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Program x4toc5

Translation of experimental data from the EXFOR format
to the computation format C5

by

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Created: 1 June 2024
Last modified: 11 June 2024

Vienna-2024

PROGRAM x4toc5

(Version 2024-06-10)

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Introduction

Enclosed is the documentation for program x4toc5. The program is designed to translate experimental data from the EXFOR format (allowing various units and flexible columns order for data and requiring a lot of text analysis) to a Computation format with a fixed units and numerical data in columns. Format C5 is built on the same basic concept as computation format C4 provided by the program X4TOC4*, using the same data columns (1-132), EXFOR reaction data classification via MF.MT providing compatibility with ENDF* data, etc. Program x4toc5 is written on java and provides important extensions of functionality and output data in C5 format: meta data, additional data columns, extended EXFOR data coverage, interpretation of uncertainties, various data recalculations, output options, etc.

* Dermott E. Cullen and Andrej Trkov, Program X4TOC4, report IAEA-NDS-80,
<https://nds.iaea.org/publications/iaea-nds/iaea-nds-0080.pdf>

* See also: EXFOR Formats Description for Uses, edited by Otto Schwerer, IAEA-NDS
https://www-nds.iaea.org/nrdc/nrdc_doc/iaea-nds-0206-200806.pdf#page=52

* ENDF-6 Formats Manual, edited by D. A. Brown, 2023, NNDC, BNL, USA
<https://www.nndc.bnl.gov/endfdocs/ENDF-102-2023.pdf>

Extensions and compatibility of C5 versus C4

Initially, program x4toc5 was created in order to provide two extensions: statistical and systematical uncertainties (in new data columns) and some “meta-data” from EXFOR, like Reaction, Method, Version, Title, Reference, etc. (new lines in the text starting with symbol #). Core structure of data line was preserved from C4 in order to provide backward compatibility for existing end-user’s software.

Later, functionality of x4toc5 was extended to generate correlation matrices on the basis of EXFOR uncertainties, recalculate data for inverse reactions, etc. C5 format was extended accordingly, but until now x4toc5 has an option (flag “-c4”) to generate C4 formatted output.

Dictionaries

x4toc5 is built on general-purpose EXFOR Java package “zv.v.x4” and uses EXFOR-CINDA Dictionaries (DICT_ARC_NEW.* files). In order to provide compatibility in data meaning and definitions with ENDF and X4TOC4, x4toc5 uses Dictionary EXFOR14A.DAT from X4TOC4 and extended table {EXFOR:SF*} \Leftrightarrow ENDF:MF.MT.LR created by V.Pronyaev (2007). For the cases when search in both dictionaries failed, but measured quantity can be identified on the basis of EXFOR Dictionaries, x4toc5 can generate data with known MF and MT=0 (this feature can be deactivated by using flag “-nomt0”).

C5 file structure

C5 file contains Begin-line, Datasets and End-line. Dataset is identified by <Subentry+Pointer> presenting data for single Reaction-code. All information taken from Entry and Subentry is nested into Dataset. In other words, there is no nesting level for Entry and Subentry - all information is repeated in each Dataset. Structure of EXFOR file: [ENTRY:[SUBENT:[Pointer:Reaction]]], C5 file:[Datasets].

- Begin-line contains “#Format-ID”, date and time of file creation, and database time stamp.
- Dataset starts with “#DATASET”, following with meta-data starting with “#”, data and ends with “#/DATASET”. Optionally, file can contain covariance data (flag “-c5m”).
- End-line contains “#/Format-ID” and few numbers - summary of content.

```
#C5M.2.3      20240610      132247      20240529
#DATASET      23114002      20130924
#SUBENT       23114002      20130924
#ENTRY        23114      20170322
#TITLE        High resolution measurements of the 241Am(n,2n)
#AUTHORS      C.Sage, V.Semkova, O.Bouland, P.Dessagne, A.Fernandez,
#AUTHOR1      C.Sage+
#YEAR         2010
#METHOD       ACTIV, GSPEC
#REACTION     95-AM-241 (N, 2N) 95-AM-240,, SIG
#C5DATA
. . . . . Data . . . .
#/C5DATA
# /DATASET    23114002
. . . . .
. . . . . Datasets . . .
. . . . .
#/C5M.2.3
```

Example of Dataset in C5M format (SUBENT 23114002)

```

#DATASET      23114002    20130924
#SUBENT       23114002    20130924
#ENTRY        23114      20170322
#TITLE        High resolution measurements of the 241Am(n,2n)
#+            reaction cross section
#AUTHORS      C.Sage, V.Semkova, O.Bouland, P.Dessagne, A.Fernandez,
#+            F.Gunsing, C.Naestren, G.Noguere, H.Ottmar,
#+            A.J.M.Plompen, P.Romain, G.Rudolf, J.Somers, F.Wastin
#AUTHOR1      C.Sage+
#YEAR         2010
#X4REF1       J,PR/C,81,064604,2010
#REFERENCE1   Jour: Physical Review, Part C, Nuclear Physics, Vol.81, p.064604 (2010)
#DATE         20130924
#INSTITUTE    2FR SAC,2ZZZGEL,2FR CAD,2FR STR,3BULBLA,1USALAS,2ZZZITU,2FR BRC
#METHOD       ACTIV,GSPEC
#REACTION     95-AM-241(N,2N)95-AM-240,,SIG
#C4Reaction   (N,2N),SIG
#ReactionType CS
#MF           3
#MT           16
#PROJ         1
#TARG         95241
#TARGET       95241          [ ]          95-AM-241          [ ]
#REAC1        N,2N
#PRODUCT      95-AM-240
#C4ReaCode    (N,2N),SIG
#Quantity     Cross section
#DataUnits0   B
#DataUnits    ?
#D4REAC       R0#
#ReaCombi     a
#C4FOUND      1
#C4BEGIN      [ 1 95241 3 16 A ]
#DATA-HDR     DATA
#VarFamily    [0 2          ]
#xVariables   1
#+            Y = Y(X1)
#ReacRatio    false
#vReacs       1
#C5EXT1       132          (4F9.0)          dSys,dStat,dOther,dTot //Absolute fully correlated, uncerrelated, partially
correlated and total uncertainties
#C5EXT2       168          (5F9.0)          dSys,dStat,dOther,dTot,dData //Relative uncertainties (dData/Data) in per-cents
#C5DATA       9

```


Columns 1-131 are the same as in C4:

- 1-5 **Proj** Projectile ZA (e.g. for neutron=1, proton=1001)
- 6-11 **Targ** Target ZA (e.g. for 26-Fe-56=26056)
- 12 **M** Target metastable state (e.g. 26-FE-56m=M)
- 3-15 **MF** MF (ENDF conventions, plus additions)
- 16-19 **MT** MT (ENDF conventions, plus additions)
- 20 **P** Product metastable state (e.g. 26-FE-56M=M)
- 21 **X** EXFOR status
- 22 **C** Center-of-mass flag (C=center-of-mass, blank=lab)
- 23-94 8 data fields (each in Fortran E9.3 format)
- 1) 23-31 **Energy** Projectile incident energy
- 2) 32-40 **dEnergy** Projectile incident energy uncertainty
- 3) 41-49 **Data** Data, e.g. cross section, angular distribution, etc.
- 4) 50-58 **dData** Data uncertainty
- 5) 59- 67 **Cos** Cosine or legendre order
- 6) 68-76 **dCos** Cosine uncertainty
- 7) 77-85 **Lvl** Identified by columns 95-97 (e.g. level E, half-life)
- 8) 86-94 **dLvl** Identified by columns 95-97 (e.g. level E, uncertainty)
- 95- 97 **I78** Identification of data fields 7 and 8 (LVL=level energy, LVN=level number, HL=half-life, E2=energy of outgoing particle, EXC=excitation energy, QVL=Q value, TMS=sample temperature, THS= sample thickness, etc.)
- 98-122 **Refer** Reference (first author and year)
- 123-127 **Entry** EXFOR Entry (accession number)
- 128-130 **Sub** Subent (sub-accession number)
- 131 **P** Pointer (multi-dimension table flag)

C5 extension.

C5 indicates center-of-mass flag for every data pair in C5 line “#C.M.Flag” and C4 flag C in 22nd column

Datasets	C.M.Flag	C	Ei	Data	Cos	E2
113,539	0000					
123	0001	I				C.M.
6,444	0010	E			C.M.	
38	0011	M			C.M.	C.M.
947	0100	C		C.M.		
666	0101	K		C.M.		C.M.
15,653	0110	G		C.M.	C.M.	
286	0111	O		C.M.	C.M.	C.M.
1,811	1000	B	C.M.			
105	1010	F	C.M.		C.M.	
195	1100	D	C.M.	C.M.		
159	1101	L	C.M.	C.M.		C.M.
438	1110	H	C.M.	C.M.	C.M.	
140,404	total					

#Datasets: number of Datasets with the Flag in C5 file generated from EXFOR-2024-05-29 (MT=0 excluded)

```
#Proj Targ M MF MT PXC Energy dEnergy Data dData Cos/LO/ZP dCos/LO/AP LVL/HL dLVL/HL I78 Refer (YY) EntrySubP
#----><---->0<--><-->000<-----><-----><-----><-----><-----><-----><-----><-----><-----><--><-->
1 95241 3 16 A 8340000.0 150000.0 0.09680001 0.006292 C.Sage, (10) 23114 2
1 95241 3 16 A 9150000.0 150000.0 0.16290.0092853 C.Sage, (10) 23114 2
1 95241 3 16 A 1.333E7 150000.0 0.24180.0111228 C.Sage, (10) 23114 2
1 95241 3 16 A 1.61E7 150000.0 0.15240.0070104 C.Sage, (10) 23114 2
1 95241 3 16 A 1.716E7 30000.0 0.11610.0051084 C.Sage, (10) 23114 2
1 95241 3 16 A 1.79E7 100000.0 0.10570.0046508 C.Sage, (10) 23114 2
1 95241 3 16 A 1.936E7 150000.0 0.0895 0.007339 C.Sage, (10) 23114 2
1 95241 3 16 A 1.995E7 70000.0 0.10210.0059218 C.Sage, (10) 23114 2
1 95241 3 16 A 2.061E7 40000.0 0.077900010.0068552 C.Sage, (10) 23114 2
```

Columns 132-212 contain detailed information about uncertainties:

132-140	dSys	fully correlated uncertainties (abs.)
141-149	dStat	uncorrelated uncertainties (abs.)
150-158	dOther	partially correlated uncertainties (abs.)
159-167	dTot	total uncertainties (abs.)
168-176	dSys%	fully correlated uncertainties (%)
177-185	dStat%	uncorrelated uncertainties (%)
186-194	dOther%	partially correlated uncertainties (%)
195-203	dTot%	total uncertainties (%)
204-212	dData%	data uncertainties (%)

Example: EXFOR 23114002.x4

```
ERR-ANALYS (ERR-T,,,P) Total uncertainty
(MONIT-ERR,,,P) 27Al(n,a) standard x-section (1.6-5.4%)
(ERR-1,,,U) Counting of 240Am activity (1.4-6.3%)
(ERR-2,,,U) Counting of 24Na activity (0.7-2.0%)
(ERR-3,,,F) Intensity of 240Am gamma line (1.2%)
(ERR-4,,,U) Number of 27Al in sample (0.1%)
(ERR-5,,,P) Number of 241Am in sample (0.3%)
(ERR-6,,,F) 24Na/240Am efficiency ratio (3.0%)
(ERR-7,,,F) Correction for decay of 240Am (0.4-0.9%)
(ERR-8,,,U) Correction for secondary neutron (<1.4%)
```

Example: 23114002.c5, columns 132-221

dSys	dStat	dOther	dTot	dSys%	dStat%	dOther%	dTot%	dData%
<----->	<----->	<----->	<----->	<----->	<----->	<----->	<----->	<----->
0.0032468	0.0049368	0.001862	0.006292	3.35	5.10	1.92	6.50	6.50
0.0053534	0.0067185	0.0031334	0.0092853	3.29	4.12	1.92	5.70	5.70
0.0078724	0.0065554	0.0039362	0.0111228	3.26	2.71	1.63	4.60	4.60
0.0050084	0.0035773	0.0030821	0.0070104	3.29	2.35	2.02	4.60	4.60
0.0038154	0.002125	0.002348	0.0051084	3.29	1.83	2.02	4.40	4.40
0.0034945	0.001596	0.0023469	0.0046508	3.31	1.51	2.22	4.40	4.40
.00294127	0.0060298	0.0027875	0.007339	3.29	6.74	3.11	8.20	8.20
0.0033553	0.002267	0.0041973	0.0059218	3.29	2.22	4.11	5.80	5.80
0.0025601	0.0047398	0.0042131	0.0068552	3.29	6.08	5.41	8.80	8.80

Program x4toc5

Translation of experimental data from the EXFOR format
to the computation format C5

User's Guide

by

Viktor Zerkín

Last modified: 12 June 2024

Vienna-2024

System environment and requirements

- 1) Operating systems: Windows, Linux, MacOS
- 2) JDK/JRE version-1.5 and higher (Java Development Kit/Java Runtime Environment)
- 3) Disk space ~100 MiB

Package distribution

The package distribution includes

1. Source codes in Java
2. Make files (bat and bash) for Windows/Linux/MacOS
3. Dictionaries in the format DICT_ARC_NEW
4. Test EXFOR files
5. Test scripts (bat and sh)
6. Plotting examples (Python + Plotly + scripts to run)
7. Test-results for checking/comparison by end-user

```
x4toc5
|   help.txt
|   LICENSE.TXT
|   make1.bat
|   make1.sh
|   README.md
|   README.md
+---bin
|       x4toc5.jar
+---doc
|       x4toc5.pdf
+---src
|   |   *.java
|   |   package-info.java
|   +---x4dict
|       |   DICT_ARC.TOP
|       |   DICT_ARC_NEW.*
+---tests
|   |   *.x4
|   |   c5file.py
|   |   c5line.py
|   |   c5plot1sig.py
|   |   c5subr.py
|   |   levels.zip
|   |   plot1.bat
|   |   plot1.sh
|   |   test1.bat
|   |   test1.sh
|   |   x4toc5.jar
+---tests-result
|   |   *.c5
|   |   *.c5m
|   |   *.html
|   |   *.png
|   |   test1.tto
|   |   ....
```

1. Preparation steps

1.1. Install Java

Example for Linux-Ubuntu:

```
$ sudo apt-get install openjdk-8-jdk
```

-or-

```
$ sudo apt-get install default-jdk
```

1.2. Check and install Python and Plotly (optional)

Example for Linux-Ubuntu:

```
$ python3 --version
```

```
$ sudo apt-get install python3-pip
```

```
$ pip3 install plotly
```

1.3. Download and check package

Example for Linux-Ubuntu:

```
$ cd ~/x4toc5
```

```
$ du -hc --time --max-depth=1
1008K  2024-06-10 11:40 ./bin
83M    2024-06-10 11:58 ./tests-result
5.6M   2024-06-10 12:25 ./src
8.8M   2024-06-10 11:47 ./tests
99M    2024-06-10 12:25 .
99M    2024-06-10 12:25 total
```

1.4. Prepare RIPL-Levels for tests (optional, to be used with flag “-mt51”)

Example for Linux-Ubuntu:

```
$ cd tests
```

```
$ unzip levels.zip
```

1.5. Recompile source codes and prepare new JAR archive (optional)

Linux/MacOS:

```
$ bash make1.sh
```

Windows:

```
$ make1.bat
```

2. Run program

The code and Dictionaries are distributed as source and binary (JAR archive) files ready to run in any Java Virtual Machine. The program can run from JAR file or compiled and run from class files:

```
$ java -jar x4toc5.jar myexfor.x4
$ javac -d . *.java
$ java zvv.x4.x4toc5 myexfor.x4
```

2.1. Display help (running without input file)

```
$ java -jar x4toc5.jar

Translate EXFOR to C5 computational format
Program x4toc5, ver. 2024-06-10
V.Zerkin, IAEA, Vienna, 2010-2024

Run:  $ java [flags] x4toc5 file.x4 [options]

Options:
  -o:file      output file, default: file.x4.c5
  -dict:dir    directory with EXFOR Dictionaries, default: -dict:x4dict/
  -dlvl:dir    directory with levels,                default: -dlvl:levels/
  -split:dir   output C5 file for every Entry to a file in directory:
                1/123/12345.c5
  -c5          output format: C5 (default)
  -c5m         output format: C5M (C5+correlation matrix)
  -c4          output format: C4
  -i           recalculate data to inverse reactions, e.g.:
                6-C-13(A,N)8-O-16,,SIG --> 8-O-16(N,A)6-C-13,,SIG
                2-HE-4(P,D)2-HE-3,,DA  --> 2-HE-3(D,P)2-HE-4,,DA
  -i:file      inverse data for the reactions listed in the file
  -cm2lab      convert EN-CM, ANG-CM, DATA-CM from C.M. to Lab. (MF4 only)
  -norr        do not convert DATA: Rutherford-Ratio to B/SR
  -noqe        do not replace Q-Value by E-Level for partial XS
  -mt51        replace MT by MT+iLevel (for MT:51,601,651,701,751,801)
  -nomt0       do not process Datasets with unknown MT
  -sort        sort data by independent variables (EN, AN, E2)
  -h[elp]      print this text
  -ps          show process
  -debug       set debug mode

Java flags:
  -Xmx<size>   set maximum Java heap size
  -cp <paths>  list of directories, JAR archives to search for class files
  -jar <path>  file with binaries (archive of classes - compiled java codes)

Examples:
  $ java x4toc5 myfile.x4
  $ java x4toc5 x4.x4 -dict:x4dict/
  $ java -Xmx400M -jar x4toc5.jar x4.x4 -i -o:x4.x4.c5i
```

3. Run tests

3.1. Tests

- 1) *Display help-info*
- 2) *Convert x4 to c5 with default options*
- 3) *Convert x4 to c5, split output by Entry*
- 4) *Convert x4 to c4*
- 5) *Inverse reaction data*
- 6) *Generate correlation matrix*
- 7) *Replace MT by MT+iLevel from RIPL-Levels for partial reactions*
- 8) *Keep Q-Value, i.e. do not replace by Energy-Level*
- 9) *Inverse reaction data for selected reaction*
- 10) *Convert C.M. to Lab system*
- 11) *Plotting Cross Sections*

3.2.a) Linux/MacOS

```
$ cd ~/x4toc5/tests
$ bash test1.sh
... Confirm next test: Press <ENTER> ...
$ bash plot1.sh
... opens window in your Web-Browser ...
```

3.2.b) MS-Windows

Press <Win/R>, type cmd ..., press <ENTER>. You should get Terminal-window.

```
$ cd C:\x4toc5\tests
$ test1.bat
... Confirm next test: Press <ENTER> ...
$ plot1.bat
... opens window in your Web-Browser ...
```

3.3. Test results

You should get new files in the “tests” directory with extensions .c5.*

Examples of output if provided in the directory “tests-result” for comparison and checking.

3.4. Plot results

If you have Python3 and Plotly installed, python-code will open two tabs in your browser:

Cross sections $\sigma(E)$: 13-AL-27(N,A)11-NA-24,,SIG #Datasets:86/86/86
EXFOR-C5, by V.Zerkin, IAEA-NDS, 2010-2024, ver.2024-06-09 //running:2024-06-10 11:53:41

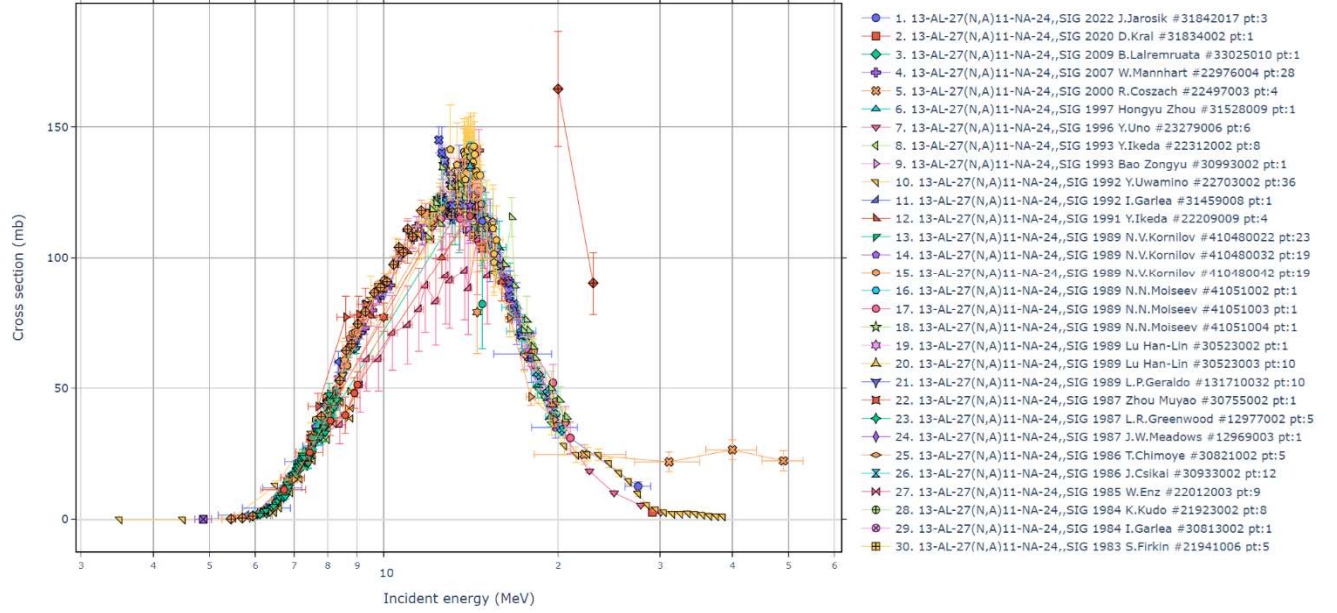


Fig.1. Data for reaction: 13-AL-27(N,A)11-NA-24,,SIG

Cross sections $\sigma(E)$: 8-O-16(N,A)6-C-13,PAR,SIG; 8-O-16(N,A)6-C-13,,SIG and inverted 6-C-13(A,N)8-O-16,,SIG #Datasets:3/3/3
EXFOR-C5, by V.Zerkin, IAEA-NDS, 2010-2024, ver.2024-06-09 //running:2024-06-10 11:53:44

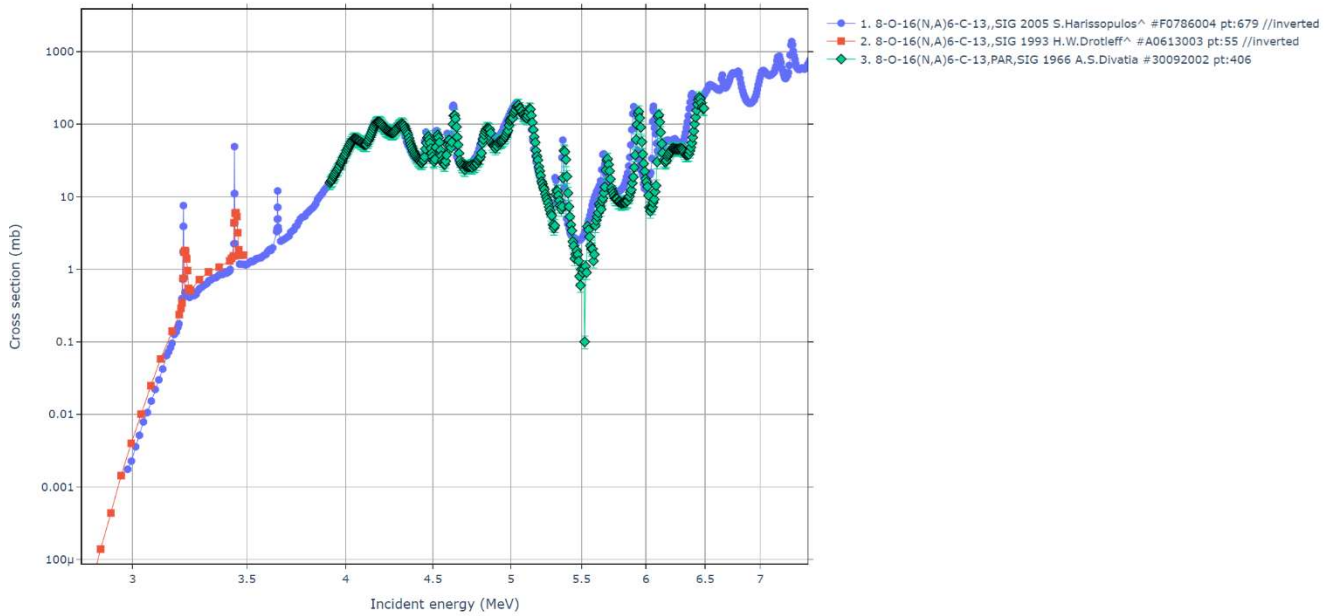


Fig.2. Data for reaction: 8-O-16(N,A)6-C-13,,SIG and inverted 6-C-13(A,N)8-O-16,,SIG