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### Observations on Processing Neutron Nuclear Data from the JEF-1 Fundamental Cross Section Library with the Karlsruhe Version of the Processing System NJOY

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#### Abstract

During the generation of a new group constant set for application in PWR fuel cycle analysis, many irregularities in the group cross sections and selfshielding factors were observed. As the fundamental cross section library the Joint Evaluated File JEF-1 was used, the processing of these data to group constants was performed with the Karlsruhe version of the processing system NJOY. Most of the irregularities occur for high concentration of the nuclide in question, especially in the unresolved resonance region. The irregularities are discussed in some detail and possible reasons for their occurrance are given. This investigation is done for all group cross sections of the heavy materials, structural materials, oxygen, boron, and hydrogen bound in water. All irregularities are removed, partly formally. The application of this new group constant library to the analysis of the PWR-fuel cycle will be described in another paper.

#### Anmerkungen zur Erstellung von Neutronenwirkungsquerschnitten von der JEF-1 Kerndatenbibliothek mit der Karlsruhe Version des Gruppenkonstantenerstellungsprogramms NJOY

#### Zusammenfassung

Bei der Erstellung eines neuen Gruppenkonstantensatzes zur Anwendung in Druckwasserreaktoren wurde eine Reihe von Irregularitäten in den Gruppenkonstanten und Selbstabschirmungsfaktoren beobachtet. Die Erstellung von Gruppenkonstanten erfolgte mit dem Code-System NJOY auf der Basis der Kerndatenbibliothek JEF-1. Die meisten Irregularitäten ergeben sich für hohe Konzentration der Nuklide, besonders für Wirkungsquerschnitte im nicht aufgelösten Resonanzbereich. Die Irregularitäten und deren mögliche Ursachen werden diskutiert. Diese Untersuchungen wurden für alle Gruppenkonstanten der schweren Isotope, der Strukturmaterialien, für Sauerstoff, Bor und gebundenen Wasserstoff durchgeführt. Alle Irregularitäten wurden beseitigt, zum Teil nur formal. Die Anwendung dieses neuen Gruppensatzes für die Analyse des Brennstoffzyklus von Druckwasserreaktoren wird in einem weiteren Bericht beschrieben

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#### 1. Introduction

The Joint Evaluated File (JEF) is in progress since 1982 in the framework of the NEA Data Bank as a collaboration between laboratories in the Member Countries. The first nuclear data library, called JEF-1, has been tested and is available to scientists in the NEA Data Bank Member Countries since 1985. Preparation and part of the validation of JEF-1 is described in /1/. The file contains interaction data for about 300 nuclei in ENDF/B - format. The evaluation work at the Nuclear Research Center Karlsruhe is integrated within the JEF project. Because JEF uses the ENDF/B - format, in consequence at Karlsruhe the processing code system MIGROS /2/, developed to process nuclear data in KEDAK - format, had to be replaced. It was decided to use the Los Alamos processing system NJOY /3/, prepared to process data in ENDF/B format. NJOY has been implemented, tested and improved at Karlsruhe /4/. In order to keep the calculational scheme for reactor analyses at Karlsruhe, the output of NJOY had to be transformed to be accepted by the reactor codes; this is done with the code JOYFOR /5/.

As a first step, the narrow-resonance (NR) approximation was used to calculate the neutron flux distribution in the resonances, following the Boundarenko -Scheme /6/ applied in Karlsruhe since the early sixties for fast reactor analysis. It is well known that for wide or intermediate-width resonances in the eV-range this approximation (i.e. the  $1/\Sigma_t$  (E) fine - flux distribution) is not accurate enough. But in the tests of NJOY this approximation allowed a fair comparison with the results of MIGROS, so that an easy familiarization with the NJOY scheme was possible. An improved calculational procedure in the eV-range will be applied in another step.

This Karlsruhe NJOY - processing scheme was applied to generate a cross section set for all available isotopes in the JEF-1 data library for PWR analyses; as a weighting spectrum the collision density of a KWO\* - PWR configuration was used, for which many tests in Karlsruhe had already been performed, and especially, because for this reactor configuration experimental results from postirradiation analyses are available.

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The tests of the JEF-1 group set on experiments and on international benchmarks are described by the author in another publication /7/, /10/. In the present report the main findings in establishing group constants for PWR calculations are given: inconsistencies, irregularities and related phenomena in the effective group cross sections, which may either be caused by the basic nuclear data, the processing code, or, for the energy range below about 0.5 keV, from the used NR - approximation.

### 2. The Generation of Group Constants Using the Processing Scheme NJOY

The cross section processing code package NJOY87 is well documented in Ref. /3/. The code NJOY was thoroughly checked in an international benchmark exercise, performed at IAEA; the results of this benchmark exercise are described by D.E. Cullen in Ref. /8/: After improvements by the authors participating in the benchmark, satisfactory agreement was found with the reference solution. At KfK an earlier version of NJOY87 was used to prepare the group sets discussed here. The results of this NJOY version were critically compared with the results from the MIGROS - System; a large number of irregularities could be removed. But, nevertheless, there remained still questionable values of group constants, which at the present stage were removed only formally. Having available now the latest version of NJOY87, a cross check between this version and the improved KfK - version probably could bring a better understanding of possible deficiencies in the calculational procedure of NJOY.

#### 2.1 General considerations on irregularities

The present paper describes the observations during the preparation of a group set for PWR - analyses, using JEF - data and NJOY processing methods.

The resonance selfshielding factors f, as proposed by Bondarenko at al, are calculated by NJOY in dividing the effective group cross section by the infinitely diluted cross section (at the same temperature); a simple method was used to make a selection of irregularities found in the results. It is well known that for a wide variety of cases the resonance selfshielding factors in an energy group g for reaction x, i.e.

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$$f_x^g(\sigma_0, T) = \sigma_x^g(\sigma_0, T) / \sigma_x^g(\infty, T)$$

are found to be smaller or equal to unity:  $0 < f_x \ge 1$ . There exist certain exceptions from this rule if the narrow resonance approximation is used:. For structural materials as e.g. Ni or Fe, f-factors are observed to be larger than unity (e.g. 1.10); this happens, if a strong and narrow p-wave capture resonance is situated very near to the minimum of the total cross section which is due to interference between potential and resonance scattering. For higher temperatures the narrow resonance is Doppler broadened and the weighting procedure with 1/ ( $\sigma_t + \sigma_0$ ),  $\sigma_0$  being the background cross section, gives a very strong weight for one flank of the broadened narrow resonance. In this cases it can be shown  $\frac{9}{1}$  that f > 1, if all the resonances (also the broad one) are described as narrow resonances. It is indicated in Ref. /9/ that a more realistic representation of resonances (e.g. a multi - level representation for the resonance and a non-NR-approximation for the flux) brings the f - factors in exess of unity down into the  $0 < f \le 1$  interval. It is not clear at present, whether f always has to stay in the interval [0,1]. In this paper the outlaying values of the f-factor are used as an indicator: if f < 0 or f > 1, then it is very probable that

- a) the fundamental resonance data in the resolved or unresolved resonance energy region are not adequate or not complete
- b) the processing code has deficiencies
- c) the resonance representation is not accurate enough (single level compared to multilevel representation, treatment of the unresolved resonance region)
- d) the method of calculationg effective cross sections via the NR-approximation ( $\phi$  (E) = F(E) /  $\Sigma_t$  (E)) is not accurate enough in wider resonances.

In any case, possible irregularities with f < 0 and f > 1 require special attention. In the following sections the observations for all materials from the JEF-1 file are listed and commented, as far as possible.

## 2.2 Indication of probable irregularities in processing cross sections of heavy nuclei

As discussed in section 2.1, possible irregularities are indicated if the values of the resonance selfshielding factors are outside the interval 10,11.

The group library was established in 69 groups, the corresponding group boundaries are given in <u>Tab. 1</u>; it should be mentioned that this group structure is identical with that given in the WIMS scheme originated in the United Kingdom.

#### 2.2.1 Indications of probable irregularities for U232:

<u>Tab. 2</u> shows the observed indications for possible irregularities for the flux weighted fission cross section and for the current-weighted total cross section.

<u>Comments</u>: The irregularities all occur for high concentration (low  $\sigma_0$ ) of U232 for all tabulated temperatures. In group 23 is the boundary between the resolved and unresolved resonance region. For 900 K and especially for 2100 K the selfshielding factor for fission is unacceptably large; for 2100 K an almost equally large f-factor appears in the unresolved energy region at its lower boundary: there seems to be a mismatch of the fission cross section at the boundary of the resolved and the unresolved resonance region. In addition, in the resolved energy range (10.5 to 53 ev) only 13 resonances are given; they are described with single level Breit-Wigner (SLBW) parameters, again a possible reason for f>1 as mentioned in section 2.1. The total cross section was weighted with the neutron current, which means a  $1/\Sigma_t^2$  weighting in energy across a resonance. The corresponding f-factor for high concentration of the material in question even becomes <u>negative</u> and reaches values up to -10 (group 20 for 2100K) or +12 (group 21, 300 K) ! These unacceptable values obviously are due to a deficiency in the description of the unresolved energy region.

In reactor analyses U232 does not appear in high concentration; but it is not clear whether for larger dilution the cross sections are reliably determined having in mind the large deviations for high concentration.

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#### 2.2.2 Indications of probable irregularities for U234

In <u>Tab\_3</u>, the irregularities found for the cross sections of U232, are listed.

<u>Comments</u>: In <u>Tab. 3</u> irregularities appear in groups 10 and 11 for neutron capture and fission at 2100 K. These irregularities occur at the upper boundary of the <u>unresolved resonance region</u> next to the continuum. The deviations are not very large and probably could be accepted in reactor analyses: U234 will be present in reactors only with low concentration.

#### 2.2.3 Indications of probable irregularities for U235

#### Tab. 4 contains the irregularities found far U235

<u>Comments</u>: It was expected that for this very important reactor material no or only very few irregularities would be found. As seen from <u>Tab. 4</u>, all irregularties occur in the <u>unresolved</u> resonance region (group 22 to group 12) for all temperatures and  $\sigma_0 = 0.001$ ,  $\sigma_0 = 10$ , and  $\sigma_0 = 100$  (for 2100 K only). This observation gives a hint that the unresolved resonance region is not properly described in the Karlsruhe NJOY-module. The deviations are usually a few percent at 300 K and 900 K; at 2100 K (groups 17 and 18) a possible error up to 9 % is indicated for neutron capture.

In general, the deviations can not be tolerated, and therefore there is a need for a better representation of the unresolved resonance region.

#### 2.2.4 Indication of probable irregularities for U236 and U238

Tab. 5 shows irregularities found far U236 and U238

<u>Comments</u>: Only a few irregularties were found for U236 and U238. For U236 there is an obscure f-factor observed in the high energy region of group 6 for the fission cross section  $\sigma_f$ : there are obviously no resonances, there happens to be an almost vanishing  $\sigma_f$  in this group ( $\sigma_f \sim 0.02$  barn); for high concentration an indication of a deviation of 4 % is found which can be due to the numerical treatment used in this case. The same effect is found for U238 in group 6. In both cases no effect will be noticed in reactor applications. Furtheron, for high concentration an irregulartiy is indicated in the resolved resonance region in group 26 and at the switch-over to the continuum in group 11. Probably the last effect is coming from a mismatch at the upper boundary of the unresolved resonance region.

#### 2.2.5 Indication of probable irregularities for Pu238

In <u>Tab. 6</u> in group 17 ( $\sim$ 2.2 keV to  $\sim$ 3.5 keV) the fission cross section shows a small deviation for high concentration from the expected values.

<u>Comments</u>: This energy range belongs to the <u>unresolved</u> resonance region,  $\sigma_f$  is about 1 parn. Very probably the resonance description in this energy region is not sufficiently accurate, so that the observed irregularity in f by 2 % to 3 % can occur, which is temperature independent and seems to become smaller for larger background cross sections  $\sigma_0$ . In reactor analyses Pu238 plays an important role for radiation after discharge of the fuel from the reactor; it always is present in low concentration (large  $\sigma_0$ ).

#### 2.2.6 Indication of probable irregularities for Pu239 and Pu240

As can be seen from <u>Tab. 7</u>, a 3 % irregularity for Pu239 seems to occur in the <u>unresolved</u> resonance region (650 eV to 30 keV).

<u>Comments</u>: The resonances are described with energy dependent resonance parameters in the unresolved resonance region (MLBW representation is used in the resolved resonance region). Because this irregularity occurs only at high temperature (2100 K), can be due to the fact that in addition to the resonance cross section generally a temperature independent cross section is added to give the properly measured (average) value. This additional cross section is usually a fitting "parameter", but it is not smooth, and in principle would need Doppler broadening, which is not foreseen in the processing code. In general, this special energy region seems not being described accurately.

For Pu240 no indication of irregularities was observed. MLBW-representation is used for the resolved resonance region, and in the unresolved resonance region all resonance parameters are energy dependent.

#### 2.2.7 Indication of probable irregularities for Pu241

In <u>Tab. 8</u> irregularities occur in the resolved resonance region (group 28) for the elastic cross section  $\sigma_{el}$ , and in the unresolved resonance region for capture and fission.

<u>Comments</u>: The irregulartiy for the resolved resonance region for  $\sigma_{el}$  is occuring in group 28 for low  $\sigma_0$ . This indication of a 3 % to 4 % irregularity was also observed by using pointwise data and numerical Doppler broadening. Thus, it gives a hint that the way of calculating the flux depression in the resonance by  $1/\Sigma_t(E)$  is not sufficient; instead the true flux distribution in the resonances, calculated for instance within the wide-resonance or intermediate resonance theory approxiamtion or with a collision probability method in a unit pin cell, could improve the accuracy.

The usually used NR-approximation in this paper could be in general the reason for an irregularity in the resolved energy region, especially in those groups covering the flanks of resonances.

In the <u>unresolved</u> resonance region again some irregularities appear, very probably caused by the used formalism, which needs improvement. It is clear that in using pointwise data in the unresolved resonance region, no resonance selfshielding can be observed - and therefore also no irregularities.

#### 2.2.8 Indication of probable irregularities for Pu242

As shown in <u>Tab. 9</u>, an irregularity is found only in the resolved resonance region, namely in the left flank of the 2.67 eV resonance, but only for  $\sigma_{el}$ .

<u>Comment</u>: This irregularity seems to be caused by the NR-approximation of the neutron flux density via  $1/\Sigma_t(E)$ , similar as for Pu241. Again the calculation from pointwise data gives the same indication.

#### 2.2.9 Indication of probable irregularities for Am241

In Tab. 10 the irregularities for Am241 are listed.

<u>Comments</u>: In the resolved resonance region (groups 28 and 30) unexpected results are observed for elastic scattering with a possible error of 2 % to 3%, in both the cases, when resonance parameters or pointwise data are used: these resonances between 2eV and 4eV do overlap, so that the  $1/\Sigma_t$  (E) approximation for the neutron flux density in the resonances is not adequate enough; this indication occurs only for high concentration of the material, which will not happen in present days reactors. The other indicated irregularity occurs again in group 6 for the fission cross section, which is very small and strongly varying with energy in this energy group: numerical effects can be responsible for this effect. No consequences will follow in reactor analyses from this behaviour at very high concentration of Am241.

#### 2.2.10 Indication of probable irregularities for Am243

In <u>Tab\_11</u> irregularities are found in elastic scattering for the resolved resonance region (group 28), in the <u>unresolved</u> resonance region for neutron capture, and in the high energy region (group 6) in the fission cross section.

<u>Comments</u>: In the resolved resonance region again the elastic cross section seems to have some error by about 3% and it appears also, when point-wise data are used. As before, a not accurate enough flux depression in this resonance is probably the reason for this behaviour. The unresolved resonance region shows irregularities for the capture cross section by 2 % to 4% for  $\sigma_0 = 10$  barn and at high temperature only: The description of the unresolved resonance region therefore needs to be improved, although in reactor calculations this relatively high concentration of Am243 will not occur.

The observed irregularity in group 6 at high energy again happens for very low fission cross sections; numerical effects may be responsible for this behaviour at very high concentration of the material: this will have no effect in reactor calculations.

## 2.3 Indication of probable irregularities for structural materials (Zr, Fe, Cr, Ni) oxygen and boron

At first, observations for irregularities for zirconium, oxygen and boron are discussed (materials present in light water reactors). Secondly the observations for Fe, Cr, Ni, structural materials in advanced PWRs and in fast reactors, are investigated.

#### 2.3.1 Indications of irregularities for zirconium, oxygen and boron No indications of irregularities were observed for natural zirconium, for oxygen, for boron 10 and boron 11.

## 2.3.2 Indications of probable irregularities for natural Fe, Cr, and Ni

As seen from <u>Tab. 12</u>, for high concentration of natural iron ( $\sigma_0 = 0.001$ ) between 25 and 41 keV a negative capture cross section was observed for 2100 K.

<u>Comments:</u> In this range, the total cross section has a very deep minimum ("window" at 25 keV), followed by a high maximum at about 28 keV. The capture cross section has in this energy region a broad s-wave resonance and some narrow p-wave resonances with about 1 barn in the peaks. The capture cross section in the valleys between the resonances (between 30 and 41 keV) decreases below 0.001 barns. The observed negative capture group cross section in group 12 was calculated to be - 0.0076 barns. The resonance representation is given in MLBW. The reasons for this irregularity can come from numerical errors, the NR  $\leftarrow 1/\Sigma_t$  (E) description of the neutron flux density in the resonances, and the use of negative "addition" cross sections, which are not Doppler broadened.

## 2.3.3 Indication of probable irregularities for hydrogen, bound in water

The JEF-1 file contains the presently best available data. They have been shown to give better results than the ENDF/B - III source, which is still in current use (see Ref. /1/). After correcting a simple error in the original file, no further irregularities were found.

2.4 Indication of probable irregularities in processing fission product cross sections.

The cross section file for fission products in JEF-1 is considered as one of the best available international data files at present. Integral data tests were used in addition to a critical review of the evaluations to verify the quality of the data (see Ref. /1/).

Fission products do not occur with high concentration in reactor burnup investigations (usually they can be considered as infinitely diluted). Inconsistencies were observed for the cross sections of a few fission product isotopes, but all of these irregularities occur at high concentration of the nuclides in question. In the resonance region, even negative cross sections appear for some nuclides in high concentration:

Tc99, Pd107, Cs133, Pr141, Nd144, Nd145, Nd148, Pm147, Sm147, Sm149, Sm151, Eu155

For some nuclides (e.g. Ru103, Pd108, Nd146, Nd188, Nd150, Pm148m, Sm149, Sm150, Sm151, Eu153, Eu154, Eu155, Gd156, G157, Tb159, Lu176), the value of f becomes larger than unity for high concentration.

Although all these irregularities occur for high concentration of the nuclides and therefore are not important in reactor calculations (it should be noted that for large dilution the irregularities with f>1 vanish and f=1 is calculated), they should be clarified. It could be that either the resonance representation (combined in some cases with an extra "addition" cross section), the use of the NR -  $1.\Sigma_t$  (E) weighting in the resonances, or insufficient data are responsible for these irregularities.

Aside from the irregularities in the cross sections of those fission product nuclei, mentioned above, the cross sections of all other fission products do not show irregularities.

#### 3. Formal Removal of observed Irregularities

For application in reactor analysis, the observed irregularities were removed formally. Reactor analysis at present in Karlsruhe is performed on the basis of the -f-factor formalism, introduced by Bondarenko et. al. /6/ within the framework of fast reactor investigations; all reactor codes at KfK are using this concept. With the introduction of JEF-1 nuclear data, the processing system NJOY replaced the KfK processing system MIGROS, but the output of NJOY had to be transformed in order to be accepted by the reactor codes: in consequence therefore resonance selfshielding factors f had to be defined via  $fx = \sigma_x (\sigma_0, T) / \sigma_x (\sigma_0 = \infty, T)$  for three values of the temperature and many values (usually 7) of the background cross section  $\sigma_0$ .

As outlined in chapter 2 of this paper, the hypothesis is used that 0 < f = 1, all deviations of f from this interval [0,1] are assumed to be irregularities due either to the resonance representation in the resolved or unresolved resonance region, to numerical deficiencies or insufficient description of the neutron flux distribution by the NR-approximation within a resonance. Although exceptions from this simple rule may perhaps be possible, which would need further investigation, following formal recipé has been used:

- 1. All values  $f_x > 1$  are put to unity
- 2. If  $f_x < 0$ , then via a suitable extrapolation formula  $f_x$  was fixed to a positive value near to zero.

This simple prescription makes it possible to use the KfK-reactor codes to investigate the quality of the group cross sections, derived from JEF-1, in benchmark calculations and in comparison with experiment. This qualification of the JEF-1 group constant set will be discussed in Ref. /10/.

#### 4. Conclusion

In this paper, probable irregularities in the group cross sections, based on the JEF-1 nuclear data library, are discussed. These irregularities were observed during the generation of a group constant set for application in PWR fuel cycle analyses. As a hypothesis, the resonance selfshielding factor is assumed to be within the interval [0,1], if the group constants are calculated with the adequate resonance representation in the resolved and unresolved resonance region, the true neutron flux density within the resonances, and with an accurate numerical treatment. The deviations from this "regular" behaviour of the resonance selfshielding factors are considered as indications of possible irregularities. The investigation is performed for all heavy nuclides present in (U, Pu) fuel cycles, important structural materials, for oxygen, boron and hydrogen, bound in water

The observed irregularities should be investigated within the framework of group constant calculations for the follow-up cross section file JEF-2. In this way it is hoped that the evaluation and the processing of the fundamental data will then be free of irregularities.

With a few exceptions the main irregularities, described in this paper, occur for the group cross section generation in the unresolved resonance region. An improved treatment of the unresolved resonance region therefore is mandatory. This is already in progress within the JEF-project.

In the processing area, NJOY87 will be applied next, together with its possibilities of adequate treatment of energy dependent flux density calculations within the resonances.

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#### 5. Tables

GROUP	ENERGY	ENERGY WIDTH	LETHARGY WIDTH	GROUP	ENERGY	ENERGY WIDTH	LETHARGY WIDTH	
1 2 3 4 5 6 7 8 9 0 11 12 14 15 14	MeV $10.0 - 6.0655$ $6.0655 - 3.679$ $3.679 - 2.231$ $2.231 - 1.353$ $1.353 - 0.821$ $0.821 - 0.500$ $0.500 - 0.3025$ $0.3025 - 0.183$ $0.183 - 0.1110$ $0.111 - 0.06734$ $0.06734 - 0.04085$ $0.04085 - 0.02478$ $0.02478 - 0.009118$	3.9345 2.3865 1.118 0.878 0.532 0.321 0.1975 0.0195 0.072 0.04366 0.02649 0.01607 0.00975 0.005912	0-49997 0-49998 0.5001 9 0.5001 3 0.49956 0.49592 0.50253 0.50260 0.49996 0.49998 0.49985 0.49987 0.49987 0.49980	28 $4.00 - 3.30$ 29 $3.30 - 2.60$ 30 $2.60 - 2.10$ 31 $2.10 - 1.50$ 32 $1.50 - 1.30$ 33 $1.30 - 1.15$ 34 $1.15 - 1.12$ 35 $1.097 - 1.07$ 36 $1.097 - 1.07$ 37 $1.071 - 1.04$ 38 $1.045 - 1.02$ 39 $1.020 - 0.99$ 40 $0.996 - 0.97$ 41 $0.972 - 0.95$ 42 $0.950 - 0.91$ 43 $0.910 - 0.85$ 44 $0.850 - 0.78$ 45 $0.780 - 0.52$ 45 $0.780 - 0.52$ 45 $0.625 - 0.50$ 45 $0.625 - 0.50$ 45 $0.625 - 0.50$ 45 $0.625 - 0.50$ 45 $0.625 - 0.50$ 45 $0.625 - 0.50$ 45 $0.625 - 0.50$ 46 $0.625 - 0.50$ 57 $0.220 - 0.18$ 58 $0.080 - 0.06$ 59 $0.067 - 0.05$ 60	ENERGY 400 - 3.30 3.30 - 2.60 2.60 - 2.10 2.10 - 1.50 1.50 - 1.30 1.30 - 1.15 1.15 - 1.123 1.123 - 1.097 1.097 - 1.071 1.071 - 1.045 1.045 - 1.020 1.020 - 0.996 0.996 - 0.972 0.972 - 0.950 0.950 - 0.910 0.910 - 0.850 0.850 - 0.780 0.780 - 0.525	4.00 - 3.30 3.30 - 2.60 2.60 - 2.10 2.10 - 1.50 1.50 - 1.30 1.30 - 1.15 1.15 - 1.123 1.097 - 1.071 1.071 - 1.045 1.045 - 1.020 1.020 - 0.996 0.996 - 0.972 0.972 - 0.950 0.950 - 0.910 0.910 - 0.850	0.700 0.700 0.500 0.600 0.200 0.150 0.027 0.026 0.026 0.026 0.026 0.025 0.024 0.022 0.022 0.020 0.040 0.060	0.19237 0.238L1 0.21357 0.33647 0.14310 0.12260 0.02376 0.02342 0.02399 0.02L58 0.02L21 0.02289 0.02L39 0.02289 0.02289 0.04302 0.06821
15 16 17 18 19 20 21 22 23 24 25 26 27	eV 911.6.0 - 5530.0 5530.0 - 3519.1 3519.1 - 2239.45 2239.45 - 1.25.1 1.25.1 - 906.898 906.898 - 367.262 367.262 - 1.28.728 1.28.728 - 75.5012 75.5012 - 28.052 1.8.052 - 27.700 27.700 - 15.968 15.968 - 9.877 9.877 - 2.00	3588 - 0 201 0 - 9 1 279 - 65 81 4 - 35 518 - 202 539 - 636 218 - 534 73 - 2266 27 - 4494 20 - 352 11 - 732 6 - 091 5 - 877	0.50006 0.45198 0.45199 0.45199 0.45197 0.90395 0.90396 0.67797 0.45187 0.55085 0.55085 0.48038 0.90391		0.850 - 0.780 0.780 - 0.625 0.625 - 0.500 0.500 - 0.400 0.500 - 0.300 0.350 - 0.320 0.320 - 0.300 0.320 - 0.280 0.280 - 0.220 0.220 - 0.180 0.180 - 0.140 0.180 - 0.140 0.140 - 0.100 0.100 - 0.080 0.080 - 0.067 0.067 - 0.058 0.058 - 0.050 0.058 - 0.050 0.058 - 0.050 0.058 - 0.050 0.058 - 0.050 0.055 - 0.030 0.030 - 0.025 0.025 - 0.020 0.020 - 0.015 0.015 - 0.010 0.010 - 0.005 0.055 - 0	0.070 0.155 0.125 0.100 0.050 0.020 0.020 0.030 0.020 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.040 0.050 0.005 0.	0.08594 0.22154 0.22314 0.22314 0.13353 0.08961 0.06454 0.06899 0.11333 0.12783 0.20067 0.25131 0.35647 0.22314 0.17733 0.14425 0.14842 0.17435 0.18232 0.15415 0.18232 0.22314 0.28768 0.40547 0.69315	

Table 1: Energy Groups and Group Boundaries for the 69 Group Cross Section Set

σ0	Т(К)	Group Number	ffis	f <sub>tot</sub> c 1)
0.001	300	23		- 0.12
		22		- 0.16
		21		12.47
	900	23	1.05	- 0 10
	500	23	1.05	- 0.13
		22		1.06
		21		- 1.00
		20		4.83
		19		1.03
	2100	23	1.30	- 0.09
		22	1.29	- 0.08
		21		- 0.39
1 <sup>1</sup>		20		- 9.30
		19		1.22
10	2100	23		1.25
		22		1.21

## Table 2:Probable Deficiencies in the Group Cross Sections of U232Indicated by Irregular f-Factors

1) c: current weighted

 
 σ₀
 T(K)
 Group Number
 fcapt
 ffis

 0.001
 2100
 11
 1.02

 10
 1.02
 1.02

## Table 3:Probable Deficiencies in the Group Cross Sections of U234Indicated by Irregular f-Factors

σ <sub>0</sub>	Т(К)	Group Number	f <sub>capt</sub>	<i>f</i> fis
0.001	300	15 14 12	1.03 1.03 1.02	
	900	13 17 16 15	1.03 1.04 1.06 1.07	1.02 1.04 1.04
	2100	14 13 17 16 15 14 13	1.06 1.04 1.08 1.09 1.09 1.07 1.05	1.04 1.03 1.06 1.07 1.06 1.05 1.03
10.	300	16 15 14	1.03 1.04 1.04	1.03 1.03 1.03
	900	13 18 17 16 15 14	1.03 1.05 1.06 1.07 1.07 1.06	1.03 1.04 1.06 1.06 1.05 1.05
	2100	13 19 18 17 16 15 14 13	1.04 1.06 1.09 1.09 1.09 1.08 1.06 1.05	1.04 1.06 1.08 1.08 1.08 1.07 1.05 1.04
100	2100	20 19 18 17 16	1.02 1.03 1.03 1.02 1.02	1.02 1.03 1.02 1.02

# Table 4:Probable Deficiencies in the Group Cross Sections of U235Indicated by Irregular f-Factors

α0	Τ(Κ)		Group Number	$f_{fis}$
		<u>U236</u>		
0.001	300		6	1.04
4	900		6	1.04
	2100		6	1.04
		<u>U238</u>		
0.001	300		6	1.03
	900		6	1.03
	2100		26	1.02
			11	1.04
			6	1.03
10	2100		11	1.03

Table 5:Probable Deficiencies in the Group Cross Sections of U236and U238 Indicated by Irregular f-Factors

σο	T(K)	Group Number	ffis
0.001	300	17	1.03
	900	17	1.03
	2100	17	1.03
	·		
10.	300	17	1.02
	900	17	1.02
	2100	17	1.02

<u>Table 6:</u> Probable Deficiencies in the Group Cross Sections of Pu238 Indicated by Irregular f-Factors

α0	Т(К)	Group Number	fcapt
10	2100	15	1.03
		14	1.03
		13	1.03

# Table ?Probable Deficiencies in the Group Cross Sections of Pu239Indicated by Irregular f-Factors

σΟ	Т(К)	Group Number	fcapt	ffis	fel
0.001	300	28			1.03
	900	28			1.03
	2100	28			1.04
		15	1.03		
		14	1.03	1.02	
10	300	28			1.03
	900	28			1.03
		16	1.03		
		15	1.03	1.03	
		14	1.03	1.03	
		13	1.02	1.02	
	2100	28			1.03
		17	1.05	1.04	
		16	1.06	1.05	
		15	1.05	1.05	
		14	1.04	1.04	
		13	1.03	1.03	

## Table 8:Probable Deficiencies in the Group Cross Sections of Pu241Indicated by Irregular f-Factors

σ0	Т(К)	Group Number	fel
0.001	300	31	1.05
	900	. 31	1.05
	2100	31	1.05
10	300	31	1.04
	900	31	1.04
	2100	31	1.04

## Table 9:Probable Deficiencies in the Group Cross Sections of Pu242Indicated by Irregular f-Factors

σ0	Т(К)	Group Number	ffis	fel
0.001	300	30		1.02
		28		1.03
		6	1.02	
	900	28		1.03
		6	1.02	
	2100	28		1.02
		6	1.02	
10	300	30		1.02
		28		1.02
	900	28		1.02

## Table 10:Probable Deficiencies in the Group Cross Sections of Am241Indicated by Irregular f-Factors

σ0	Т(К)	Group Number	fcapt	ffis	fel
0.001	300	29			1.03
		6		1.02	
	900	29			1.03
		6		1.02	
	2100	29			1.03
		6		1.02	
10.	300	29			1.02
	900	29			1.03
		15	1.02		
	2100	29			1.03
		17	1.04		
		16	1.04		
		15	1.04		
		14	1.02		

## Table 11:Probable Deficiencies in the Group Cross Sections of Am243Indicated by Irregular f-Factors

α0	Т(К)		Group Number	f <sub>capt</sub>
		<u>Fe</u>		
0.001	2100		12	-0.4
		<u>Ni</u>	· .	
0.001	2100		16	1.02

Table 12:Probable Deficiencies in the Group Cross Sections of NaturalFe and Ni Indicated by Irregular f-Factors

#### References

- / 1/ J. Rowlands, N. Tubbs: The Joint Evaluated File: A New Nuclear Data Library for Reactor Calculations, Proc. of Int. Conf. on "Nuclear Data for Basic and Applied science, Vol. 2, p. 1493, Santa Fé, NM (1985)
- / 2/ I. Broeders, B. Krieg: MIGROS-3: A Code for the Generation of Group Constants for Reactor Calculations from Neutron Nuclear Data in KEDAK Format, KfK 2388, Februar 1977
- / 3/ R.E. MacFarlane and D.W. Muir: "NJOY 87.0", Los Alamos National Laboratory Memo T-2-L-10991, June 1987
- / 4/ B. Krieg, I. Broeders: The KfK-Version of the Neutron and Photon Cross Section Generation Code NJOY: Implementation, Verification and Modification of the Code, Internal KfK-Report, JEF-DOC, Kernforschungszentrum Karlsruhe (1987)
- / 5/ B. Krieg, I. Broeders: JOYFOR a Program for Tranformation on NJOY Results in MATXS-Format to the MITRA Input Format, KfK 4179, Kernforschungszentrum Karlsruhe, Februar 1987
- / 6/ L.P. Abagjan, N.O. Bazazjanc, I.I. Bondarenko, M.N. Nikolaev: Gruppenkonstanten schneller und intermediärer Neutronen für die Berechnung von Kernreaktoren, KfK-tr-144 (1965)
- / 7/ A. Mateeva, H. Küsters: Testing of JEF-1 Data on the Burnup Behaviour of PWR-Fuel up to 33 GWd/t, JEF-DOC (1987)
- / 8/ D.E. Cullen: Report on the IAEA Cross Section Processing Code Verification Project, INDC (NDS)-170/NI (1985)
- / 9/ F.H. Fröhner: Self-shielding Factors Greater than Unity in Narrow-Resonance Approximation, Internal KfK-Report, Kernforschungszentrum Karlsruhe (1978)
- A. Mateeva: Qualification of the JEF-1 Nuclear Data Library for Pressurized
   Water Reactors, KfK-4461, Kernforschungszentrum Karlsruhe (1988)