

INDC(HUN)–34 Distr.: G+R

[N D C INTERNATIONAL NUCLEAR DATA COMMITTEE

The Group Version of the International Reactor Dosimetry File IRDF–90 for Use in the Neutron Metrology File NMF–90 (IRDF–90/NMF–G)

E. J. Szondi Institute of Nuclear Techniques Technical University of Budapest, Hungary

October 1999

IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

Produced by the IAEA in Austria October 1999

The Group Version of the International Reactor Dosimetry File IRDF–90 for Use in the Neutron Metrology File NMF–90 (IRDF–90/NMF–G)

E. J. Szondi Institute of Nuclear Techniques Technical University of Budapest, Hungary

Abstract

The International Reactor Dosimetry File IRDF–90 of the Nuclear Data Section of the IAEA has been developed for neutron metrology purposes. Its second version was distributed in October 1993.

In frame of the evaluation of the Neutron Metrology File NMF–90 a systematic revision of IRDF–90 has been performed. The format of this cross section library has been adjusted to the ENDF–6 format rules, and the integrity of covariance information of several reactions has been improved. The library includes data on 53 reactions of 37 detector materials, furthermore 9 cross section sets without covariance information (cover materials, dpa calculation). The cross sections are available in a 640 groups (extended SAND II) histogram format.

This version of the library noted IRDF–90/NMF–G is distributed in PC DOS format. Programs for installation and integrity test are also supplied.

October 1999

Contents

Introduction	7
The structure of the library	8
The content of the IRDF–90/NMF–G	9
Summary of the modifications to the 2nd version of the IRDF-90 to include that library in the NMF–90	12
Installation of the library on a personal computer	15
References	16

Introduction

The cross section library *International Reactor Dosimetry File IRDF–90* of the Nuclear Data Section of the International Atomic Energy Agency (IAEA NDS) (2nd version, released in September 1993 [1]) was compiled in ENDF–6 format [2]. The aim of this library was to supply a consistent data base for neutron metrology investigations.

In the mean-time the Neutron Metrology File NMF–90 [3] has been developed. This file contains cross section processing and neutron spectrum adjustment modules elaborated by different institutes (Institute of Nuclear Techniques of the Technical University of Budapest; Netherlands Energy Research Foundation, ECN, Petten; Physikalisch–Technische Bundesanstalt, Braunschweig; Oak Ridge National Laboratory). It will be distributed by IAEA NDS. An improved version of the file IRDF–90 has been produced in order to be applied as common cross section library for the different modules of NMF–90.

The name "**IRDF–90/NMF–G**" was assigned to this library, where the letter "G" means that the cross section data are given in 640 groups, in histogram form in the "extended SAND II" energy grid [4] from 0.0001 eV to 20 MeV.

This report contains a technical description on the library.

The Structure of the Library

The numerical data in file MF = 3 are interpreted as *sums of the smooth background cross sections and of the resonance contribution*, therefore the file MF = 2 is not needed for further processing. Similar structure is required for describing the uncertainty information of the cross sections, *i.e.* the uncertainty due to the resonance contribution which is given in file MF = 32, has been summed up with the uncertainty of the smooth background cross section (MF = 33) and stored *only* in file MF = 33.

The following ENDF–6 notations occur in the description:

- HEAD the first record in a section
- HSUB eye-readable identifier for the library
- IREV revision number
- LRP flag that indicates whether resolved and/or unresolved resonance parameters are given in File 2
- MAT unique material identification number
- MF file label
- MT section
- NLIB library identifier
- NSUB sublibrary number
- NTAPE tape number
- XMF1 floating point form of a file number referenced for covariance data

The Content of the IRDF-90/NMF-G

This description refers to the library the tape number of which is NTAPE = 9404. The library identifier is the same as the one in the IRDF-90 Version 2: NLIB = 34.

The library contains the cross sections and their uncertainties (in form of covariance matrices) for the target materials and reactions listed in Table 1.

			Table 1
Reaction	Evaluator(s), Laboratory	Evaluation DATE	Material MAT
${}_{3}^{6}Li(n,{}_{1}^{3}H){}_{2}^{4}He$	G. M. Hale, P. G. Young, LANL*	April 1989	325
${}^{10}_{5}B(n,\alpha)^{7}_{3}Li$	G. M. Hale, P. G. Young, LANL*	November 1989	525
${}^{19}_{9}F(n,2n){}^{18}_{9}F$	M. Wagner et al, IRK	June 1980	925
$^{23}_{11}Na(n,\gamma)^{24}_{11}Na$	Yuan Hanrong, CNDC	April 1990	1123
${}^{24}_{12}Mg(n,p){}^{24}_{11}Na$	M. Wagner et al., IRK	April 1990	1225
${}^{27}_{13}Al(n,p){}^{27}_{12}Mg$	D.M. Hetrick, C.Y. Fu, ORNL	April 1990	1325
$^{27}_{13}Al(n,\alpha)^{24}_{11}Na$	M. Wagner et al., IRK	April 1990	1325
${}^{31}_{15}P(n,p){}^{31}_{14}Si$	M. Wagner et al., IRK	June 1980	1525
${}^{32}_{16}S(n,p){}^{32}_{15}P$	D.M. Hetrick, C.Y. Fu, ORNL	1989	1625
$^{45}_{21}Sc(n,\gamma)^{46}_{21}Sc$	Z. X. Zhao, CNDC	February 1991	2126
${}^{46}_{22}Ti(n,p){}^{45}_{21}Sc$	D.M. Hetrick, C.Y. Fu, ORNL	1989	2225
${}^{47}_{22}Ti(n,np){}^{46}_{21}Sc$	C. Philis et al., ANL	January 1977	2228
${}^{47}_{22}Ti(n,p){}^{47}_{21}Sc$	C.Y. Fu, ORNL	1991	2228
${}^{48}_{22}Ti(n,np){}^{47}_{21}Sc$	C.Y. Fu, ORNL	January 1977	2231
$\frac{{}^{48}_{22}}{Ti(n,p)}^{48}_{21}Sc$	D.M. Hetrick, C.Y. Fu, ORNL	1989	2231
$\frac{nat}{23}V(n,p)$	A. Smith, D. Smith, ANL	June 1988	2300
$^{52}_{24}Cr(n,2n)^{51}_{24}Cr$	M. Wagner et al., IRK	April 1990	2431
${}^{55}_{25}Mn(n,2n){}^{54}_{25}Mn$	K. Shibata, JAERI, ORNL	March 1988	2525
$^{55}_{25}Mn(n,\gamma)^{56}_{25}Mn$	K. Shibata, JAERI, ORNL	March 1988	2525
${}^{54}_{26}Fe(n,p){}^{54}_{25}Mn$	D. M. Hetrick et al., ORNL	November 1989	2625
${}^{56}_{26}Fe(n,p){}^{56}_{25}Mn$	C. Y. Fu et al., ORNL	November 1989	2631
$\frac{58}{26}Fe(n,\gamma)\frac{59}{26}Fe$	N. M. Larson, ORNL	November 1989	2637
$\frac{59}{27}Co(n,2n)^{58}_{27}Co$	M. Wagner et al., IRK	April 1990	2725
$^{59}_{27}Co(n,\gamma)^{60}_{27}Co$	S. Mughabghab, BNL	1977	2725
$\frac{59}{27}Co(n,\alpha)^{56}_{25}Mn$	A. Smith et al, ANL	April 1990	2725

Dosimetry reactions in IRDF-90/NMF-G

Reaction	Evaluator(s), Laboratory	Evaluation	Material
		DATE	MAT
$^{58}_{28}Ni(n,2n)^{57}_{28}Ni$	M. Wagner et al., IRK	April 1990	2825
$^{58}_{28}Ni(n,p)^{58}_{27}Co$	N. Larson et al., ORNL	1989	2825
${}^{60}_{28}Ni(n,p){}^{60}_{27}Co$	N. Larson et al., ORNL	October 1989	2831
$^{63}_{29}Cu(n,2n)^{62}_{29}Cu$	M. Wagner et al., IRK	November 1989	2925
$^{63}_{29}Cu(n,\gamma)^{64}_{29}Cu$	C.Y. Fu et al., ORNL	November 1989	2925
$^{63}_{29}Cu(n,\alpha)^{60}_{27}Co$	C.Y. Fu et al., ORNL	November 1989	2925
$^{65}_{29}Cu(n,2n)^{64}_{29}Cu$	Hetrick, Fu, Larson, ORNL	November 1989	2931
${}^{64}_{30}$ Zn(n, p) ${}^{64}_{29}$ Cu	M. Wagner et al., IRK	April 1990	3025
${}^{89}_{39}Y(n,2n){}^{88}_{39}Y$	R. Howerton et al., LLNL, ANL	January 1986	3925
${}^{90}_{40}Zr(n,2n){}^{89}_{40}Zr$	M. Wagner et al., IRK	April 1990	4025
$^{93}_{41}Nb(n,2n)^{92}_{41}Nb$	M. Wagner et al., IRK	July 1991	4125
${}^{93}_{41}Nb(n,n_1){}^{93m}_{41}Nb$	M. Wagner et al., IRK	July 1991	4125
$^{93}_{41}Nb(n,\gamma)^{94}_{41}Nb$	A. Smith et al., ANL, LLL	July 1991	4125
${}^{103}_{45}Rh(n,n_1){}^{103m}_{45}Rh$	M. Wagner et al., IRK	June 1980	4525
$^{109}_{47}Ag(n,\gamma)^{110}_{47}Ag$	Z. X. Zhao, CNDC	June 1991	4731
$^{115}_{49}In(n,2n)^{114}_{49}In$	C. Dunjiu, CNDC	January 1990	4931
$^{115}_{49}In(n,n_1)^{115m}_{49}In$	S. Chiba, D. L. Smith, ANL	January 1990	4931
$^{115}_{49}$ In (n,γ)	F. Schmittroth, HEDL	January 1990	4931
$^{127}_{53}I(n,2n)^{126}_{53}I$	ZhaoWenrong. Lu Hanlin et al, CNDC	June 1990	5325
$^{197}_{79}Au(n,2n)^{196}_{79}Au$	M. Wagner et al., IRK	April 1990	7925
$^{197}_{79}Au(n,\gamma)^{198}_{79}Au$	P. G. Young et al., LANL*	April 1990	7925
$^{232}_{90}Th(n,f)$	M. Bhat et al, BNL, ANL	December 1977	9040
$^{232}_{90}Th(n,\gamma)^{233}_{90}Th$	M. Bhat et al, BNL, ANL	December 1977	9040
${}^{235}_{92}U(n,f)$	L. W. Weston et al., ORNL, LANL*	April 1989	9228
$\frac{238}{92}U(n,f)$	L. W. Weston et al., ORNL, LANL*	April 1989	9237
$^{238}_{92}U(n,\gamma)^{239}_{92}U$	L. W. Weston et al., ORNL, LANL*	April 1989	9237
$^{237}_{93}Np(n,f)$	F. Mann et al., HEDL, SRL	April 1978	9337
$^{239}_{94}Pu(n,f)$	P. Young et al., LANL*	April 1989	9437

* - The cross sections and covariance martices for ${}^{6}Li(n,\alpha)$, ${}^{10}B(n,\alpha_{0})$, ${}^{10}B(n,\alpha_{1})$, ${}^{197}Au(n,\gamma)$, ${}^{235}U(n,f)$, ${}^{238}U(n,f)$ and ${}^{239}Pu(n,f)$ are taken from unreleased version of ENDF/B-VI evaluation prepared by A. Carlson, G. Hale, W.P. Poenitz and R. Peelle as combined R-matrix and least square fitting of correlated data sets for these reaction. The total cross sections of generally used cover materials listed in Table 2 are given without covariance information.

The cross section for the widely used radiation exposure parameter *displacement per target atom* (dpa) is given for three *components of stainless steels*, as listed in Table 3. These cross sections have been assigned by the reaction codes MT = 900 and MT = 901.

			Table 2
Reaction	Evaluator(s), Laboratory	Evaluation	Material
		EDATE	MAT
$^{10}_{5}B(n,total)$	G. M. Hale, P. G. Young, LANL	November 1989	525
$^{nat}_{48}Cd(n,total)$	S. Pearlstein, BNL	May 1974	4800
$^{nat}_{48}Cd(n,\gamma)$	S. Pearlstein, BNL	May 1974	4800
$^{nat}_{64}Gd(n,total)$	IAEA NDS	August 1990	6400
$^{nat}_{64}Gd(n,\gamma)$	IAEA NDS	August 1990	6400

Cross sections for detector cover materials

Cross sections for dpa calculation

	<i>J</i> 1		Table 3
Reaction	Evaluator(s), Laboratory	Evaluation EDATE	Material MAT
$^{nat}_{24}Cr(n,dpa)$	W. L. Zijp, ECN	1985	2400
$\frac{hat}{26}Fe(n,dpa)$	W. L. Zijp, ECN	1985	2600
$^{nat}_{28}Ni(n,dpa)$	W. L. Zijp, ECN	1985	2800

Summary of the Modifications to the 2nd Version of the IRDF–90 to Include that Library in the NMF–90

The majority of the illegal format elements present in the first version of IRDF–90 (see *e.g.* in [5]) has been corrected in the second issue [1]. However, some shortcomings still remained also in the second version. Depending on the processing code, the format irregularities present in the library might lead to undefined results. To prevent these effects, the non-standard format elements have been adjusted to the ENDF–6 rules. Furthermore, some numerical data of certain reaction cross section covariance matrices have also been modified to make the data in the library consistent. These actions are described in this chapter.

Modifications introduced:

In general, in the HSUB records, the NLIB–NVER symbols on the first card have been changed to "IRDF–90/NMF–G" where the extension to the original "IRDF–90" notation refers to the group version of the Neutron Metrology File NMF–90. The library number, NLIB = 34 hasn't been modified.

The format errors in the positional parameters are corrected (eg the keyword "MATERIAL" was inserted).

Generally, the basic concept of the "group" version of the IRDF–90 libraries was applied consequently. It means that the file MF = 3 shall contain the *sum of the smooth background cross section and the resonance contribution*. Therefore, the resonance parameters of the file MF = 2 are not needed as input data for processing in NMF–90. The NMF–90 version uses the LRP = 0 value for all dosimeter materials. (The unnecessary information has been removed, and the lacking files MF = 2 have been added.) In case of the materials for which no covariance data with the reaction cross sections are given (cover materials, dpa), the value LRP = –1 has been assigned, in spite of the fact, that isn't allowed for incident neutrons. (*E.g.*, the scattering radius, the only value for the LRP = 0 cannot be interpreted for "mixtures" of isotopes.)

The data on the dpa cross sections have been rewritten using the ENDF–6 format rules instead of the ENDF–5.

Furthermore, the following particular modifications have been done:

6–S–32, MAT = 1625: To reduce the size of the file MF = 33, the first sub-subsection has been partitioned. The new covariance matrices describe the same information as the original ones did. Furthermore, the discrepancy of the files MF = 3 and MF = 33 has been eliminated by extrapolating the covariance data downwards (3rd sub-subsection of the second subsection). To sign these modifications the value of REVISION was changed from IREV = 0 to 1.

21–Sc–45, MAT = 2126: Besides the revision of the file MF = 1, the value of DDATE has been included.

The most important modification in the data set of this material was that the structure of the uncertainty information was adapted to "group" conception of the IRDF libraries [6]. In frame of this work the contents of file MF = 32 has been converted into format MF = 33, and inserted there as second subsection. The calculations resulted in the new covariance matrices for the reaction (n,γ) , *i.e.* for MT = 102. The file MF = 32 has been removed.

To sign these modifications the value of REVISION was was to IREV = 1.

22–Ti–46, MAT = 2225: A new sub-subsection was inserted into file MF = 33 to extrapolate the covariance matrix of the (n,p) cross section (MT = 103) downwards from 2.4 to 1.6 MeV.

22–Ti–47, MAT = 2228: A new sub-subsection was inserted into file MF = 33 to extrapolate the covariance matrix of the (n,p) cross section (MT = 103) downwards from 0.80 to 0.69 MeV.

22–Ti–48, MAT = 2231: A new sub-subsection was inserted into file MF = 33 to extrapolate the covariance matrix of the (n,p) cross section (MT = 103) downwards from 4.0 to 3.2 MeV.

29–Cu–63, MAT = 2925: A new sub-subsection was inserted into file MF = 33 to extrapolate the covariance matrix of the (n,α) cross section (MT = 107) downwards from 2.0 to 1.0 MeV.

29-Cu-65, MAT = 2931: The lower energy boundary of the covariance information in file MF = 33 has been modified from 10.1 to 10.0 MeV.

49–In–115, MAT = 4931: In file MF = 33, the value in the field #5 of the HEAD record, furthermore the XMF1 values have been corrected.

Warning: the library doesn't contain the files MF = 8 and MF = 9, therefore the fraction of the production of the ^{116m}In with half life 54 min is given only in a free text of section 451. As the MT = 102 refers to the (n, γ) reaction and **not** to the product of the reaction, the reaction rate that is used in the neutron spectrum adjustment, has to be calculated dividing the saturation activity of ^{116m}In by 0.79.

53–I–127, MAT = 5325: The higher energy boundary of covariance information in file MF = 33 has been modified from 19.89 to 20.00 MeV.

92-U-238, MAT = 9237: The structure of the file MF = 33 has been modified omitting the cross-material covariance terms referring to MAT = 525, MT = 800 and MT = 801, as these reactions aren't present in the library. On the other side, the missing reference in the section MT = 102 to MAT = 9237, MT = 18 has been evaluated and inserted. The reference to MAT = 325, MT = 700 has been renamed to MAT = 325, MT = 105.

The high end of the energy grid in file MF = 33 is 2.3 MeV in IRDF–90 Version 2. To make the files MF = 3 and MF = 33 consistent, a new sub-subsection has been inserted the numerical data of which have been taken from the International Reactor Dosimetry File IRDF–85 [7]. The uncertainty figures became pessimistic this way: the relative standard deviation in the energy region 1.0 to 2.3 MeV in the IRDF–85 is 10 %, while the corresponding values in IRDF–90 Version 2 lie between 1.5 and 2.0 %. Nevertheless, due to

the lack of data, the following IRDF–85 values have to be used: from 2.3 to 4.5 MeV: 11 %, from 4.5 to 5.5 MeV: 16 %, from 5.5 to 20.0 MeV: 30 %. (The cross sections are very low above 2.3 MeV, therefore the importance of these high uncertainty values is negligible.)

93-Np-237, MAT = 9337: The uncertainty information in file MF = 33 has been extrapolated downwards from 10 to 10^{-4} eV inserting a relative standard deviation value of 30 %. (The cross sections are very low below 10 eV, therefore the importance of this high value is negligible [6].)

Installation of the Library on a Personal Computer

The installation of the library on a personal computer is performed using a utility program present on the distribution diskette.

Put the diskette into the selected drive and type at the DOS prompt:

INSTALL <source drive>: <target drive>: Enter

The installing program will check the integrity of the data files on the diskette, expand the library on the target drive, and check the integrity of the generated new library. The results of the test are written in a disk file.

The generated files are: IRDF90NG.DAT (the library), IRDF90NG.DIR (index file), and INSTALL.LOG (CRC values and their references).

REFERENCES

- [1] *N. P. Kocherov, P. K. McLaughlin*: The International Reactor Dosimetry File (IRDF– 90 Version 2). Report IAEA–NDS–141, Rev. 2, October 1993.
- [2] *P. F. Rose, C. L. Dunford*: ENDF–6 Formats Manual. Version of Oct. 1991. Report IAEA–NDS–76. Rev. 4, Jan. 1992.
- [3] É. M. Zsolnay, H. J. Nolthenius, L. R. Greenwood, E. J. Szondi: Reference data file for neutron spectrum adjustment and related damage calculations. = Proc. of the 7th ASTM-Euratom Symposium on Reactor Dosimetry, Strasbourg, France, 27–31 August 1990. ISBN 0–7923–1792–0. pp. 299–306.
- [4] *W. N. McElroy* et al.: SAND II. Neutron flux spectra determinations by multiple foil activation iterative method. Oak Ridge National Laboratory, RSIC Computer Code Collection CCC-112. May 1969.
- [5] *E. J. Szondi*: Internal consistency of the covariance information in the International Reactor Dosimetry File IRDF–90. = Proc. of a Specialists' Meeting on Evaluation and Processing of Covariance Data. Oak Ridge National Laboratory, USA, 7th–9th October 1992. Report NEA/NSC/DOC(93)3. OECD, Paris, 1993. pp. 265–278.
- [6] Sz. Czifrus: Evaluation of resonance region covariance information. Report BME–TR– RES–21/93. Institute of Nuclear Techniques of the Technical University of Budapest, Oct. 1993. ISBN 963 420 414 7.
- [7] *D. E. Cullen, P. K. McLaughlin*: The International Reactor Dosimetry File (IRDF–85). Report IAEA–NDS–41, Rev. 1., April 1993.

ine mornar
1) 26007
VIENNA
1-12645
00-21710
)