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## What's the deal with Exfor entry 41245.022?

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#### Abstract:

While collecting data to fill in the "*Current knowledge*"" section in "Applying Random Sampling methods to data analysis..." [1], the author stumbled on what seems to be an inconsistency in Exfor entry 41245.022[2] between the cross-section value given in the database and code predictions / experimental values. This document looks into bibliographical documents, Talys calculations, and experimental results in order to understand the value quoted in the Exfor entry and make recommendation on how to use it in future works.

### Context

Exfor entry 41245.022[2] is listed as (74-W-183(N,INL)74-W-183,PAR,SIG,G). Therefore, the value given is expected to be the production cross section of  $\gamma$  rays of energy 210  $\pm$  30 keV, resulting from the inelastic scattering of neutron off <sup>183</sup>W at an incident energy of 3 MeV (see in the entry [2] for details).

However, upon comparison with Talys [3] calculations, the value in the entry is doubtful, as it is too large to reflect the cross section predicted by the code, even when accounting for uncertainties, as shown in figure 1.



Figure 1. Plot of the Exfor entry value (black) against predictions by Talys (colored lines). The transitions are identified using Talys' convention [4].

## What's in the bibliography?

The Exfor entry [2] references several sources for the value. The main one is *"Vop.At.Nauki i Tekhn.,Ser.Yaderno-Reak.Konstanty, Issue.2, p.59 (1996), Russia"* [5]. The article is not easy to find [6], and even if you find it, apart from the abstract, it is in Russian. Fortunately, the Exfor team keeps copy of all references attached with the entries, which finally allowed a consultation of the document, and automatic images recognition services paired with automatic translation made it possible to get a reasonably accurate English version of the paper.

Even before the English version of the text, we can see, in the Exfor entry and in the table of the article, that our direct interpretation of the (74-W-183(N,INL)74-W-183,PAR,SIG,G) listing might be wrong. Indeed, the Exfor entry contains the following lines:

CORRECTION Corrections were made on gamma-quanta registration efficiency, on gamma-quanta self-absorption, neutron flux attenuation and multiple scattering in samples, on registration system's fallouts, on internal conversion of gamma-quanta, on gamma-quanta angular distribution

The internal conversion of gamma-quanta hints that the quoted cross section might not be a  $\gamma$  production one has expected, but a transition cross section (i.e. corrected for internal conversion).

Additionally, in the article's *Table 2*, showing the values reported in Exfor, the line corresponding to entry 41425.022 clearly refers to several isotopes, as shown in figure 2.

Элемент	Энергия гамма- квантов, МэВ (из схем распада)	Изотоп	Средняя энергия гамма-квантов, МэВ	Сечение выхода гамма- квантов, мб
Вольфрам	0,198 0,207 0,215 0,215	186W 183W 184W 186W	0.21±0,03	2523±730

Figure 2. Excerpt of table 2 from [5]. Auto-translations of the column titles gives: "Element", "Energy of gamma quanta, MeV (from decay schemes)", "Isotope", "Average energy of gamma quanta, MeV", and "Gamma quanta output cross section, mb"

This indicates that the cross section given in Exfor correspond to some sort of combination of isotopic contributions.

We see that the first transition mentioned is identified as one from <sup>186</sup>W, with no transition from <sup>182</sup>W listed. However, there is a 198 keV transition in <sup>182</sup>W (198.4 keV, L12L08), and no matching transition in <sup>186</sup>W, so we can assume a transcription error and the table should read 182 for that line, instead of 186.

The most obvious meaning would be that the  $\gamma$  cross section has been determined from a natural Tungsten target, with a 26, 14, 30, 28 % mix of 182, 183, 184 and 186 W respectively. But this

contradicts the internal conversion information mentioned earlier, as not all the transitions listed in the Table 2 have the same ICC.

After this careful reading of the bibliography, one can now explore several hypotheses: Is the quoted cross section for  $\gamma$  production or transition, meaning "Is the data corrected for internal conversion, and if yes, using what ICC values?". Also, "Is the measurement done on isotopic or natural tungsten, and what is the isotopic abundances?"

# Looking into $^{nat}W(n, n' \gamma_{210\pm 30 keV})$

Using Talys default calculation, we can extract all transitions that present an energy in the specified  $210 \pm 30$  keV range, and select those with a large enough cross section (arbitrarily, > 10 mbarns). The list is given in table 1. For these *contributing* transition (identified using Talys' convention [4]), we look for their Multipolarity in the NNDC database and their Internal Conversion Coefficient (ICC) (as reported in RIPL3).

We see in the table that some transition energies are a bit off, compared to the table in figure 2 (207 keV vs. 208.8 keV from the L04L00 in <sup>183</sup>W). This is not too much of a bother considering that the measurement is done using an NaI scintillator, and that the main peak is contaminated by other transitions.

More importantly, the multipolarity and ICC of the different contributing transitions vary a lot. This will have an impact on the internal conversion correction.

To disentangle the different hypotheses (with or without internal conversion, mix of isotopes, ...) we performed a series of calculations of the W(n, n'  $\gamma_{210\pm30keV}$  cross section, using Talys [3] (default calculation, and two set of predictions specifically tuned for W isotopes [7] [8]), and experimental values ([1] [9]).

We investigate four hypotheses:

- Natural abundance weighted  $\gamma$  production summation of contributing transitions (noted Ab.W.d Sum $\gamma$ ).
- Natural abundance weighted *transition* cross section summation of contributing transitions (i.e. using ICC coefficient) (noted Ab.W.d Sum transitions).
- Unweighted (i.e. each isotope contribute fully)  $\gamma$  production summation of contributing transitions (noted UnW.d Sum  $\gamma$ ).
- Unweighted transition cross section summation of contributing transitions (noted UnW.d Sum transition).

The computation using Talys default and experimental data is available in this repository.

Isotope	Label	Energy [keV]	$(n, n'\gamma)$ cross section at 3 MeV [mbarns]	Multipolarity	ICC
<sup>182</sup> W					
	L02L01	229.3	789.4	E2	0.196
	L12L08	198.4	38.5	E2	0.317
	L14L09	222.1	57	E1	0.048
	L17L11	217.5	14.5	(E1)	0.051
	L24L15	189.6	11.8	M1+E2	0.740
<sup>183</sup> W					
	L04L00	208.8	13	M1+E2	0.527
	L06L02	209.9	241.2	E2	0.262
	L08L03	205.1	13.8	M1+E2	0.611
	L17L13	188.8	12.9		0.581
	L19L16	219.4	14.7		
	L28L18	201.9	45.2		
<sup>184</sup> W					
	L08L04	226.7	207.8	E1+M2+E3	0.059
	L10L06	215.3	61.3	E1+M2+E3	0.052
	L16L08	215.3	39.7		0.353
	L17L07	238.9	11.4		0.245
	L19L10	203.7	10.5	[E1]	0.060
	L22L11	224.7	13.2	E2	0.210
	L24L13	216.5	23.2	E2	0.237
<sup>186</sup> W					
	L07L03	214.8	402.8	E1	0.053
	L11L05	183.1	35.4	E1	0.079
	L13L07	218.9	22.9		0.332
	L26L18	195.1	17.2	[E2]	0.339

Table 1. List of transitions with  $\gamma$  energy in the 210  $\pm$  30 keV range, as listed in Talys calculations, with their multipolarity and Internal Conversion Coefficient.

### **Results**

The results of the computations using Talys default parameters are shown in figure 3 and figure 4. Each scenario (Natural abundances *vs.* No weight,  $\gamma$  *vs.* transition) is tested. Both when considering  $\gamma$  and transition cross section, the natural abundance weighted sum scenario (Ab.W.d Sum) is too small (by a factor 5) compared to the Exfor value. The non weighted values (UnW.d Sum) are much closer, with the UnW.d Sum transition cross section being very close to the Exfor reference value.



Figure 3. Result of summation computations using  $\gamma$  cross section. The cross section used for these plots come from Talys default calculations. Contributing cross sections are represented by the full lines, color codes by isotopes. The summed contributions by isotope at 3 MeV are represented by the thin horizontal dash using the same color code. The full Abundance weighed summed contribution (Ab.W.d Sum  $\gamma$ ) is represented by the thick dark blue dash, the unweighted sum (UnW.d Sum  $\gamma$ ) by the thick light-blue one.



Figure 4. Result of summation computations using transition cross section. The cross section used

for these plots come from Talys default calculations. Contributing cross sections are represented by the full lines, color codes by isotopes. The summed contributions by isotope at 3 MeV are represented by the thin horizontal dash using the same color code. The full Abundance weighed summed contribution (Ab.W.d Sum transition) is represented by the thick dark blue dash, the unweighted sum (UnW.d Sum transition) by the thick light-blue one.

### **Comparison to Experimental values.**

We try to confirm the results obtained with Talys calculations by using experimental (n, n'  $\gamma$ ) cross section, measured with HPGe detectors (as opposed to scintillator in [5]) and isotopic targets [9] [1] [10].

As not all the  $\gamma$  rays listed in Table 1 are accessible experimentally, the sum of experimental cross sections should be considered as a *lower bound*, in particular compared to the measurement in [5], obtained with a scintillator detector, lacking the fine resolution of HPGe detectors.

Figure 5 presents the result using the experimental  $(n, n' \gamma)$  cross sections.



Figure 5. Same exercise as in figures 3 and 4, but using experimental values [1].

### **Summary of results**

The table 2 gathers the results from the different hypotheses testing, with different sets of Talys calculation [8] [3], as well as the experimental (n, n'  $\gamma$ ) cross sections.

$\sigma$ in mbars	Exfor 41242.022	Talys 1.96 (default)	Talys (P. Romain[8])	Talys (M. Dupuis <b>[7])</b>	Exp. (n, n' γ)
	2523 ± 730				
Ab.W.d Sum transitionγ		544.3	485.0	464.2	352.0 ± 18
Ab.W.d Sum transition		635.0	562.5	538.5	408.3 ± 23
UnW.d Sumγ		2122.6	1845.0	1795.0	1330.6 ± 41
UnW.d Sum transition		2510.6	2140.2	2082.2	1544.5 ± 53

Table 2. Summary of cross sections obtained with the different hypotheses, with different Talys calculations([3], [7], [8]), and experimental values [1]. All cross sections are given in mbarns. See figure 6 for a graphical representation.



Figure 6. Summary of values obtained with the different hypotheses, with different Talys calculations([3], [7], [8]), and experimental values [1]. See table 2 for the details of numerical values.

## Interpretation

The best compatibility of result with the value quote in the Exfor entry is obtained by considering the Unweighted sum of transition contribution. The fact that it might be transition cross section rather than  $\gamma$  one is supported by several elements. But the Unweighted aspect is most puzzling. Indeed, not only does the Unweighted sum value presents no physical, or practical, interest, but being able to compute it would require the knowledge of isotopic cross sections top begin with. And these would likely have been quoted directly if they had been available.

A possible reason could be that the determination was done using different target with the isotopic composition not known accurately enough, or with isotopic purity high enough, to allow a full disentangling of the isotopic contributions, leading to a value from unweighted sum, but that is really stretching the possible scenario into the *unlikely* domain.

It is more logical to dismiss the agreement as a *happy* accident and look for other explanations.

The value quoted is more likely the abundance weighted (i.e. determined from a natural W sample) transition cross section. *But* either the internal the conversion correction, or/and the correction for angular distribution introduced significant errors leading to an overestimated value.

Not having the detail of the analysis or supporting publications, it is very hard to conclude further.

### Take away message

- The Exfor entry 41245.022 most likely refers to transition cross section, on a mix of isotopes.
- The entry value is to be taken with extreme care (or dismiss all together).
- Other entries related to the same publication may suffer from the same issue. To test this, the same comparison between quoted value and Talys calculation has been done for all other W transitions quoted in the paper [5] and yield discrepancy in all cases. However, not systematic bias is observed, so no direct *correction factor* could be inferred from these additional comparisons.

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#### References

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- 2. Gamma-quanta production cross sections at neutron inelastic scattering at the energy 3 MeV EXFOR/41245.022
- 3. Talys Nuclear Reaction Code. Arjan Koning, Stephane Hilaire, Stephane Goriely. https://nds.iaea.org/talys/
- 4. We use Talys-style transitions labeling, with LiiLff, where ii and ff are the indices of the initial and final states (starting from 00 = the ground state, and going up in energy, whatever the spin and parity).
- 5. Vop.At.Nauki i Tekhn.,Ser.Yaderno-Reak.Konstanty, Issue.2, p.59 (1996), Russia
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Code and Data availability statement

The code used to perform the analysis, as well as Talys default calculations can be found at the following URL: https://gitlab.in2p3.fr/greg.henning/investigating-exfor-entry-41245.022