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Addendum

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Translation of Selected Reports on Neutron Spectrum Unfolding

by Kh. Ya. Bondars, et al

Institute of Physics
Academy of Sciences of the Latvian SSR.
P. Stuchka Latvian State University

Translated by the IAEA

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PHYSICS OF THE ATOMIC NUCLEUS AND ATOMIC AND MOLECULAR SPECTROSCOPY

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METHODS OF NEUTRON SPECTRUM CALCULATION FROM MEASURED REACTION RATES IN SAIPS PART III. NEUTRON CROSS-SECTION LIBRARIES

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ABSTRACT

The paper provides the information needed by users of the SAIPS information system on the neutron cross-section libraries accessible and on the principles upon which they are based. Neutron cross-section integrals in fission and fusion spectra are given.

1. INTRODUCTION

In SAIPS [2, 3] some of the neutron cross-section libraries most frequently used in laboratories for unfolding neutron spectra have been adapted and approved and are brought up to date and recommended for calculations. Neutron cross-section libraries differ with regard to their compositions, evaluated cross-sections, the principles on which they are based and so on. It is not possible to select a single "correct" cross-section library, since subjective assumptions are involved in the establishment of any of these libraries. There thus arises a need for periodic review of the cross-sections recommended. This is particularly important when they are to be used in new fields, for example, for controlled nuclear fusion devices.

In this paper questions arising in connection with the selection of the set of detectors used for unfolding neutron spectra and with the evaluation of the quality of different laboratories are discussed.

2. PROCESSING AND EVALUATION OF MEASURED CROSS-SECTIONS IN THE SETTING UP OF THE ZACRSS DOSIMETRY LIBRARY

Over a number of years we have been setting up a dosimetry library based on the evaluation of measured neutron cross-sections. It has also been modified, approved, used in calculations, compared with other cross-section libraries and so on. At the same time, software for processing neutron cross-sections has been developed and improved.

We presented the first cross-section evaluations in Ref. [5] in the form of figures, while the numerical data were sent to the Scientific Research Institute for Power Physics at Obninsk. At the Second All-Union Meeting on Measurement of Neutron Radiation in Reactors and Accelerators the techniques used for performing these evaluations were described [4]. In Ref. [9] the data were presented in the form of tables. The latest version of the cross-section library, which has been called "ZACRSS", is described in Ref. [1] and has been sent to the Obninsk Institute and to the computer centre of the Radiation Shielding Information Center (RSIC) at Oak Ridge, United States. In ZACRSS, 28 threshold reactions are evaluated (see Table 2). The first cross-section evaluations were made with the Minsk-32 computer, and experimental data were collected from the literature. With developments in computer technology and international contacts, as well as in the work of the Obninsk Institute, the methods used for evaluating and processing experimental cross-section measurements have been improved. On the ES-1022 we have now developed the software for automation of the processing of neutron cross-sections. It can be used for preliminary processing of sets of data containing cross-sections in the EXFOR exchange format, i.e. copying, correction of physical and logical errors, sorting, selection of the cross-sections required etc. With this preliminary processing it is possible to assemble a set of data containing neutron cross-sections to be used for evaluation and a set of data providing additional information.

Cross-sections are evaluated by the least-squares method using a polynomial approximation of experimental cross-section measurements [8]. The evaluation program has been constructed on the basis of the programs of Ref. [10]. Apart from its adaptation on the ES-1022 computer, some additional features were added: a freer format for initial input data; a wider determination of weights; identification of the argument range required (in this case the energy range); compression of the argument variation range etc. For the approximation, orthogonal polynomials are used [8]. The degree of the polynomial k at which the best approximation is reached was determined from the condition of the minimum in relation to k of the value.

$$\varepsilon_0(k)=\sum_{n=1}^{N}(\sigma_n-\sigma_n^{(k)})^2 p_n/(N-k)N,$$

where N is the number of experimental data points over which the approximation is made, p_n is the weight of the measured cross-sections at the n-th point and $\sigma_n^{(k)}$ is the polynomially approximated cross-section at the n-th point. Various methods were used for performing the evaluation: the energy range was divided up into overlapping parts and different weights were used. This was necessary because of the great differences in the evaluated cross-sections, the deterioration in the conditionality of the problem with an increase in the number of orthogonal polynomials and experimental values [7], and the complex nature of the cross-sectional dependence of certain reactions. The results obtained were matched. At the same time, the error in the evaluation was calculated on the basis of the propagation of errors [8].

The evaluated data are presented in the form of coefficients of a polynomial or in terms of data points. If required, they may be given in the form of tables, displayed with a plotter or put in the form required for adaptation in SAIPS.

3. EVALUATED CROSS-SECTION LIBRARIES

The cross-section libraries ENDF/B-IV, ENDF/B-V (the dosimetry part), ENDL 76 (78), JENDL-1 and the library set up at the Institute of Heat and Mass Exchange of the Byelorussian Academy of Sciences have been adapted in SAIPS in ENDF/B format. The advantage of ENDF/B format lies in the fact that, in addition to the figures, further information is provided for the data shown. For processing these data a set of programs has been constructed for searching and displaying the data required, calculating cross-sections in the resonance region, presenting cross-sections in the SAIPS dosimetry library format, print-out, plotting, visual display etc., of the data required. The set of programs consists of rewritten and adapted programs for processing data in ENDF/B format.

In SAIPS the adapted version of the BOSPOR 78 libraries contains evaluated cross-sections at energy points [6].

As a rule the unfolding programs adapted in SAIPS contain ther own dosimetry libraries of cross-sections. These programs include: (1) SAND II, which came with the DETAN 74 library; (2) WINDOWS, which came with the dosimetry cross-section libraries from ENDF/B-IV, DETAN 74 and some libraries for which the source of cross-sections is not given; (3) GIN, which contains some resonance cross-sections; and (4) RFSP JÜL, which came with a cross-section library for which the source is not given. When setting up the cross-section library for their own calculation programs the authors ignore the need for additional information on cross-sections, which renders determination of the quality of cross-sections in libraries difficult. Thus, although for SAIPS users cross-sections from libraries of all the unfolding programs mentioned are available, they are not shown in the summary tables 1 and 2. Exceptions are the resonance cross-sections from the GIN program library, which are not found in other dosimetry libraries.

4. THE CONTENT OF AND CHARACTERISTICS OF CROSS-SECTIONS IN VARIOUS LIBRARIES

Tables 1 and 2 give lists of adapted cross-sections and some of their characteristics. The integrals are calculated from the formula

$$A_i = \int_0^{18\ \text{МэВ}} \sigma(E)\varphi(E)\,dE,$$

where $\sigma(E)$ are the neutron cross-sections as a function of the energy E, $\phi(E)$ or the fission spectrum in the Watt form

$$\varphi(E) = 0{,}484 e^{-E}\,\mathrm{sh}\,(\sqrt{2E})$$

and the spectrum of the thermonuclear fusion model shown in Table 3. The table shows the energy range in which detectors make a 90% contribution, rejecting ± 5% in the direction of high and low energies.

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Integrals of adapted resonance detector cross-sections*/

Table 1

№	Reaction	Spectrum No.	Cross-section source				Limits of 90% of energy range	
			DETAN 74	ENDF/B-IV	ENDF/B-V	Australian library	Low	High
1	2	3	4	5	6	7	8	9
1	$^{23}Na(n,\gamma)^{24}Na$	1	2,647E−28	2,621E−28	3,071E−28		5,750E−02	4,400E+00
		2	3,359E−28	2,989E−28	3,051E−28		1,425E−01	1,420E+01
2	$^{45}Sc(n,\gamma)^{46}Sc$	1	6,097E−27	5,653E−27	6,733E−27		4,500E−02	3,200E+00
		2	5,375E−27	5,119E-27	4,571E−27		1,150E−01	1,360E+01
3	$^{55}Mn(n,\gamma)^{56}Mn$	1	3,558E−27				3,400E−02	3,800E+00
		2	2,911E−27				1,100E−01	1,360E+01
4	$^{58}Fe(n,\gamma)^{59}Fe$	1	2,814E−27	2,033E−27	1,623E−27		1,600E−01	3,200E+00
		2	1,977E−27	3,710E−27	3,727E−27		1,350E−01	6,200E+00
5	$^{59}Co(n,\gamma)^{60}Co$	1	5,187E−27	6,237E−27	6,035E−27		1,900E−02	2,300E+00
		2	4,370E−27	5,204E−27	4,356E−27		1,100E−01	3,100E+00
6	$^{63}Cu(n,\gamma)^{64}Cu$	1	1,073E−26	1,077E−26	9,942E−27		2,700E−02	4,000E+00
		2	8,836E−27	7,113E−27	7,811E−27		1,200E−01	1,380E+01
7	$^{98}Mo(n,\gamma)^{99}Mo$	1				3,896E−26	1,100E−01	3,100E+00
		2				2,591E−26	1,275E−01	2,700E+00
8	$^{109}Ag(n,\gamma)^{110}AgM$	1	1,138E−26				6,300E−02	4,300E+00
		2	1,106E−26				1,275E−01	1,400E+01
9	$^{115}In(n,\gamma)^{116}InM$	1	1,463E−25	1,349E−25	1,259E−25		1,050E−01	3,100E+00
		2	9,057E−26	8,465E−26	7,759E−26		1,275E−01	4,300E+00
10	$^{139}La(n,\gamma)^{140}La$	1				6,363E−27	5,250E−02	2,600E+00
		2				4,321E−27	1,200E−01	2,100E+00
11	$^{152}Sm(n,\gamma)^{153}Sm$	1				6,057E−26	5,000E−02	2,800E+00
		2				4,049E−26	1,150E−01	2,600E+00
12	$^{164}Dy(n,\gamma)^{165}Dy$	1				1,757E−26	1,000E−01	3,200E+00
		2				1,165E−26	1,200E−01	2,800E+00
13	$^{186}W(n,\gamma)^{187}W$	1				3,663E−26	1,000E−01	3,300E+00
		2				2,537E−26	1,200E−01	4,500E+00
14	$^{197}Au(n,\gamma)^{198}Au$	1	8,082E−26	8,235E−26	8,035E−26		3,800E−02	2,500E+00
		2	7,064E−26	6,671E−26	6,092E−26		1,150E−01	6,900E+00
15	$^{232}Th(n,\gamma)^{233}Th$	1	1,018E−25	9,921E−26	9,053E−26		8,400E−02	3,000E+00
		2	7,528E−26	7,190E−26	6,237E−26		1,150E−01	4,200E+00
16	$^{238}U(n,\gamma)^{239}U$	1	8,701E−26	7,297E−26	6,558E−26		9,200E−02	2,800E+00
		2	5,788E−26	4,884E−26	4,818E−26		1,275E−01	3,300E+00

*/ 1 – fission spectrum

2 – hybrid-reactor spectrum

Table 2

Cross-section integrals for spectrum of fission and hybrid thermonuclear tokamak reactor threshold detectors

№	Reaction	Cross-section source					Limits of 90% of energy range	
		DETAN 74	ENDF/B-IV	ENDF/B-V	ZACRSS	BOSPOR-78	Low	High
1	2	3	4	5	6	7	8	9
1	$^{6}Li(n, \alpha)^{3}H$		4,795E−25 5,714E−25				1,700E−01 1,700E−01	5,500E+00 1,410E+01
2	$^{10}B(n, \alpha)^{7}Li$		5,037E−25 6,085E−25				6,600E−02 1,275E−01	5,200E+00 1,420E+01
3	$^{19}F(n, 2n)^{18}F$				6,730E−30 1,445E−26		1,220E+01 1,300E+01	1,650E+01 1,440E+01
4	$^{24}Mg(n, p)^{24}Na$	1,497E−27 8,904E−26			1,488E−27 8,366E−26		6,600E+00 1,120E+01	1,140E+01 1,430E+01
5	$^{27}Al(n, \alpha)^{24}Na$	6,633E−28 5,299E−26	6,848E−28 5,229E−26	6,848E−28 5,216E−26	6,803E−28 5,029E−26		6,500E+00 1,150E+01	1,180E+01 1,430E+01
6	$^{27}Al(n, p)^{27}Mg$	3,841E−27 3,982E−26	4,091E−27 3,762E−26	4,091E−27 3,740E−26	3,981E−27 3,955E−26		3,500E+00 6,600E+00	9,200E+00 1,430E+01
7	$^{28}Si(n, p)^{28}Al$	9,737E−27 1,713E−25					5,500E+00 8,200E+00	1,010E+01 1,430E+01
8	$^{31}P(n, p)^{31}Si$	3,302E−26 5,705E−26					2,200E+00 3,000E+00	6,900E+00 1,420E+01
9	$^{32}S(n, p)^{32}P$	6,055E−26 1,555E−25	6,505E−26 1,553E−25		6,469E−26 1,557E−25		2,500E+00 3,900E+00	7,400E+00 1,430E+01
10	$^{34}S(n, \alpha)^{31}Si$	2,234E−27 5,451E−26					5,200E+00 9,900E+00	1,030E+01 1,430E+01
11	$^{35}Cl(n, \alpha)^{32}P$	1,327E−26 5,761E−26					3,200E+00 4,500E+00	7,900E+00 1,430E+01
12	$^{46}Ti(n, p)^{46}Sc$	1,129E−26 1,322E−25	9,927E−27 1,207E−25	1,075E−26 1,181E−25	1,046E−26 1,295E−25		3,400E+00 6,800E+00	9,100E+00 1,430E+01

Table 2 continued

13	$^{47}Ti(n,p)^{47}Sc$	1,774E−26 3,893E−26	2,176E−26 6,200E−26	2,191E−26 6,402E−26	2,063E−26 5,970E−26		2,100E+00 3,000E+00	6,900E+00 1,430E+01
14	$^{48}Ti(n,p)^{48}Sc$	2,367E−28 3,722E−26	1,696E−28 2,503E−26	2,684E−28 2,566E−26	1,657E−28 2,573E−26		6,600E+00 1,230E+01	1,280E+01 1,440E+01
15	$^{52}Cr(n,p)^{52}V$					7,486E−28 4,398E−26	5,700E+00 1,120E+01	1,140E+01 1,430E+01
16	$^{54}Fe(n,p)^{54}Mn$	7,886E−26 2,209E−25	7,852E−26 2,203E−25	7,887E−26 2,125E−25	7,707E−26 2,163E−25	8,315E−26 2,366E−25	2,300E+00 4,000E+00	7,700E+00 1,430E+01
17	$^{55}Mn(n,2n)^{54}Mn$		2,322E−28 2,796E−25	1,911E−28 2,583E−25	1,988E−28 2,990E−25		1,110E+01 1,290E+01	1,540E+01 1,440E+01
18	$^{56}Fe(n,p)^{56}Mn$	1,086E−27 4,710E−26	1,036E−27 4,671E−26	9,900E−28 4,606E−26	1,088E−27 4,574E−26	9,980E−28 4,743E−26	5,500E+00 1,090E+01	1,100E+01 1,430E+01
19	$^{58}Ni(n,p)^{58}Co$	1,056E−25 2,582E−25	1,029E−25 2,442E−25	1,023E−25 2,533E−25	1,059E−25 2,555E−25	9,671E−26 2,551E−25	2,100E+00 3,700E+00	7,400E+00 1,430E+01
20	$^{58}Ni(n,2n)^{57}Ni$	2,396E−30 5,585E−27	2,541E−30 6,280E−27	2,580E−30 6,634E−27	2,472E−30 5,872E−27		1,320E+01 1,330E+01	1,700E+01 1,450E+01
21	$^{59}Co(n,\alpha)^{56}Mn$	1,466E−28 1,171E−26	1,457E−28 1,171E−26	1,421E−28 1,172E−26	1,494E−28 1,157E−26		5,900E+00 1,170E+01	1,180E+01 1,430E+01
22	$^{59}Co(n,2n)^{58}Co$		1,625E−28 2,268E−25	1,722E−28 2,593E−25			1,130E+01 1,290E+01	1,560E+01 1,440E+01
23	$^{60}Ni(n,p)^{60}Co$	5,306E−27 5,878E−26	2,444E−27 5,851E−26	2,496E−27 5,715E−26		2,382E−27 6,490E−26	2,700E+00 7,500E+00	9,500E+00 1,430E+01
24	$^{63}Cu(n,\alpha)^{60}Co$	4,908E−28 1,688E−26	3,473E−28 1,620E−26	5,335E−28 1,906E−26	3,651E−28 1,640E−26		3,900E+00 1,010E+01	1,090E+01 1,430E+01
25	$^{63}Cu(n,\alpha)^{60}CoM$	4,521E−28 1,686E−26					5,900E+00 1,020E+01	1,100E+01 1,430E+01
26	$^{63}Cu(n,2n)^{62}Cu$	8,474E−29 1,686E−25			7,338E−29 1,493E−25		1,190E+01 1,300E+01	1,630E+01 1,440E+01
27	$^{64}Zn(n,p)^{64}Cu$	3,801E−26 1,194E−25			3,571E−26 1,227E−25	3,485E−26 1,121E−25	2,400E+00 4,000E+00	7,700E+00 1,430E+01

Table 2 continued

1	2	3	4	5	6	7	8	9
28	$^{64}Zn(n, 2n)^{63}Zn$				1,635E−29 3,537E−26		1,300E+01 1,320E+01	1,700E+00 1,450E+01
29	$^{65}Cu(n, 2n)^{64}Cu$		2,978E−28 3,270E−25	2,909E−28 3,121E−25	2,901E−28 3,041E−25		1,090E+01 1,280E+01	1,530E+01 1,440E+01
30	$^{90}Zr(n, 2n)^{89}Zr$	7,956E−29 1,849E−25					1,260E+01 1,310E+01	1,670E+01 1,440E+01
31	$^{90}Zr(n, p)^{90}J$				3,568E−28 1,807E−26		4,600E+00 1,130E+01	1,120E+01 1,430E+01
32	$^{93}Nb(n, 2n)^{92}Nb$				3,754E−28 1,805E−25		9,800E+00 1,250E+01	1,410E+01 1,430E+01
33	$^{103}Rh(n, n)^{103}RhM$				7,077E−25 5,151E−25		8,000E−01 7,600E−01	5,900E+00 1,400E+01
34	$^{115}In(n, n)^{115}InM$	1,855E−25 1,198E−25	1,705E−25 1,129E−25	1,767E−25 1,139E−25	1,829E−25 1,180E−25		1,200E+00 1,300E+00	5,800E+00 1,400E+01
35	$^{127}J(n, 2n)^{126}J$	6,868E−28 4,888E−25	1,150E−27 6,212E−25	1,150E−27 6,232E−25	6,667E−28 5,042E−25	4,522E−28 4,348E−25	1,010E+01 1,270E+01	1,460E+01 1,440E+01
36	$^{203}Tl(n, 2n)^{202}Tl$					2,834E−27 7,954E−25	8,700E+00 1,220E+01	1,350E+01 1,440E+01
37	$^{232}Th(n, f)FP$	7,141E−26 1,828E−25	7,074E−26 1,761E−25	7,379E−26 1,764E−25	7,089E−26 1,727E−25		1,600E+00 2,500E+00	7,100E+00 1,430E+01
38	$^{232}Th(n, 2n)^{231}Th$				1,541E−26 6,571E−25		7,100E+00 1,020E+01	1,110E+01 1,430E+01
39	$^{235}U(n, f)FP$	1,230E−24 1,593E−24	1,236E−24 1,586E−24	1,231E−24 1,555E−24			2,000E−01 2,100E−01	5,100E+00 1,420E+01
40	$^{237}Np(n, f)FP$	1,292E−24 1,644E−24	1,337E−24 1,602E−24	1,339E−24 1,600E−24	1,303E−24 1,601E−24		6,900E−01 8,800E−01	5,400E+00 1,430E+01
41	$^{238}U(n, f)FP$	2,873E−25 5,865−25	3,018E−25 7,260E−25	2,997E−25 5,867E−25	2,868E−25 5,885E−25		1,500E+00 2,200E+00	6,700E+00 1,430E+01
42	$^{239}Pu(n, f)FP$	1,762E−24 2,036E−24	1,782E−24 2,027E−24	1,786E−24 2,028E−24			2,700E−01 2,550E−01	5,100E+00 1,420E+01

Table 3

Spectrum of hybrid thermonuclear tokamak reactor [11]

№	Energy MeV	$\phi(E)$, $\frac{n}{cm^2 \cdot MeV \cdot s}$	№	Energy MeV	$\phi(E)$, $\frac{n}{cm^2 \cdot MeV \cdot s}$	№	Energy MeV	$\phi(E)$, $\frac{n}{cm^2 \cdot MeV \cdot s}$
1	0,1125	18,02	21	1,1	0,88	41	7,75	0,02
2	0,1375	18,16	22	1,3	0,65	42	8,25	0,01
3	0,1625	18,32	23	1,5	0,45	43	8,75	0,01
4	0,1875	12,86	24	1,7	0,39	44	9,5	0,05
5	0,2115	14,64	25	1,9	0,27	45	10,5	0,01
6	0,2375	10,08	26	2,125	0,29	46	11,5	0,008
7	0,2625	13,48	27	2,375	0,24	47	12,25	0,02
8	0,29	10,72	28	2,625	0,22	48	12,75	0,03
9	0,325	9,16	29	2,825	0,14	49	13,35	0,2
10	0,375	8,98	30	3,125	0,14	50	13,85	1,05
11	0,425	5,9	31	3,375	0,12	51	14,05	1,27
12	0,475	5,74	32	3,625	0,1	52	14,6	1,23
13	0,525	5,06	33	3,875	0,1	53	14,3	1,01
14	0,575	4,36	34	4,25	0,11	54	14,5	0,54
15	0,625	4,6	35	4,75	0,06	55	14,7	0,16
16	0,675	3,71	36	5,25	0,046	56	14,9	0,03
17	0,725	3,28	37	5,75	0,04	57	15,1	0,00
18	0,775	2,18	38	6,25	0,03	58	15,3	0,00
19	0,85	2,12	39	6,75	0,03	59	15,5	0,00
20	0,95	1,54	40	7,25	0,02	60	15,6	0,00