DRAFT

PROPOSAL FOR ENDF/B FORMAT IMPROVEMENTS IN THE RESONANCE REGIONS

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Two basic stipulations can be made:

1 - The ENDF format results from choices made some 30 years ago; the needs, the searches for accuracy and completeness, the informatics context have greatly change since then. Recent modifications bump against limitations resulting from these choices. For the future, it is necessary to consider the definition of a format independent of the past (i.e., in practice, of the actual ENDF format); the set-up of this new, with a wider scope format should involve a wider range of physicists than those actually working with the ENDF format.

2 - An evaluator does not have to account for in their evaluation for the processing paths or codes, but should be able to include in the evaluated data as much as possible of the present knowledge on the nuclei. It's the duty of the processing code or of the processor (by using options) to neglect or approximate parts of this knowledge if they felt it necessary.

Hereafter we consider modifications with respect to the general organisation of ENDF-B. The two first proposals imply no modification of the format, but just modifications of the specifications

1 - LIBERTY (and exactness) FOR THE NUMBER OF DEGREES OF FREEDOM in the URR range.

According ENDF-102 the number of degrees of freedom AMU* characterising the distribution of partial widths are real numbers with the following restrictions:

1.0 <= AMUN <= 2.0	for the neutron width,
1.0 <= AMUF <= 4.0	for the fission width[1],
1.0 <= AMUX <= 2.0	for the "competitive" width (generally the inelastic),
At present AMUG = 0.0	for the radiation width, what means a constant value

But in practice AMUN, AMUX, AMUF **are always integer values**, while the checking routine just detects values outside the specified ranges; furthermore an ENDF convention for the neutron width implies that it be an integer value (cf. 1-3).

There are reasons to introduce non-integer values, possibly outside the specified ranges:

1-1 Nuclear physics justifications

a) <u>Widths distribution for a single channel</u>: the theory, based on statistical hypothesis, concludes that the widths for a single channel are distributed according a χ^2 law with **one**

1 There is also the case LFW=1, LRF=1, scarcely used, which states that MUF is an integer such that 1<= MUF <= 4

degree of freedom. But this assume a completely statistical process, while several experimental analysis of the neutron width distributions conclude that $\nu>1$. (cf. Pa92).

According to our knowledge all experimental determinations of ν conclude to $\nu>1$, while most common experimental errors should increase the variance, i.e. should decrease the experimental value of ν.

b) The sum of a few partial widths: the sum of 2 partial widths Γ_1 and Γ_2 distributed according $\chi2$ law with ν_1 and ν_2 is distributed according a $\chi2$ law with $\nu_1+\nu_2$ degrees of liberty **only** if the averages $\overline{\Gamma}_1$ and $\overline{\Gamma}_2$ are proportional to ν_1 and ν_2, what is not always true; the description of the sum by a $\chi2$ law is an approximation, which required a non-integer value of ν.

For example if $\overline{\Gamma}_1=1.$ and $\overline{\Gamma}_2=0.5$, the sum can be properly describe by a $\chi2$ law with $\overline{\Gamma}=1.5$ and $\nu=1.8$.

c) Fluctuations of Γ_γ. It seems that it is widely accepted that the radiation width, Γ_γ, has significant fluctuations, and that a constant value is not appropriate; ENDF-102 states (2.4.20, 3) that "it is not worthwhile deciding if AMUG is 30 or 40.". It's a matter of accuracy (see below).

1-2 Neutronics justifications. In order to check the need for a better description in the URR range we did some calculations, introducing some modifications of the available tools, in order to check the influence of several parameters (Mo92, Ri**). Calculations have been done for 238U and for 235U; we give, hereafter, some results for 10 barns dilution .

effect on the self-shielding factor of a non standard value of ν
i.e. either non-integer value, or non-0 (indeed, infinite) value of ν

Nucleus		values of the self-shielding factor f	effect on f of a non-standard value of ν
238U	$\Gamma_n : \nu=1.1$	0.88 <==> 0.94	0.003 <==> 0.005
238U	$\Gamma_\gamma : \nu=100.$	0.85 <==> 0.94	0.015
235U	$\Gamma_f : \nu=2.5$	0.95 <==> 0.97	0.0003 <==> 0.0015

The effect is not negligible for the neutron width (even more if $\nu=1.25$), and important for the radiation width, contrarily to the ENDF-B assumption!

1-3 : Exactness of AMUN. The number of channels for the neutron (elastic) widths may be equal to 2 if I>0 and l>0 : in that case we will have some values AMUN=2 (see examples below).

But there is a strange mixture of data for the neutron widths according ENDF-102: "2.4.20. Degrees of freedom...

... It is assumed.... that $<\Gamma_n>$ is the sum of two equal average partial widths. In Appendix D this factor of two is absorbed into the definition of $<\Gamma_n>$,...."

Apparently the value which has to be inserted as the average neutron width is not $<\Gamma_n(J)>$, but $<\Gamma_n(J,s)>$, the width for a single channel. And processing codes have to multiply the $<\Gamma_n>$ value by the number of degrees of freedom to obtain the right average neutron width.

That **prohibits the use of non-integer values for Γ_n^2**, and is a source of confusion: all the average widths are the sum over the several channels contributing to this width, except the neutron average width which is the width for 1 channel, even if there are 2 of them!

This is a source of error.

For 239Pu for example, I=1/2, for l=1, we have:

	J	ν	$<\Gamma_n>/<D>$
JEF-2	0	1	1.6352E-4
	1	2	1.6357E-4
	2	1	1.6356E-4
JEF-3	0	1	1.6352E-4
ENDF-B6	1	1	1.6357E-4
	2	1	1.6356E-4

The two evaluations provides the same parameters, the neutron width for l=1,J=1 is half the true neutron width, and evaluations JEF-3 and ENDF-B6 are wrong. We should have :

	J	ν	$<\Gamma_n>/<D>$
JEF-3	0	1	1.6352E-4
ENDF-B7	1	2	3.2714E-4
	2	1	1.6356E-4

Of such errors have effects on the average cross-sections; we calculate the effect at 20 keV.

Effect of the ν value on the 239Pu cross-sections at 20 keV

		Total cs	Fission cs
Average (infinite dilution)	ν=1 ν =2	14.704(35) 14.936	1.736(33) 1.936(34)
sigma-d = 10 barns	ν =1 ν =2	14.488(38) 14.719(38)	1.689(31) 1.888(32)

Conclusion: we suggest to state that the neutron width is the real neutron width for the (l,J) considered;

we suggest to reject any restriction upon the values of ν, keeping the convention that ν=0. means a constant value of the width.

2 - Inclusion of resolved resonances in the Unresolved energy Range. It's always better to replace random information by the actual one; i.e., if some great resonances have been analysed in the URR, why not included them in the evaluation? leaving to the processing code the duty to neglect this information, or to process it more or less accurately.

The inclusion of resolved resonances in the URR may also presents other advantages. Fig represents the total and the fission cross-sections of 238U around 28000 eV. The total

[2] We did some tests with NJOY: if we insert a value ν=1.3 for the neutron widths, the cross-sections are increased. CALENDF print a diagnostic of anomaly but use the nearest integer value (1 or 2), and average cross-sections are unchanged..

cross-section results from a random generation of resonances; the fission provides from the rough description given in file 3: it is not a resonance, but a cluster of few resonances.

Calculated by CALENDF between 28160. and 28260. eV, the self-shielding coefficient is 0.95 for capture, 1.02 for the fission, for there is no correlation between the randomly generated total cs and the fission cs.

What we suggest in this case, in order to obtain a better physical description of this sub-threshold fission, is that the evaluator includes a few random resonances with adjusted fission widths.

3 – GENERALISATION OF THE RESONANCE PARAMETERS REPRESENTATION

The actual format allows only up to 4 partial widths, which are a-priori defined. We propose to make possible to have an a-priori **undetermined number** of a-priori **undetermined partial widths.**

For this purpose it's necessary to define the number of partial widths (NPW), and to identify them; using the MT number can do this identification.

A sequence of resonance parameters would be preceded by a line defining the number of partial widths, and their identification; it could be necessary to continue data on a second line

The ENDF format split the resolved resonances according to their angular momentum l, but mix the spins J; there is no serious justification to this practice, which results from history (cf.); here after we assumes we preserve this presentation. Also we will not write the total width.

We give, here after, a few examples and their advantages.

3-1 Resolved Resonance Range:

3-1-1 Few academic examples.

Elastic scattering, capture, two inelastic channels: NPW=4

4		2	102	51	52
ER(1)	J(1)	Γn(1)	Γγ(1)	Γin1(1)	Γin2(1)
ER(2)	J(2)	Γn(2)	Γγ (2)	Γin1(2)	Γin2(2)

b) Elastic scattering, capture, (n,α): NPW=3

3		2	102	107
ER(1)	J(1)	Γn(1)	Γγ (1)	Γnα (1)
ER(2)	J(2)	Γn(2)	Γγ (2)	Γnα (2)

3-1-2 The case of 27Al. It's a 5/2-spin nucleus, and then there are 2 possible (elastic) neutron channels, of spin 2 and 3. The possible spins of resonances are given in the following table:

^{27}Al (I=5/2) - Possible spin states of the compound nucleus ^{28}Al according to the orbital momentum l

channel spin	J, spin of the compound nucleus		
	l=0	l=1	l=2
2	2^+	$1^-,2^-,3^-$	$0^+,1^+,2^+,3^+,4^+$
3	3^+	$2^-,3^-,4^-$	$1^+,2^+,3^+,4^+,5^+$

Then a 2+ resonance, for example, can be formed by 3 different ways, i.e. will have 3 neutron partial widths (elastic scattering). Furthermore these widths should have a sign (i.e. the sign of the channel amplitude) which is of importance:

- for interferences in the angular distribution of scattered neutrons, even between resonances of different orbital momenta,
- for interferences in the cross sections (total, i.e. integrated over angles) between resonances of the same orbital momentum if there are more than one neutron channel ,

It's clear that the actual ENDF format does not allows the description of these data, if available. And they are partly available.

For this nucleus has been carefully studied both in US and in Europe; part of the experimental data was the same. At ORNL Herve Derrien et al. (De01) analysed transmission and capture data, Stephan Kopecky et al. at IRMM analysed transmission and inelastic data; both laboratories used the code SAMMY.

a) The ORNL simplification. The single channel neutron widths are very spread (variance ~ 2.). Then when there are several possible channels one of them is generally much greater than the other ones. This is the basis of what may be called the ORNL simplification: only one channel is taken into account for every resonance. And from this results a proposal by Nancy Larson et al. (LA99), which has the great advantage to require no modification of the format; it has already been applied for a tentative evaluation of 27Al (see below).

Its principle is the following: a sign is given to the resonance spin; there are two possibilities, one will characterise the channel spin s=I-1/2, the other the channel spin s=I+1/2.

In their first proposal these authors associate the sign + of the spin to the channel spin s=I-1/2, and inversely; but, as shown below, for l=0 the evaluation clearly associates the sign - to the channel spin s=I-1/2, and inversely. For l=2 the data are inconsistent for the sign + introduces simultaneously the spin J=0 and J=5, what is not possible. It has to be noticed that if we can distinguish the two channel spins from each other, we are unable to assess properly the right channel spin of a neutron channel, what is of no practical importance.

Extract from ENDF-B-7 evaluation of Al27; resonances parameters,
l=0 and l=2, from 500 to 800 keV

```
l=0
 5.261958+5  3.00000+0 5.141200+3 9.788000-1 0.000000+0 0.000000+0 1325
 5.862400+5  3.00000+0 4.596000+3 1.376000+0 0.000000+0 0.000000+0 1325
 6.145694+5  3.00000+0 1.364600+4 7.095900-1 0.000000+0 0.000000+0 1325
 7.149034+5 -2.00000+0 1.452400+3 2.210000+0 0.000000+0 0.000000+0 1325
 7.867095+5  3.00000+0 2.424100+4 2.210000+0 0.000000+0 0.000000+0 1325

l=2
 5.212374+5  0.00000+0 3.591300+4 3.348000+0 0.000000+0 0.000000+0 1325
 5.458745+5  1.00000+0 1.480000+2 6.724000-1 0.000000+0 0.000000+0 1325
 5.462643+5 -1.00000+0 9.545000+1 7.350000-1 0.000000+0 0.000000+0 1325
 5.862856+5 -3.00000+0 1.055000+2 3.599000-1 0.000000+0 0.000000+0 1325
 5.927221+5  4.00000+0 4.400000+0 3.500000-1 0.000000+0 0.000000+0 1325
```

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6.029096+5  4.00000+0 4.737000+1 2.114000-1 0.000000+0 0.000000+0 1325
6.546094+5  2.00000+0 1.615000+2 1.964000-1 0.000000+0 0.000000+0 1325
6.550861+5  3.00000+0 2.569000+2 1.734000-1 0.000000+0 0.000000+0 1325
6.989209+5 -1.00000+0 5.355000+1 1.090000+0 0.000000+0 0.000000+0 1325
7.063424+5  5.00000+0 1.295800+3 1.090000+0 0.000000+0 0.000000+0 1325
7.593513+5  2.00000+0 6.600900+3 1.090000+0 0.000000+0 0.000000+0 1325
7.663373+5 -3.00000+0 3.189000+2 1.402000+0 0.000000+0 0.000000+0 1325
7.861063+5  5.00000+0 1.113700+4 1.090000+0 0.000000+0 0.000000+0 1325
```

b) The generalised representation of ORNL data. The preceding data for 27Al(ORNL) would be described in this manner:

l=0 : NPW=3

3		2	2	102
526195.8	3.	0.	5141.2	0.9788
586240.0	3.	0.	4596.0	1.376
614569.4	3.	0.	13646.	0.70959
714903.4	2.	1452.4	0.	2.210
786709.5	3.	0.	24241.	2.210

l=2 : NPW=3

3		2	2	102
521237.4	0.	35913.	0.	3.348
545874.5	1.	0.	148.	0.6724
546264.3	1.	95.45	0.	0.735
586285.6	3.	105.5	0.	0.3599
592722.1	4.	0.	4.4	0.350
602909.6	4.	0.	47.37	0.2114
654609.4	2	0.	161.5	0.1964
655086.1	3.	0.	256.9	0.1734
698920.9	1	53.55	0.	1.090
706342.4	5.	0.	1295.8	1.090
759351.3	2	0.	6600.9	1.090
766337.3	3	318.9	0.	1.402
786106.3	5.	0.	11137.	1.090

It has to be notice that it is useless to specified the channel spin for l=0, and the first table could be so written :

l=0 : NPW=2

2		2	102
526195.8	3.	5141.2	0.9788
586240.0	3.	4596.0	1.376
614569.4	3.	13646.	0.70959
714903.4	2.	1452.4	2.210
786709.5	3.	24241.	2.210

c) The generalised representation of IRMM data. The ORNL simplification is unable to represents the results of Stephan Kopecky et al., who took into account (only) 2 neutron elastic channels for every resonance; their data are given in the following table.

for l=0 : NPW=4

4		2	-2	-2	102
526536.0	2	7975.7	0.	0.	2.00
588126.4	3	3765.5	6586.7	0.	2.00
617210.6	3	14847	108.64	0.	2.00
652952.8	2	750.86	0.	631.51	2.00
726807.8	3	113.77	226.21	0.	2.00
746438.0	2	6580.5	0.	0.	2.00

for l=2: NPW=4

4		2	2	-2	102
526814.6	4	2752.6	8231.2.	0.	2.00
547056.0	4	127.65.	0.	0.	2.00
588126.4	3	6586.7	0.	3765.5	2.00
604067.0	4	58.343	0.	0.	2.00
617210.6.	3	108.64	0.	14847	2.00
651773.0	4	9996.9	1587.6	0.	2.00
652952.8	2	0.	631.51	750.86	2.00
717133.6	1	4746.9	50.335	0.	2.00
726807.8	3	226.21	0.	113.77	2.00
747701.4	2	0.	4539.9	0.	2.00
768120.1	4	114.75	123.31	0.	2.00

Comments: the resonance 526536.0 eV has a neutron width only for l=0;
the resonance 547056.0 eV has a neutron width only for l=2;
there are 2 neutron channels with l=2 for the 526814.6 eV resonance, none for l=0;
the resonance 588126.4eV has one neutron width for l=0 and one for l=2, this resonance appears in the 2 tables, **with the same parameters**. Such is the case for the 617210., 652952. and 726807. resonances.

It's clear that the resonances (l=0,J=2) and (l=0,J=3) does not belong to the same channel spin; but it is not necessary to specify this difference; this would also be true for resonances (l=2,J=0) and (l=2,J=5), if any.

d) The generalised representation with inelastic channels. Stephan Kopecky analysed data up to 2 MeV, and introduces inelastic channels to describe the inelastic widths for decay to excited levels $3/2^+$ at 843 keV and $1/2^+$ at 1015 keV. Depending on the resonance's spin, there are several channels for each inelastic level: for instance, 3 channels for 2^+ resonances to the first exited level $3/2^+$. Stephan Kopecky simplified by introducing only one channel for each inelastic level. We give what would be the presentation of the parameters for resonances of even parity from 1100. keV to 1200. keV:

l=0, NPW=6

6		2	-2	-2	51	52	102
1108960.	2.	196.54	0.	6630.9	66.36	4.399	2.00
1110340.	2.	11754.	0.	32159.	0.2065	-0.220	2.00

1148087.	2.	208.11	0.	-6901.7	-4911.8	-16029.	2.00
1148373.	3.	99.122	16.063	0.	-10.782	766.51	2.00
1192306.	2.	1820.9	0.	2388.5	1137.8	1152.1	2.00
1199176.	3.	124.60	43.389	0.	-10.531	-5388.1	2.00

l=2, NPW=6

6		2	2	-2	51	52	102
1108960.	2.	0.	6630.9	196.54	66.36	4.399	2.00
1110340.	2.	0.	32159.	11754.	0.2065	-0.220	2.00
1137538.	1.	7694.6	20375.	0.	6.488	2.957	2.00
1148087.	2.	0.	-6901.7	208.11	-4911.8	-16029.	2.00
1148373.	3.	16.063	0.	99.122	-10.782	766.51	2.00
1153127.	4.	101.36	7.357	0.	359.61	559.91	2.00
1192306.	2.	0.	2388.5	1820.9	1137.8	1152.1	2.00
1199176.	3.	43.389	0.	124.60	-10.531	-5388.1	2.00

l=4, NPW=4

4		2	51	52	102
1195860.	6.	-462.79	1.437	0.775	2.00

e) Simplification of data for actual processing codes.

We know that the present processing codes cannot take into account all these data, even if they are valuable. Each code will have to simplify them, according its possibilities, accepting then some approximations. For example, the 27Al of IRMM could be, in a first step, simplify by merging the chanels, as in the ORNL simplification, i.e. adding the widths in the most importnt channel:

l=0

3		2	4	102
1148373.	3.	115.19	777.29	2.00
1199176.	3.	167.99	-5398.6	2.00

l=2

3		2	4	102
1108960.	2.	6827.4	70.76	2.00
1110340.	2.	43913.	-0.4265	2.00
1137538.	1.	28070.	9.445	2.00
1148087.	2.	-7109.8	-20941.	2.00
1153127.	4.	108.72	919.52	2.00
1192306.	2.	4209.4	2289.9	2.00

l=4

3		2	4	102
1195860.	6.	-462.79	2.212	2.00

3-2 Unresolved Resonance Range. We propose the same approach than for the resolved range, i.e. defining the number of partial widths (NPW), identifing them by the MT numbers, but also providing the values of ν, the number of degrees of liberty for every partial widths.

As shown here after by few academic examples this would allows much more flexibility than permitted by the actual ENDF format.

a) scattering, capture and two fission widths (ν=1. and 1.8), the second one being the sum of two channels: NPW=4

4		2	102	18	18
		1.2	0.	1.	1.8
EU (1)	D(1)	$\Gamma_n(1)$	$\Gamma_\gamma(1)$	$\Gamma_{f1}(1)$	$\Gamma_{f2}(1)$
EU (2)	D(2)	$\Gamma_n(2)$	$\Gamma_\gamma(2)$	$\Gamma_{f1}(2)$	$\Gamma_{f2}(2)$

b) This may allows to take into account the (n,γf) process for 239Pu.
For example: elastic scattering (n=1.2), capture (n=80.), (n,gf) process (n=0., i.e. constant width), one channel fission: NPW=4

4		2	102	18	18
		1.2	80.	0.	1.
EU(1)	D(1)	Γn(1)	Γγ(1)	Γγf(1)	Γf(1)
EU(2)	D(2)	Γn(2)	Γγ(2)	Γγf(2)	Γf(2)

The processing code will have the liberty to treat independently the two fission process, with no interference for the first one; or two merge them into a unique Γ_f distribution.

c) The evaluator may want to explicit some information on the gamma decay; for example: NPW=4

4		2	102	102	102
		1.2	1.	8.	0.
EU(1)	D(1)	Γn(1)	0.003	0.005	0.015

The total radiation width is 0.023 eV; processing can be done by taking into account interferences for the first partial radiation width (likely to be the ground transition); or can merge them as a unique width of average value 0.023 eV distributed according a χ^2 law with ν= 43.6 (same variance).

3-3 General organisation and consistency: this presentation accepts the general organisation of the ENDF-B format: the resolved resonances are ordered according to the orbital momentum of the neutron wave which may form this resonance, what implies that resonances may have to be duplicated (as seen above). But they are not split according their spin.

It has to be noticed that, on the contrary, a more basic approach would imply a classification by spin (and parity), the partial widths being given for every process associated to this resonance.

3.3.1 Classification by spin. The Committee for ENDF/B-VII Formats has already considered the possibility to have resonances classified under external loop over J-values.

3.3.2 Total widths of resolved resonances. They are not explicitly given in what is called the "Reich-Moore formalism", for there were no place. The suppression of the resonance spin and the use of the generalised resonance format would allow the re-introduction of the total width, what is a useful check against errors.

3.3.3 Exactness of calculations. Formally the processing codes should read the resonance parameters, and regroup resonances described under different orbital momenta, and then process them in the proper way. This would be a great modification.
We suggest to continue the resonance processing by orbital momenta, i.e. that resonances obtained by 2 different neutron waves would be processed twice, and the result added. The total (i.e. integrated over angles) cross-sections will be exact; the angular distribution of elastic scattered neutrons would be erroneous, for this process implies the neglect of interferences between scattered neutrons associated to different orbital momenta. But this may be not dramatic.data the same presentation of resonances according the orbital momenta

It has to be emphasised that treating separately the data as independent resonances will provides exact value for the cross-sections, but that the angular distribution will be incorrect for the correlation between the l=0 and l=2 scattering will be ignored; we are unable to assess the importance of this approximation, when the angular distribution is calculated.

4 –OTHER PROPERTIES of interest, but which seems difficult to include within the ENDF-B format

CONCLUSIONS

Respecting the general organisation of ENDF-B can include the modifications that we suggest in 2 and 3. They would allow evaluators to be more exact.

The processing codes would have to deal with them in two steps:
interpreting them in order to reduce the data to their present capabilities;
later on, and according the needs and the possibilities, taking more properly these information into account.

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Figure 1 : total and fission(*1000.) cross-sections of 238U between 28160. and 28260. eV; the total cs results from a random generation of parameters, defined by the file 2 of the evaluation; the fission cs results from the rough description introduced in file 3 (as a point wise cs).

(20020513, 16h30)

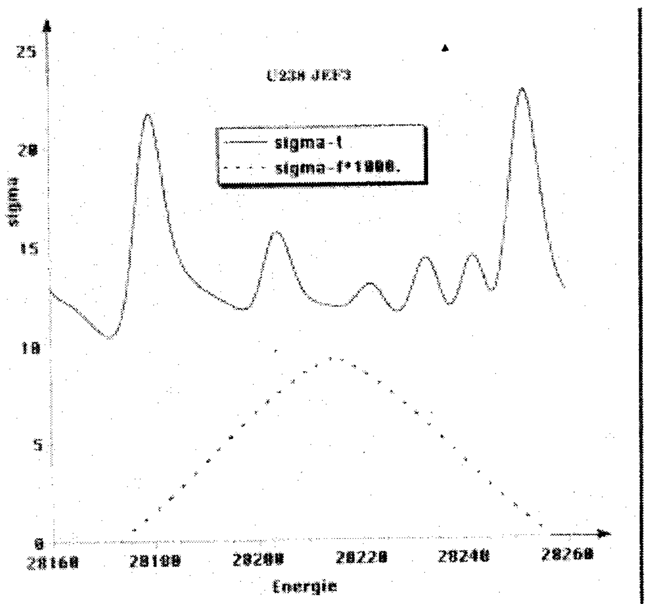

Figure 1 : total and fission(*1000.) cross-sections of 238U between 28160. and 28260. eV; the total cs results from a random generation of parameters, defined by the file 2 of the evaluation; the fission cs results from the rough description introduced in file 3 (as a point wise cs).