WP2009-14

Isotopic abundance as coded information

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1. Coding of isotopic abundance under SAMPLE

Activation cross sections measured by natural samples can be converted to cross sections for enriched samples by using natural isotopic abundances. When experimentalists tabulate such cross sections, they often tabulate isotopic abundances values as well as other parameters (e.g. decay data). We would propose a new formalism for coding of isotopic abundance values used by authors for.

Example 1: ^{47}Ti(n,p)^{47}Sc cross section measured by natural titanium sample

`SAMPLE (22-TI-47,NAT=0.0744) Normalized to the number of Ti-47 nuclei`

This means authors obtained the cross section for enriched samples as follows:

$$\sigma[^{47}\mathrm{Ti(n,p)}^{47}\mathrm{Sc}] = \sigma[^{nat}\mathrm{Ti(n,x)}^{47}\mathrm{Sc}] / 0.0744$$

2. New modifier for ratio of isotopic abundance - RAB

Conversion explained above is sometimes applied when more than two reaction channels open:

Example2: ^{47}Ti(n,p)^{47}Sc cross section measured by natural titanium sample

Above equation is not valid when neutron energy is higher than 9.4 MeV:

En< 9.4 MeV:

$\sigma[^{47}\mathrm{Ti(n,p)}^{47}\mathrm{Sc}]$

9.4 MeV < En < 17.7 MeV:

$\sigma[^{47}\mathrm{Ti(n,p)}^{47}\mathrm{Sc}] + \sigma[^{48}\mathrm{Ti(n,x)}^{47}\mathrm{Sc}]\ \mathbf{[a(^{48}Ti)/a(^{47}Ti)]}$

17.7 MeV<En < …

$\sigma[^{47}\mathrm{Ti(n,p)}^{47}\mathrm{Sc}] + \sigma[^{48}\mathrm{Ti(n,x)}^{47}\mathrm{Sc}]\ \mathbf{[a(^{48}Ti)/a(^{47}Ti)]} + \sigma[^{49}\mathrm{Ti(n,x)}^{47}\mathrm{Sc}]\ \mathbf{[a(^{49}Ti)/a(^{47}Ti)]}$

… ("a" stands for natural isotopic abundances.)

So far such quantity has been coded with general quantity modifier FCT

```
(22-TI-47(N,P)21-SC-47,,SIG)+(22-TI-48(N,X)21-SC-47,,SIG,,FCT)
(22-TI-47(N,P)21-SC-47,,SIG)+(22-TI-48(N,X)21-SC-47,,SIG,,FCT)+
(22-TI-49(N,X)21-SC-47,,SIG,,FCT)
```

For attention to users, we would propose to use a new modifier **RAB** (Ratio of ABundances) instead of FCT.

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Memo CP-D/546

Date: 24 February 2009
To: Distribution
From: N. Otsuka, O. Schwerer, W. Mannhart

Subject: **Coding of elemental cross section divided by isotopic abundance**

Sometimes cross section for natural targets (elemental cross sections) divided by natural isotopic abundances are reported [1].

Example: ^{nat}Ti(n,x)^{47}Sc
Below 9.4 MeV, only ^{47}Ti(n,p)^{47}Sc contributes to the ^{47}Sc production. Above 9.4 and 11.7 MeV, ^{48}Ti(n,d)^{47}Sc and ^{48}Ti(n,np)^{47}Sc channels open, respectively. (The channel ^{49}Ti(n,x)^{47}Sc opens above 17.7 MeV). Four EXFOR subentries give elemental cross sections divided by the natural isotopic abundance of ^{47}Ti between 9.4 and 17.7 MeV:

$$\sigma(\text{given}) = \sigma(^{nat}\text{Ti(n,x)}^{47}\text{Sc}) / a(^{47}\text{Ti})$$
$$= \sigma(^{47}\text{Ti(n,p)}^{47}\text{Sc}) + [a(^{48}\text{Ti})/a(^{47}\text{Ti})]\ \sigma(^{48}\text{Ti(n,x)}^{47}\text{Sc})$$

Subentry	Emin (MeV)	Emax (MeV)	REACTION (current)
21941.003	14.1	14.1	(22-TI-47(N,P)21-SC-47,,SIG)+ (22-TI-48(N,N+P)21-SC-47,,SIG,,A)
21999.011	14.7	14.7	(22-TI-47(N,P)21-SC-47,,SIG)+ (22-TI-48(N,D)21-SC-47,,SIG)
22976.009	7.4	14.9	(22-TI-47(N,P)21-SC-47,,SIG)+ (22-TI-48(N,X)21-SC-47,,SIG,,FCT)
30627.003	13.8	14.9	(22-TI-47(N,P)21-SC-47,,SIG)+ (22-TI-48(N,N+P)21-SC-47,,SIG)

These cross sections are plotted in **Fig.1** with the cross sections measured with an enriched target by Y. Ikeda (22089.027). Only 22976.009 is coded well. Other REACTIONs should be corrected.

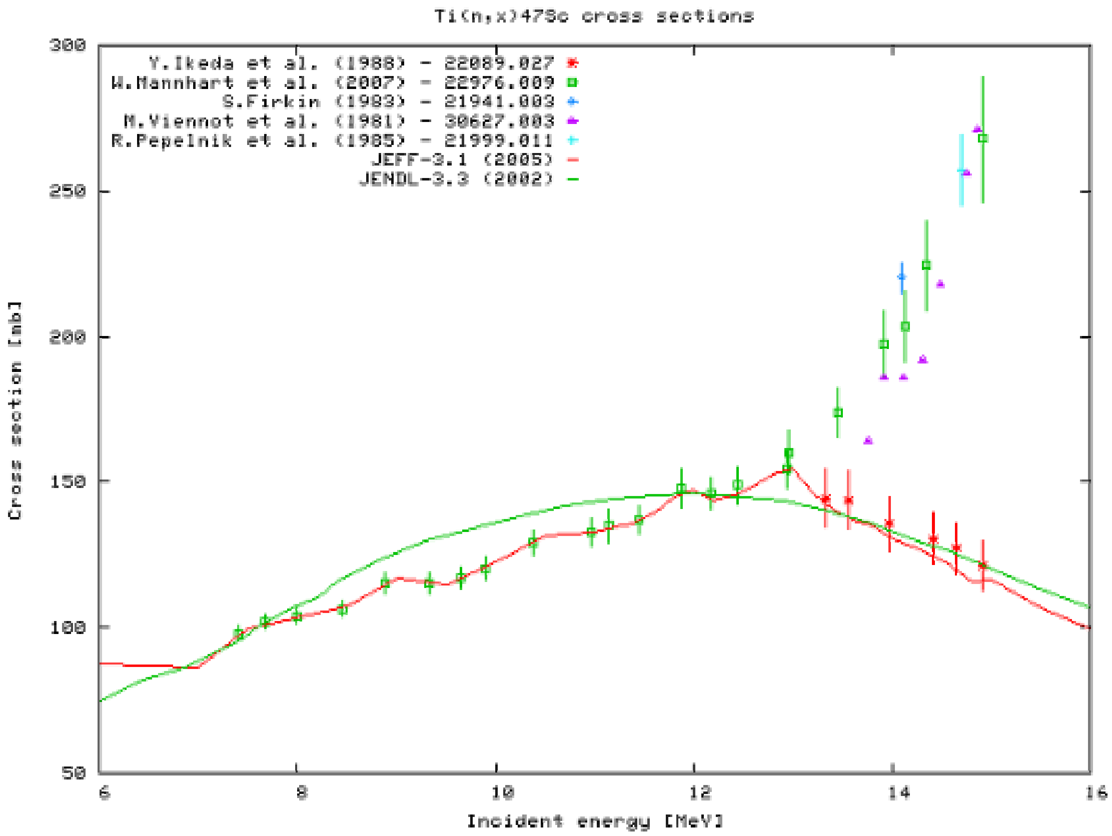


Fig. 1. σ (^{nat}Ti(n,x)^{47}Sc) / a(^{47}Ti) in EXFOR with σ (^{47}Ti(n,p)^{47}Sc) in JEFF-3.1 and JENDL-3.3 (=ENDF-B/VII)

Remarks

(1) We prefer the expression of the REACTION sum because it states exactly the contributing reaction channels. Because FCT is a generic code for multiplication of any constant, we would introduce a new modifier (say RAB):

Above 9.4 MeV

```
(22-TI-47(N,P)21-SC-47,,SIG)+(22-TI-48(N,X)21-SC-47,,SIG,,RAB)
```

Above 17.7 MeV

```
(22-TI-47(N,P)21-SC-47,,SIG)+(22-TI-48(N,X)21-SC-47,,SIG,,RAB)+
(22-TI-49(N,X)21-SC-47,,SIG,,RAB)
```

, etc. We would propose the following new modifier and quantity codes

Dictionary 34 (Modifiers)

RAB	Times natural isotopic abundance, divided by abundance of target of first term of REACTION sum

Dictionary 236 (Quantities)

,SIG,,RAB	Cross section times natural isotopic abundance, divided by abundance of target of first term of REACTION sum

(2) They are normalized by the natural isotopic abundances and therefore depend on the values of abundances adopted by authors. Actually we often see that authors tabulate values of abundances. For future renormalization, it would be better to code the value used by authors as follows:

```
SAMPLE (22-TI-47,NAT=0.0744) Normalized to the number of Ti-47 nuclei
```

Only the values explicitly given in the articles may be given. A update of LEXFOR entry is proposed below.

SAMPLE. Used to give information on the structure, composition, shape, *etc*., of the measurement sample. May contain codes and/or free text, see below.

1. Presence of this keyword is optional. However, presence is obligatory and must contain coded information when the data modifier RAB is coded in the REACTION.
2. Coded information may be given also for enriched samples.
3. The general format of the code is : (nuclide, abundance)

Nuclide field: A code of the form *Z-S-A-X*.

Abundance field: The field identifier `NAT=` or `ENR=` followed by the isotopic abundance of the natural or enriched sample, respectively. Only the values assumed by the author for obtaining the data are given.

Examples:

```
SAMPLE (22-TI-47,NAT=0.0744) Normalized to the number of Ti-47 nuclei

SAMPLE (22-TI-46,ENR=0.955) Enriched sample, 95.5% Ti-46, 3.5% Ti-48
       (22-TI-48,ENR=0.035)
```

Two documents are appended:
Appendix I: $^{nat}Ti(n,x)^{46}Sc$ and $^{nat}Pt(n,x)^{195m}Pt$
Appendix II: Comments on the draft of this memo from W.M.

Reference

[1] For example, W. Mannhart and D. Schmidt, Report PTB-N-53 (2007)

Appendix I: ^{nat}Ti(n,x)^{46}Sc and ^{nat}Pt(n,x)^{195m}Pt

Two similar examples in EXFOR are also investigated.

1. ^{46}Ti(n,p)^{46}Sc and ^{47}Ti(n,x)^{46}Sc

Threshold energies: 1.6 MeV for ^{46}Ti(n,p)^{46}Sc, 8.4 MeV for ^{47}Ti(n,d)^{46}Sc, 10.7 MeV for ^{47}Ti(n,np)^{46}Sc, 17.7 MeV for ^{48}Ti(n,x)^{46}Sc. Some activation cross sections measured with natural samples are summarized below.

#	Subentry	REACTION (current)	E (MeV)	σ (mb) 14.5 MeV	a(^{46}Ti)
1	13586.002	(22-TI-46(N,P)21-SC-46,,SIG)+	10.0	-	8.0%
	13586.012	(22-TI-47(N,N+P)21-SC-46,,SIG)	14.7	~300	
2	21999.010	(22-TI-46(N,P)21-SC-46,,SIG)+ (22-TI-47(N,D)21-SC-46,,SIG)	14.7	~300	?
3	22657.002	(22-TI-46(N,P)21-SC-46,,SIG)+ (22-TI-47(N,N+P)21-SC-46,,SIG)	14.7	~310	8.0%
4	22763.002	22-TI-0(N,X)21-SC-46,,SIG	12.6-**19.6**	~300	8.2%
5	31419.002	22-TI-0(N,X)21-SC-46,,SIG	7.5	-	8.2%
6	32592.003	22-TI-46(N,P)21-SC-46,,SIG	13.5-14.8	~300	8.0%
7	32619.003	22-TI-0(N,X)21-SC-46,,SIG	4.5-**18.0**	~290	7.93%

They are consistent with σ(^{nat}Ti(n,x)^{46}Sc) / a(^{46}Ti) (**Fig.2**). Articles of #1 - #5 explicitly mention that σ(^{nat}Ti(n,x)^{46}Sc) divided by *a*(^{46}Ti) are given. Authors of #6 and #7 do not explain such normalization, but contribution of ^{47}Ti(n,p+n), (n,n+p) and (n,d)^{46}Sc is mentioned. Therefore the current REACTIONs should be corrected to (22-TI-46(N,P)21-SC-46,,SIG)+(22-TI-47(N,X)21-SC-46,,SIG,,RAB) etc.

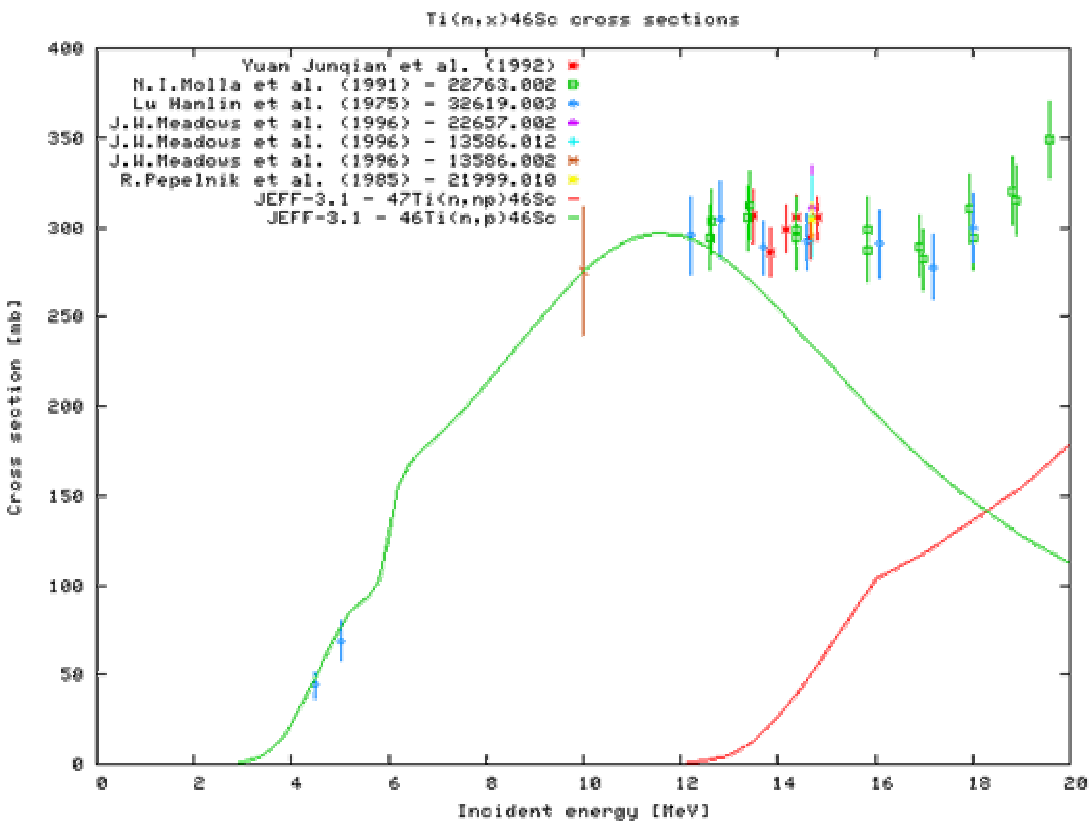


Fig. 2. $\sigma(^{nat}Ti(n,x)^{46}Sc)$ / $a(^{46}Ti)$ in EXFOR compared with $\sigma(^{46}Ti\ (n,p)^{46}Sc)$ and $\sigma(^{47}Ti(n,np)^{46}Sc)$ in JEFF-3.1

2. $^{195}Pt(n,n')^{195m}Pt$ and $^{196}Pt(n,2n)^{195m}Pt$

Threshold energies are 1.6 MeV for $^{195}Pt(n,n)^{195m}Pt$, 8.4 MeV for $^{196}Pt(n,2n)^{195m}Pt$, 21.7 MeV for $^{175}Pt(n,3n)^{195m}Pt$. The capture reaction $^{194}Pt(n,\gamma)^{195m}Pt$ also contributes to the cross section (in order of a few milli-barn). Some activation cross sections measured with natural samples are summarized below.

#	Subentry	REACTION (current)	E (MeV)	σ (mb) 14.5 MeV	$a(^{196}Pt)$
1	10244.004	(78-PT-196(N,2N)78-PT-195-M,,SIG,,(A))+(78-PT-195(N,INL)78-PT-195-M,,SIG,,(A))	14.4	~460	-
	30715.002		0.1-1.0	-	-
	30715.003		1.4-5.6	-	-
2	30715.004	78-PT-0(N,X)78-PT-195-M,,SIG	13.7-17.8	~410	-
	30715.005		13.0-17.4	~440	-
3	30733.013	78-PT-0(N,X)78-PT-195-M,,SIG	8.5	-	-
4	31622.009	(78-PT-196(N,2N)78-PT-195-M,,SIG,,A)+(78-PT-195(N,INL)78-PT-195-M,,SIG,,A)	13.5-14.6	~600	25.3%

They are consistent with $\sigma(^{nat}Pt(n,x)^{195m}Pt)$ except for 31622.009 (**Fig.3**). For 10244.004, We proposes to replace modifiers `(A)` by `A`. (then the REACTION code is equivalent to `78-PT-0(N,X)78-PT-195-M,,SIG`). The energy dependence of 31622.009 looks strange..

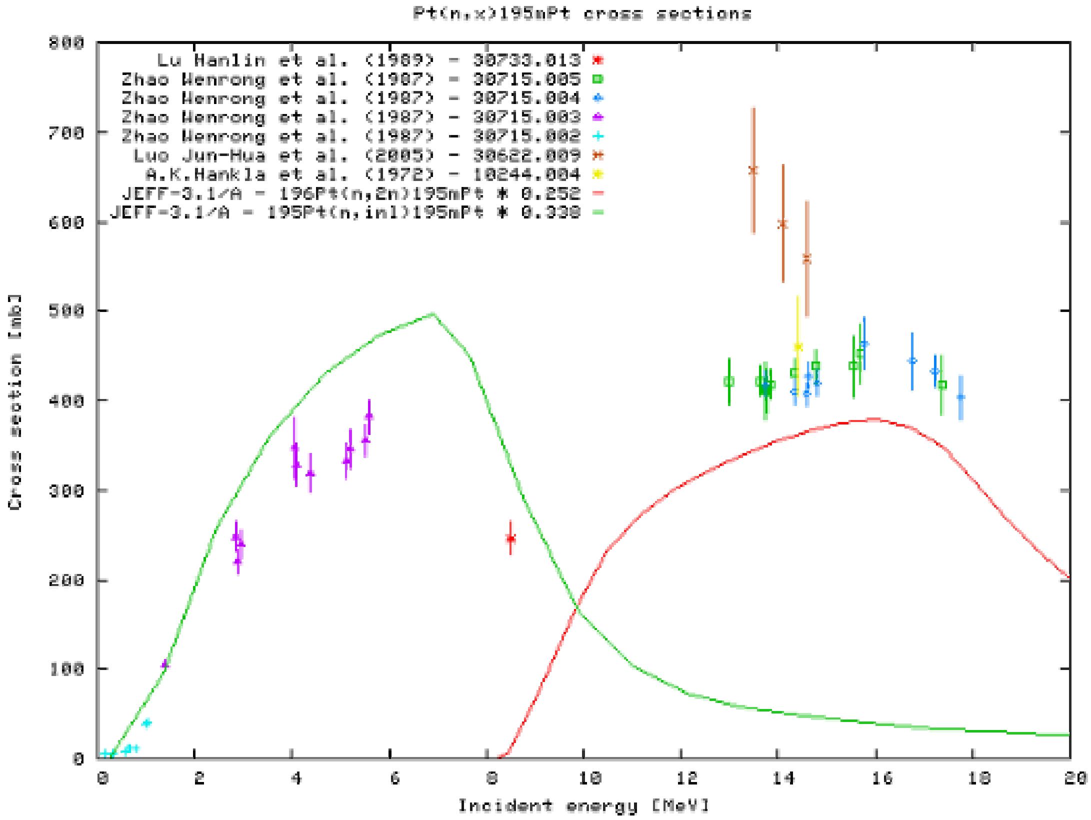


Fig. 3. σ(^{nat}Pt(n,x)^{195m}Pt) in EXFOR with σ(^{195}Pt(n,inl)^{195m}Pt * a(^{195}Pt) and σ(^{196}Pt(n,2n)^{195m}Pt * a(^{196}Pt) in JEFF-3.1/A

(Note: In the legend of this Fig.3, the accession no. pertaining to Luo Jun-Hua should be 31622.)

Appendix II: Comments on the draft of this memo from Dr. W. Mannhart (Feb 6, 2009)

Point 1:

In the discussion of the appropriate coding of the cross sections I will use the reaction ^{47}Ti(n,p)^{47}Sc + ^{48}Ti(n,x)^{47}Sc as an illustrative example.

I believe we have to consider in our discussion two aspects in parallel:

a) Which values were given in the experiments, isotopic or elemental cross sections?
b) How work the EXFOR search and plot routines with such data.

a) Given cross sections of experiments performed with elemental samples

Isotopic cross section (normalized to the number of ^{47}Ti nuclei = [N_{Ti} a(^{47}Ti)])

σ (given) = σ (^{47}Ti(n,p)^{47}Sc) + [a(^{48}Ti)/a(^{47}Ti)] σ (^{48}Ti(n,x)^{47}Sc) (1)
[primary reaction] [secondary reaction]

or elemental cross section (normalized to the number of ^{nat}Ti nuclei = N_{Ti})

σ (given) = σ (^{nat}Ti(n,x)^{47}Sc) (2)

With eqn. (1) we have the following alternatives in coding:

((22-TI-47(N;P)21-SC-47,,SIG) + (22-TI-48(N,X)21-SC-47,,SIG,,FCT)) (C1)

(22-TI-0(N,X)21-SC-47,,SIG,,**FCT**) being **σ(^{nat}Ti(n,x)^{47}Sc) / a(^{47}Ti)** (C2)

(22-TI-47(N,P)21-SC-47),,SIG,,**NAT**) (C3)

and with eqn.(2)

(22-TI-0(N,X)21-SC-47,,SIG) (C4)

For the coding C1-C3 the value of a(^{47}Ti) used must be quoted. In the case of C1 (see also eqn. (1)), there is no real need to give the numerical value of a(^{48}Ti). This value is optional.

The coding C1 is the most precise one. It indicates that the given cross section is the sum of two isotopic cross sections with a factor, and states exactly the contributing reaction channels.

The coding C2 is formally correct. However, the coding of C2 is too similar to C4 and will result, at 14.5 MeV, in quite different numerical values of ~220 mb (C2) and ~20 mb (C4), both with a common reaction string of (22-TI-0(N,X)21-SC-47,,SIG).

The coding C3 is an alternative to C1. The disadvantage of C3 (and of C4) is that the user has to investigate which additional reaction channel contributes to the cross section at a given neutron energy.

b) EXFOR search und plot routines

I have done two EXFOR searches. The result of the search of "Ti-47(n,p)" is shown in the attached file **plot_example.doc** and the result of the second search of "Ti-0(n,x)Sc-47" is shown in the file named **plot_example_2.doc**. The results were converted to the given plots which show at the right hand side the data sets used. We have to note that isotopic and elemental cross sections can only be handled in different searches.

In the isotopic search, let us first regard the data set 22976.009 (my experiment). The data cover the energy range below **and** above the threshold of the ^{48}Ti(n,x)^{47}Sc reaction. One recognizes clearly that the data below 11.7 MeV correspond to the ^{47}Ti(n,p)^{47}Sc cross section. And above 11.7 MeV, one can see that the secondary reaction channel has opened. Similar data sets are "Firkin 83", "Pepelnik 85" and "Viennot 81, even if the reaction codes given are not always correct. In the plot, the only experiment performed with isotopic samples is "Ikeda 88". All other data given in the plot were measured with elemental samples.

With the elemental search one obtains at all only three experiments. The elemental cross sections can only be compared with other elemental data. The data of "Greenwood 87" and "Meadows 87" are elemental cross sections. The data of "Molla 91" look for elemental cross sections, but were actually normalized in a quite **unorthodox** way with a(^{47}Ti)+a(^{48}Ti) = 81.2%. (The normalization value of 8.2% given in the EXFOR file is wrong and extremely misleading). The numerical values exceed the elemental cross section by 23% and should be coded as:

(22-TI-0(N,X)21-SC-47,,SIG,,**MSC**)

to state the crazy normalization.

However, this experiment demonstrates also what happens if other data are coded in EXFOR with C2, a format which differs only in the qualifier:

(22-TI-0(N,X)21-SC-47,,SIG,,**FCT**).

We would get elemental cross sections in the EXFOR file which represent data sets of different magnitudes (220 mb and 20 mb, here). In the case of "Molla 91" there remains probably no alternative. In all other cases we should avoid reaction codes which are misleading and will confuse the users.

In summary:

The limited possibilities to compare data in the elemental EXFOR search suggest to code with C4 only such data which are directly given by the authors as elemental cross sections.

All other data should be coded with C1 (or eventually with C3) and in both cases the modifier, FCT or NAT, **requires** that the relevant isotopic abundance must be specified. The second term in the coding of C1 is a distinct warning that the primary cross section is only valid up to the threshold of the secondary reaction.

The coding with C2 cannot be recommeded. It will produce data which are to a high degree misleading.

With increasing neutron energy, further reaction channels will open. This means that eqn. (1) can only be applied in a limited energy region (in the neighbourhood of the threshold of the secondary reaction). With increasing complexity the form of eqn. (4) and the coding with C4 becomes automatically mandatory.

Point 2:

I agree completely with you in the following. In the experiments the isotopic abundance is of similar importance as the monitor cross section and the decay data used. All three data are needed to allow a proper renormalization of the EXFOR cross sections with the latest values of the mentioned quantities. I support strongly your proposal to introduce a new format in the future:

Instead of

SAMPLE **(22-TI-47,7.44)** Natural (elemental) sample

I would recommend a more precise definition:

DATA NORM **(22-TI-47,7.44%)** Elemental sample used

The format will replace the "free text" and can be combined with both reaction codes, C1 and C3.

Point 3:

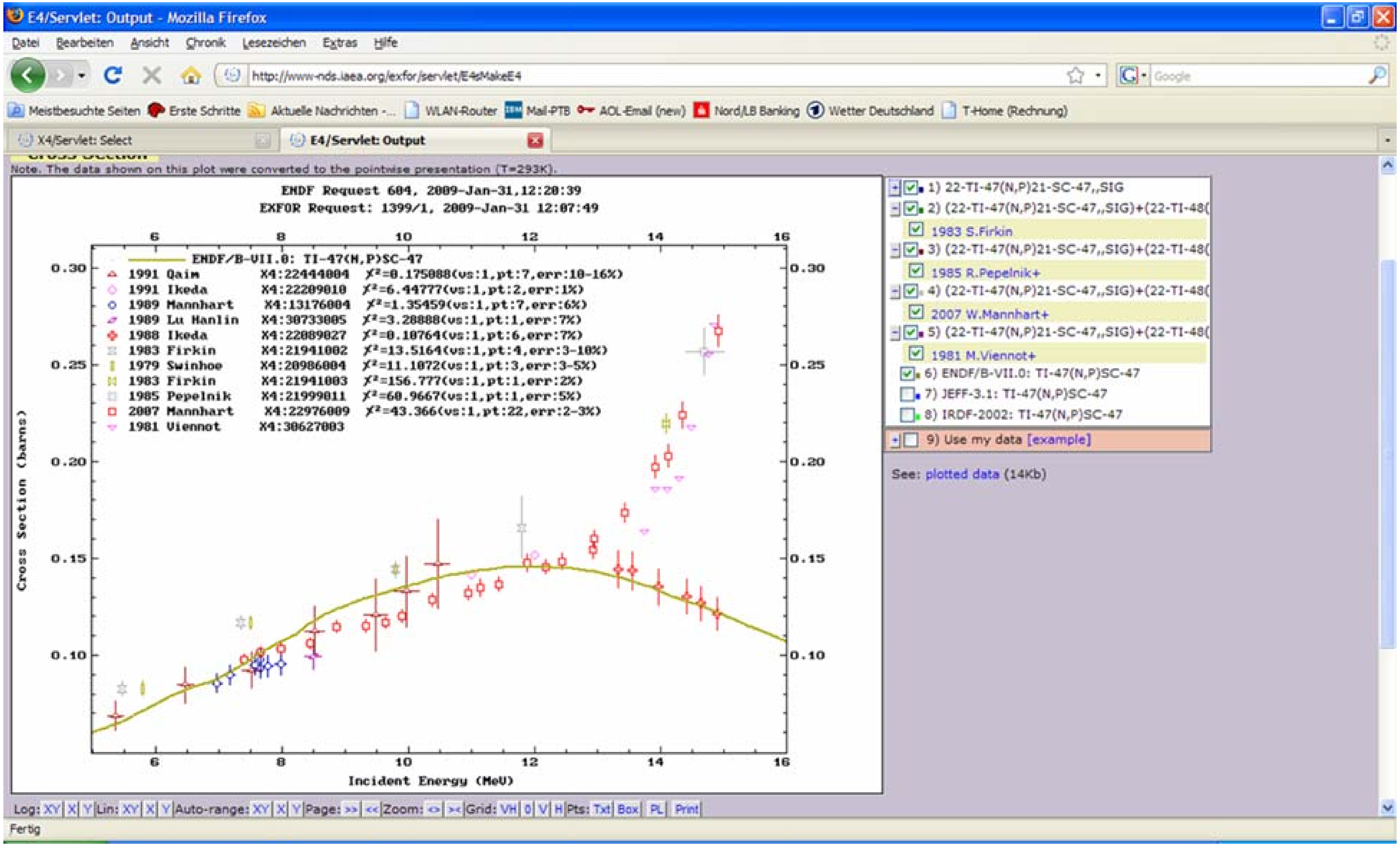
Read chapter 3.1 of my report PTB-N-53. The chapter explains why the threshold of the (n,n+p) reaction is more important than that of the (n,d) reaction and it explains also the advantages and the limits of cross sections given in the form of eqn. (1).

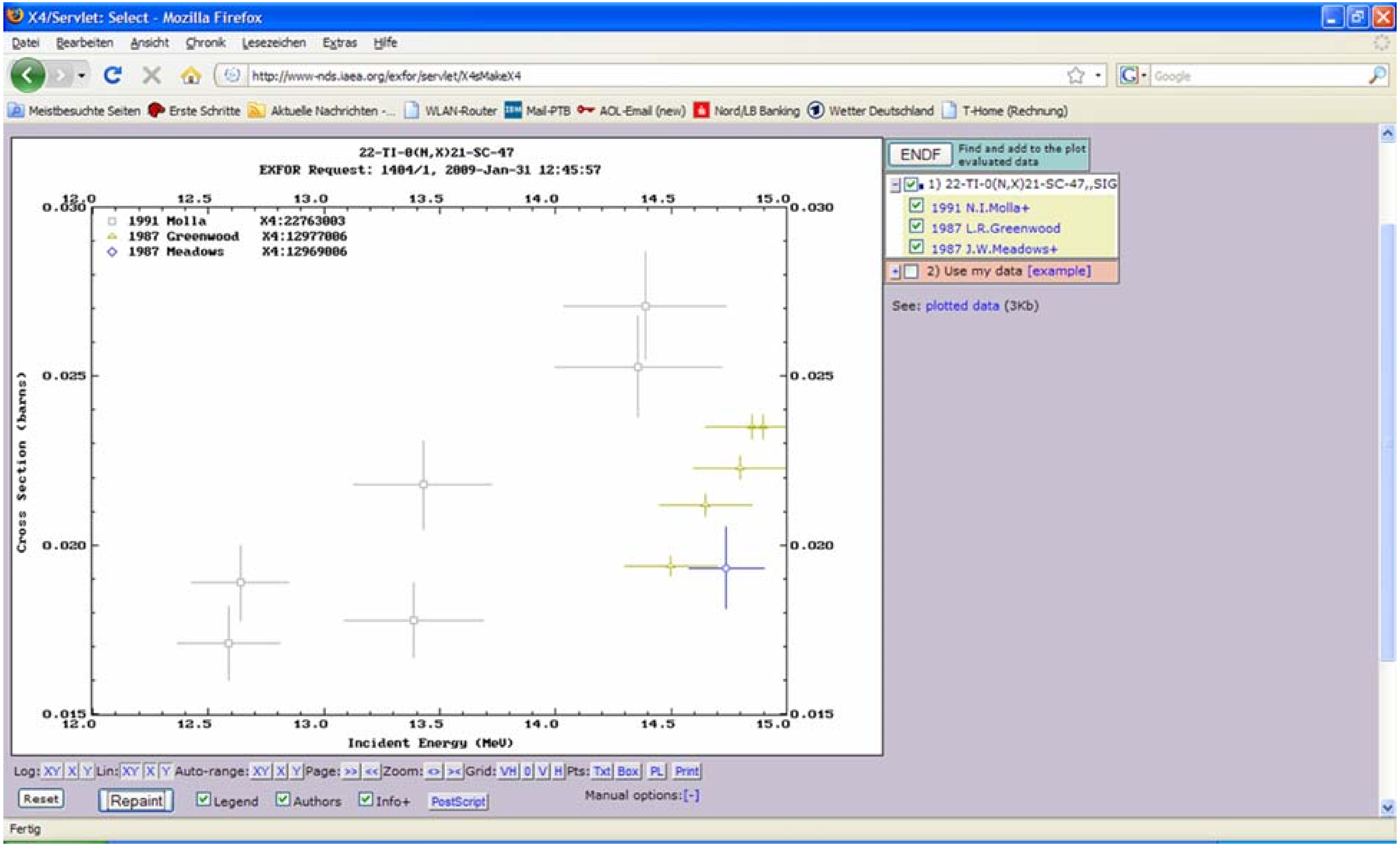
By the way, in the table given at the bottom of page 2 of your memo CP-D/54a the heading of the (n,d) and the (n,n+p) data is wrong. The 50 mb data are (n,n+p) and the 1 mb data are (n,d).

Point 4:

The file 22976_rev.txt contains all corrections given in the file X4_22976_new.doc. Stanislav Maev did an excellent job and the file should be loaded as it is.

In your email of January 2, 2009 you mentioned that only one uncertainty value is allowed of the given MB and PER-CENT with the recommendation to drop one of the values. I don't agree with you. The MB are needed to allow plots of the data **with error bars** as shown in the attached file plot_eample.doc. The PER-CENT values of ERR-T form together with the MISC2 value the relative covariance matrix. This means both quantities are needed. I recommend to tolerate both values if the space in the line is not occupied with other information. An alternative to that is the definition of a new format for the representation of the covariance matrix which is similar compact as given.


E4/Servlet: Output - Mozilla Firefox
Datei Bearbeiten Ansicht Chronik Lesezeichen Extras Hilfe
http://www-nds.iaea.org/exfor/servlet/E4sMakeE4
Meistbesuchte Seiten Erste Schritte Aktuelle Nachrichten -... WLAN-Router Mail-PTB AOL-Email (new) Nord/LB Banking Wetter Deutschland T-Home (Rechnung)
X4/Servlet: Select
E4/Servlet: Output
Note. The data shown on this plot were converted to the pointwise presentation (T=293K).
ENDF Request 604, 2009-Jan-31,12:20:39
EXFOR Request: 1399/1, 2009-Jan-31 12:07:49
ENDF/B-VII.0: TI-47(N,P)SC-47
1991 Qaim X4:22444004 χ²=0.175088(vs:1,pt:7,err:10-16%)
1991 Ikeda X4:22209010 χ²=6.44777(vs:1,pt:2,err:1%)
1989 Mannhart X4:13176004 χ²=1.35459(vs:1,pt:7,err:6%)
1989 Lu Hanlin X4:30733005 χ²=3.28888(vs:1,pt:1,err:7%)
1988 Ikeda X4:22089027 χ²=0.10764(vs:1,pt:6,err:7%)
1983 Firkin X4:21941002 χ²=13.5164(vs:1,pt:4,err:3-10%)
1979 Swinhoe X4:20986004 χ²=11.1072(vs:1,pt:3,err:3-5%)
1983 Firkin X4:21941003 χ²=156.777(vs:1,pt:1,err:2%)
1985 Pepelnik X4:21999011 χ²=60.9667(vs:1,pt:1,err:5%)
2007 Mannhart X4:22976009 χ²=43.366(vs:1,pt:22,err:2-3%)
1981 Viennot X4:30627003
Cross Section (barns)
Incident Energy (MeV)
0.10 0.15 0.20 0.25 0.30
6 8 10 12 14 16
1) 22-TI-47(N,P)21-SC-47,,SIG
2) (22-TI-47(N,P)21-SC-47,,SIG)+(22-TI-48(
1983 S.Firkin
3) (22-TI-47(N,P)21-SC-47,,SIG)+(22-TI-48(
1985 R.Pepelnik+
4) (22-TI-47(N,P)21-SC-47,,SIG)+(22-TI-48(
2007 W.Mannhart+
5) (22-TI-47(N,P)21-SC-47,,SIG)+(22-TI-48(
1981 M.Viennot+
6) ENDF/B-VII.0: TI-47(N,P)SC-47
7) JEFF-3.1: TI-47(N,P)SC-47
8) IRDF-2002: TI-47(N,P)SC-47
9) Use my data [example]
See: plotted data (14Kb)
Log: XY X Y Lin: XY X Y Auto-range: XY X Y Page: >> << Zoom: <> >< Grid: VH 0 V H Pts: Txt Box PL Print
Fertig


X4/Servlet: Select - Mozilla Firefox
http://www-nds.iaea.org/exfor/servlet/X4sMakeX4
22-TI-0(N,X)21-SC-47
EXFOR Request: 1404/1, 2009-Jan-31 12:45:57
1991 Molla X4:22763003
1987 Greenwood X4:12977006
1987 Meadows X4:12969006
Cross Section (barns)
Incident Energy (MeV)
ENDF
Find and add to the plot evaluated data
1) 22-TI-0(N,X)21-SC-47,,SIG
1991 N.I.Molla+
1987 L.R.Greenwood
1987 J.W.Meadows+
2) Use my data [example]
See: plotted data (3Kb)
Log: XY X Y Lin: XY X Y Auto-range: XY X Y Page: >> << Zoom: <> >< Grid: VH 0 V H Pts: Txt Box PL Print
Reset Repaint Legend Authors Info+ PostScript
Manual options: [-]
Fertig