA|MB|180.0|21343012
8-O-16(N,A)6-C-13,,SIG|EN|MEV|13.0|DATA|MB|150.0|21343012
8-O-16(N,A)6-C-13,,SIG|EN|MEV|14.1|DATA|MB|295.0|21343012
8-O-16(N,A)6-C-13,,SIG|EN|MEV|16.0|DATA|MB|360.0|21343012
8-O-16(N,A)6-C-13,,SIG|EN|MEV|16.9|DATA|MB|345.0|21343012
8-O-16(N,A)6-C-13,,SIG|EN|MEV|18.0|DATA|MB|240.0|21343012
8-O-16(N,A)6-C-13,,SIG|EN|MEV|19.5|DATA|MB|215.0|21343012
8-O-16(N,A)6-C-13,,SIG|EN|MEV|14.9|DATA|MB|250.0|21461002
8-O-16(N,A)6-C-13,,SIG|EN|MEV|7.136|DATA|MB|86.1|21474003
...
```

Conversion of Cross Sections to IR

Three SQL scripts returned

- ~69k data points for cross sections (Z-S-A in SF4)
- ~15k data points for cross sections (ELEM/MASS in SF4)
- ~9k data points for IR

They were converted to an unified **C4-like format** by a Python script (table.py).

```
#S.K.Ghorai+ (74)
#10359.003     37-RB-85(N,2N)37-RB-84-M,,SIG
#10359.002     37-RB-85(N,2N)37-RB-84,,SIG
# PROJ.   TARG.  PROD.  ISO.1  ISO.2    DATA1-ID    DATA2-ID         EN      DATA1  DATA1-ERR      DATA2  DATA2-ERR        M/T    M/T-ERR
#-----><-----o<-----><-----><-----><--------.o<--------.o<---------><---------><---------><---------><---------><---------><--------->
      1  37085   37084      M      T 10359.003   10359.002   1.5000E+07 6.6200E-01 8.3000E-02 1.1250E+00 1.4100E-01 5.8844E-01 1.0432E-01
      1  37085   37084      M      T 10359.003   10359.002   1.6200E+07 6.8800E-01 8.7000E-02 1.1770E+00 1.4800E-01 5.8454E-01 1.0424E-01
      1  37085   37084      M      T 10359.003   10359.002   1.7000E+07 7.6500E-01 9.9000E-02 1.2350E+00 1.6200E-01 6.1943E-01 1.1414E-01
```

Conversion of Cross Sections to IR (Cont)

of reactions and points converted to the C4-like files

Projectile	γ	n	p	d	^{3}He	α	Total
Reactions	2	186	470	127	34	143	962
Points	9	2,229	4,883	1,915	624	2,653	12,313

Validation of Output

We checked the C4-like output

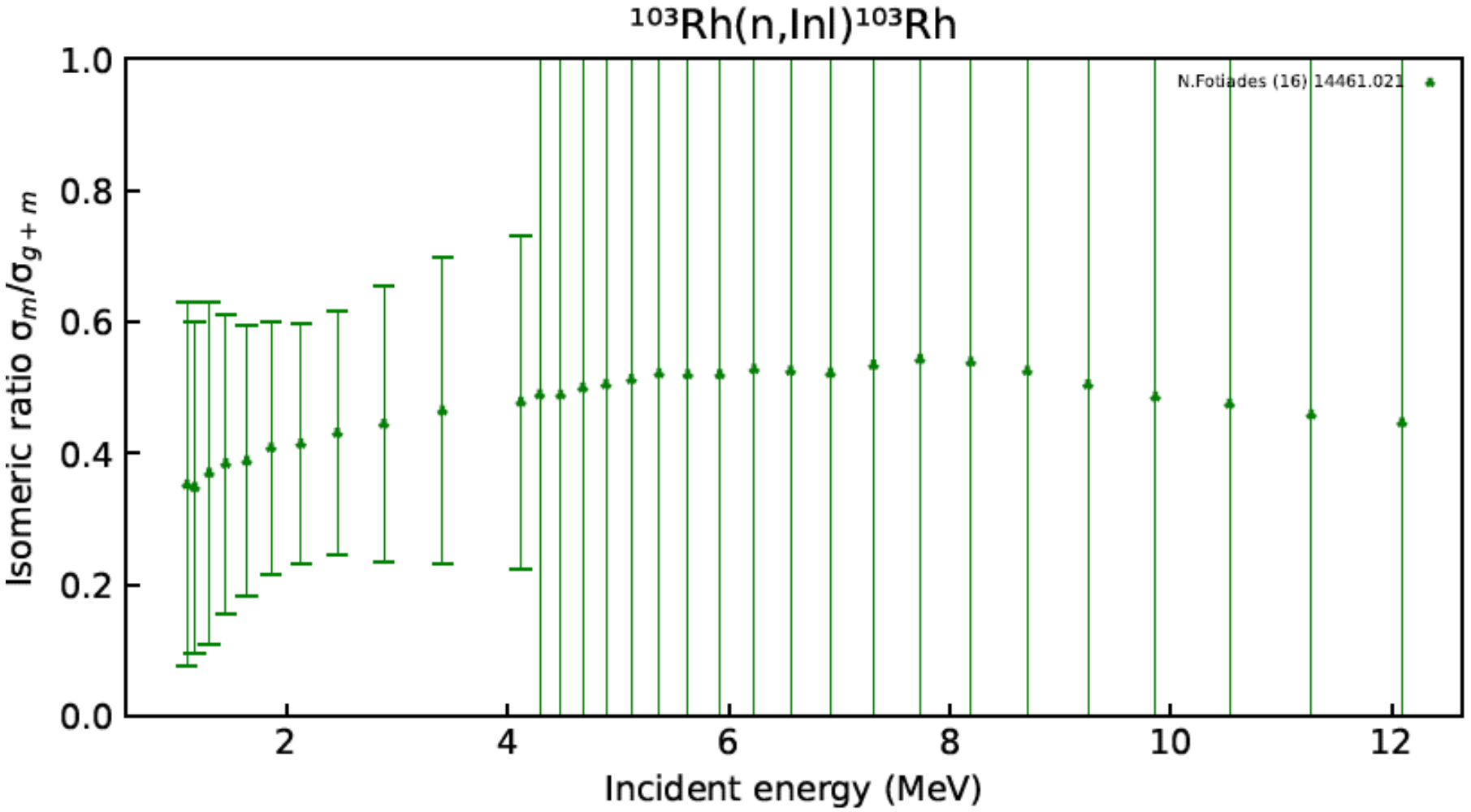
1. numerically for some conditions like $\sigma_m / (\sigma_g+\sigma_m) < 1$, $\sigma_t = \sigma_g+\sigma_m$
2. graphically (Outlier)

and found a lot of problems!!!

- duplication, violation of compilation rule, … (our fault)
- typo in source article, … (publisher / author's fault)

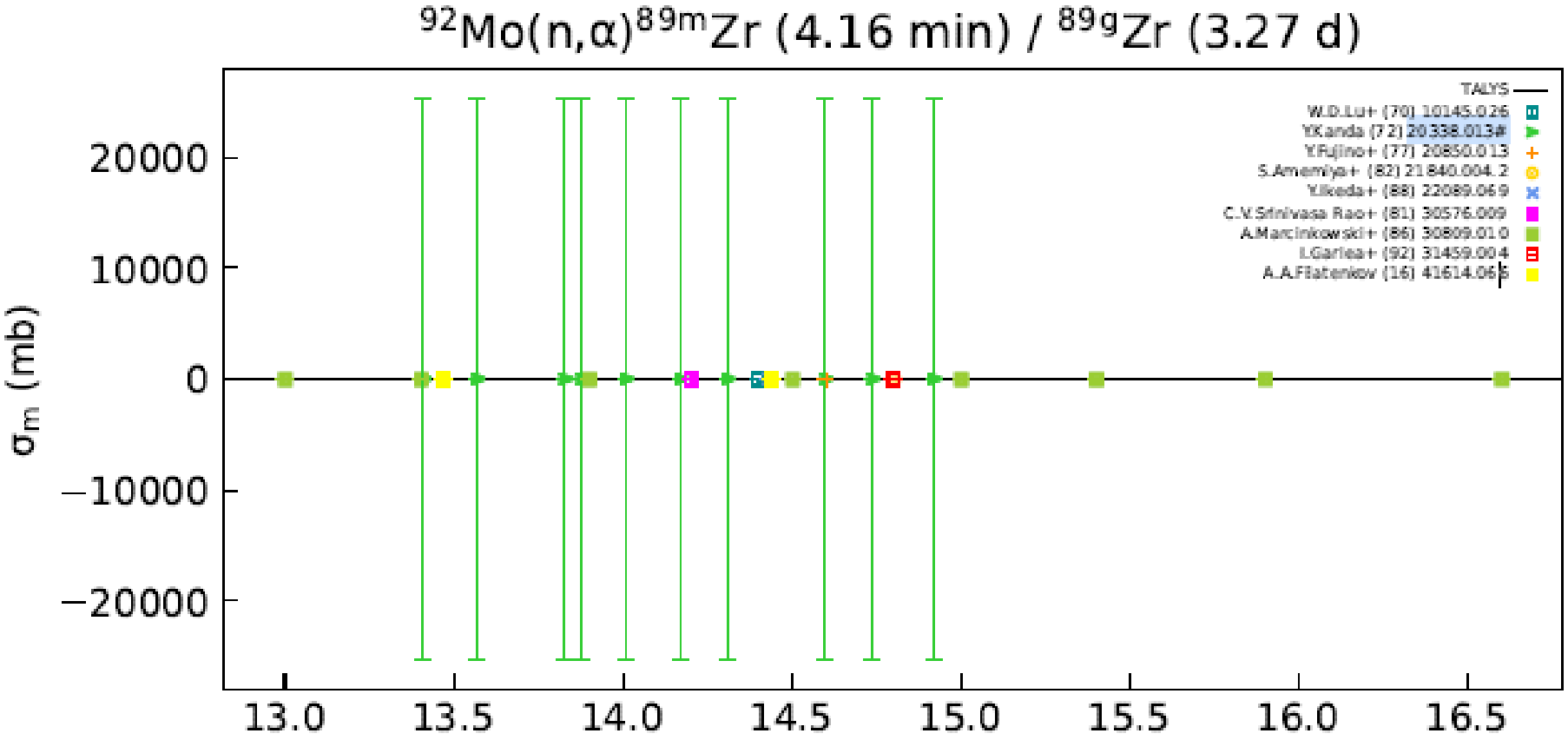
They were checked with authors and fixed manually for our processing (very time consuming process), but also registered in the EXFOR Feedback List.

Validation of Output (Cont)



Compiled IR uncertainties 100 times larger than the actual ones

Validation of Output (Cont)



Trouble due to compilation of ERR-T in both barn and %.

Repetition of headings may cause a serious problem!

Application – Tuning of spin cut-off parameter

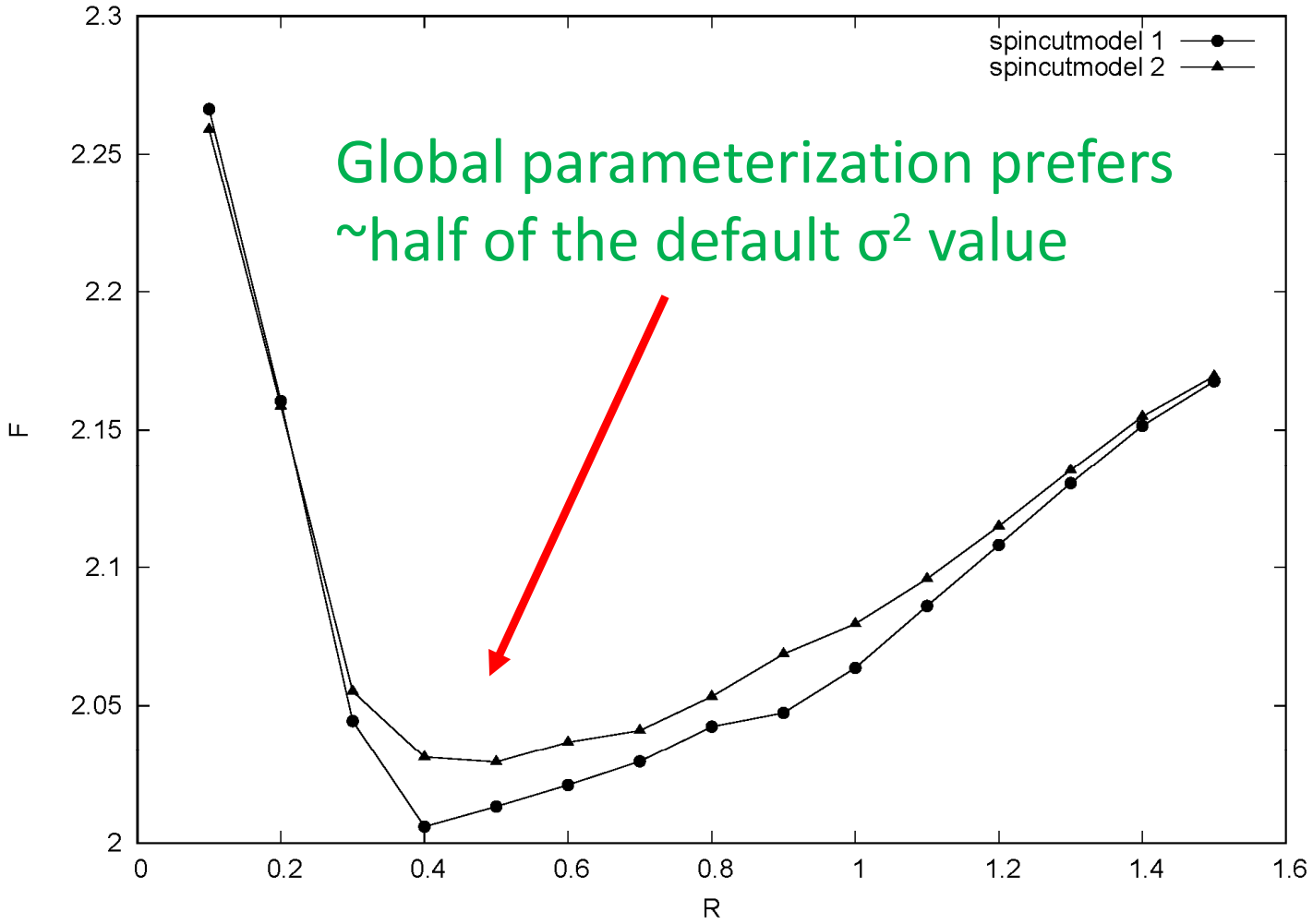
- IR strongly depends on spin distribution of intermediate or final product nuclides.

- Parametrization of spin distribution in Gaussian with spin cut-off parameter σ^2 (SCO in EXFOR!):

$$(2J+1)\exp\left[-\frac{(J+1/2)^2}{(2\sigma^2)}\right]$$

- Adjustment of $R=\sigma^2/\sigma^2_{rig}$ for ~12k experimental IRs by TALYS

Application – Tuning of spin cut-off parameter (Cont)



X4Pro for Preparation of Citation List

X4Pro also helped creation of a citation list for more than 900 EXFOR references, except for the title, for example,

Extraction from X4Pro (=from TITLE in EXFOR)

-MEASUREMENTS OF NEUTRON ACTIVATION CROSS SECTIONS AT 14.4 MEV FOR ZN-68 AND ZR-90-

Actual

Measurements of neutron activation cross-sections at 14.4 MeV for ^{68}Zn and ^{90}Zr

I want to have TITLE more close to the printed one!

Summary

- ~12k of IR values of light-particle induced reactions compiled.
- X4Pro helped a lot. (Thanks, Viktor!) Could be a NRDC product?
- Conversion of EXFOR to SQL, JSON etc. helps users for better readability. But users still need good knowledge of EXFOR (and physics) for proper uses!
- Discovered many compilation errors (not always due to our fault)
- Repetition of heading makes troubles and must be avoided.
- I want to have TITLE close to the printed one.

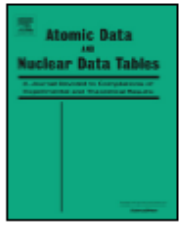
Our Data File and Plots will be Released Soon!

Atomic Data and Nuclear Data Tables xxx (xxxx) xxx

Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt



Compilation of isomeric ratios of light particle induced nuclear reactions

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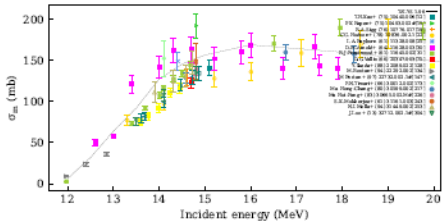
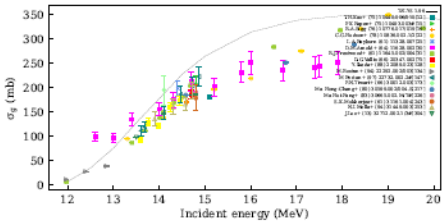
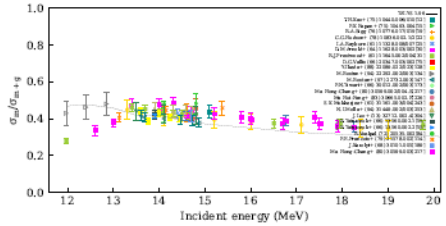
ABSTRACT

Experimental isomeric ratios of light (A ≤ 4) particle-induced nuclear reactions we

```
999999999999999999
  0  0 36 86 36 85 R  86Kr(g,n)85Kr
  0  0 36 86 36 85 H   3.3854E+08        4.5        +1 1.6128E+04        0.5         -1
  0  0 36 86 36 85 D   1.1000E+01                      1.4340E-02 9.9000E-04 1.8010E-02 1.2000E-03     0.
  0  0 36 86 36 85 D   1.1500E+01                      1.6100E-02 9.0000E-04 2.7410E-02 2.5600E-03     0.
  0  0 36 86 36 85 D   1.2000E+01                      1.8500E-02 1.0200E-03 3.5720E-02 3.1500E-03     0.
999999999999999999
  0  0 73181 73180 R  181Ta(g,n)180Ta
  0  0 73181 73180 H   2.9354E+04
  0  0 73181 73180 D   9.2000E+00                      3.0000E-03 3.2000E-03 4.8000E-02 2.1100E-03     0.
  0  0 73181 73180 D   9.7000E+00                      6.0000E-03 3.9000E-03 7.3000E-02 3.2100E-03     0.
  0  0 73181 73180 D   1.0500E+01                      6.0000E-03 2.9000E-03 1.0900E-01 4.8000E-03     0.
  0  0 73181 73180 D   1.0900E+01                      1.3000E-02 4.1000E-03 1.4300E-01 6.2900E-03     0.
  0  0 73181 73180 D   1.1500E+01                      1.5000E-02 5.2000E-03 2.3400E-01 1.0300E-02     0.
  0  0 73181 73180 D   1.2300E+01                      5.4000E-02 2.9000E-02 3.8300E-01 2.7000E-02     0.
999999999999999999
  0  1 17 35 17 34 R  35Cl(n,2n)34Cl
```







Our thanks to the helpful reviewer and editor-in-chief!

And More - INDC(SPN)-4 Arranged by UPM

Comparison with EXFOR and TALYS with TENDL-2019, JEFF-3.3, ENDF/B-VIII.0 extracted from JANIS by Oscar Cabellos

68Zn(n,g)69Zn

T1/2(g.s.)= 56.40 min Jpi(g.s.)= 1/2-
T1/2(m.s.)= 13.75 h Jpi(m.s.)= 9/2+

En (MeV)	Experiment	TENDL	JEFF	ENDF/B
2.5000E-08	0.0730+/-0.0050	0.0672	0.1074	0.0660
2.4000E-02	0.1772+/-0.0765	0.1276	0.1274	0.0724
2.4000E-02	0.1852+/-0.0365	0.1276	0.1274	0.0724
1.9800E-01	0.1890+/-0.0260	0.1746	0.1744	0.0829
2.5700E-01	0.1920+/-0.0140	0.1841	0.1844	0.0864
3.1600E-01	0.2110+/-0.0290	0.1943	0.1942	0.0896

TENDL-2019
JEFF-3.3
ENDF/B-VIII.0
TALYS 1.96
R.Booth+ (58) 11429.010/011
A.K.Chaubey+ (66) 30079.005/006
A.G.Dovbenko+ (73) 40344.004

σ_m/σ_{m+g}

1.0
0.8
0.6
0.4
0.2
0.0

10^{-7} 10^{-5} 10^{-3} 10^{-1} 10^{1}

Incident energy (MeV)

Thank you!

(by Dr. Kazu Nagashima, IAEA NS)