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Institut für Neutronenphysik und Reaktortechnik

Card Image Format of the Karlsruhe Evaluated Nuclear Data File KEDAK

D. Woll

GESELLSCHAFT FÜR KERNFORSCHUNG M. B. H.

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KEDAK *

by

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GESELLSCHAFT FÜR KERNFORSCHUNG M.B.H. KARLSRUHE

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*) Work performed within the association in the field of fast reactors between the European Atomic Energy Community and Gesellschaft für Kernforschung mbH, Karlsruhe

Contents

1. Introduction

The Karlsruhe evaluated nuclear data file KEDAK is a magnetic tape file consisting of one or more tapes. It contains evaluated microscopic neutron cross sections and other nuclear data of reactor materials. In this report the external KEDAK file in "card-image" format is described.

2. Logical structure of the nuclear data file

2.1. Basic ideas

2.1.1. A word means

a) an integer number with a maximum of 7 digits,

b) a floating point number of the form $\pm\ X \cdot 10^{Y}$, where X is a mantissa with 8 digits with $0.1 \leq X < 1.0$ and Y the exponent of the base 10 with $-50 \leq Y \leq 49$.

2.1.2. A field means a number of one or more words, which are considered as logically correlated,

2.1.3. A data set consists of three fields,

a) the name field with NN words, i.e. material names, data type names, possible further names, e.g. the energy of an excited nuclear level,

b) the argument field with NA words,

c) the value field with NW words containing the functional values belonging to the arguments.

For microscopic neutron cross sections e.g. the name field contains material and data type names, the argument field a neutron incident energy, the value field the particular cross section belonging to this energy.

2.1.4. A subgroup means the number of all data sets with equal material, data and possible further names.

2.1.5. A group means the number of all data sets with equal material and data names.

2.1.6. A file means the number of all groups contained in the nuclear data file.

3. Formal contents of the data fields

3.1. Contents of the name field

3.1.1. Material name

Each material is characterized by a fixed point number of the structure

$$Z_1Z_2Z_3A_1A_2A_3$$

where

$Z_1Z_2Z_3$ = atomic number,
$A_1A_2A_3$ = atomic weight (mass number) as integer number,
X = one digit compound reference number for characterisation of a chemical compound.

If a material is a natural element, then $A_1A_2A_3$ is set equal to 000. The compound reference number X is 0 for elements and isotopes and $\neq 0$, when compounds of the material concerned with other materials have to be treated separately. Table 1 contains the names of the materials contained in the nuclear data file KEDAK.

3.1.2. Data type name

Each data type is characterized by a fixed point number of the structure

$$KG_1G_2G_3S$$

where

K = data class,
$G_1G_2G_3$ = data group,
S = coordinate system.

The class reference numbers correspond to those of the ENDF/B format, the group reference numbers, in the case of equal data types, are taken from the ENDF/B format; in the case of different data types they are chosen in accordance with the ENDF/B-rules for the assignment of group reference numbers (see BNL - 50066 (T - 467), ENDF 102, 1967).

K	class
1	general information
2	resonance parameters
3	cross sections and other nuclear data

4	secondary angular distributions
5	secondary energy distributions

S	coordinate system
0	for the classes 1,2,3 and 5
1	laboratory system } in class 4
2	center-of-mass system } in class 4

For all data types foreseen on the nuclear data file (KEDAK) the reference numbers are specified in table II.

3.1.3. Further names

If for the full characterisation of a data type energy or other specifications are necessary these are contained in the further names as floating point numbers.

3.2. Contents of the argument field

The argument field contains the arguments for the description of the values of the respective nuclear data type as floating point numbers.

3.3. Contents of the functional value field

The functional value field contains the values belonging to the respective arguments as floating point numbers.

3.4. Units of the data

All energies and data with the unit of an energy contained in the nuclear data file are stored in eV, all cross sections in barn, all differential cross sections in barn/sterad. Further dimensions when needed are given in table II.

4. Structure of the information on tape

4.1. Records

The Karlsruhe nuclear data file KEDAK in "card-image" format contains information in records of 80 characters.

4.2. Subdivision of the records

The information part of the records, i.e. the columns 1-72 contain the data, the identification part, i.e. the columns 73 - 80, contains an identification.

4.2.1. Structure of the information part

The information part contains a maximum of 6 words with respectively max. 12 characters. The representation of the words corresponds to the FØRTRAN-field descriptors I 12 resp. E 12.6.

4.2.2. Structure of the identification part

The identification part contains in the columns

73 - 74 the position at which the material appears in the description of the material contents
or
0 in the description of the material contents

75 - 76 the position at which the data type appears in the material dependent description of the data type contents
or
0 in the description of the data type contents

77 - 80 the current adress of the record in the subgroup
or
0 in a name record.

4.3. Contents of the records

4.3.1. Description of material contents

The description of the material contents contains in the

1. record	tape number date number of the materials on the tape
2. and following records	material names

4.3.2. Description of data type contents

For each material the description of the data type contents contains in the

1. record	material name number of data types
2. and following records	data type names

4.3.3. Records for one group

4.3.3.1. Name records

For each data type and each material the name records contain

material name

data type name

number of further names

number of arguments

number of functional values

in the case of further names:

number of combinations of the further names

otherwise

0

4.3.3.2. Records with further names

If there are further names, the combination of the further names for the respective subgroup is contained in one record.

4.3.3.3. Records with number of data sets

On this record the number of data sets of the respective subgroup is given.

4.3.3.4. Data records

The data records contain arguments and functional values of the data sets. If several data sets fit into one record, arguments and functional values are repeated as long as they fit completely into one record, otherwise, if one data set needs continuation records, each data set begins with a new record.

Be ND the number of arguments and functional values per data set. Then the following numbers of data sets per record result:

ND = 2	3 data sets per record
ND = 3	2 data sets per record
$4 \leq ND \leq 6$	1 data set per record
$6 < ND \leq 12$	2 records per data set
$12 < ND \leq 18$	3 records per data set

The data sets are ordered according to increasing arguments.

4.4. Order of the information on tape

The order of the information on tape is governed by the following scheme:

Description of the material contents

for each material in the order of its appearance in the description of the material contents

description of the data type contents

for each data type of the material

name record

in the case of further names

for each subgroup a record with the further names

record with the number of data sets

data records of the subgroups

otherwise

record with the number of data sets

data records of the group

4.5. Subdivision of the file into several tapes

When more than one tape is needed for storing the file, each tape contains complete information for one or more materials with the pertinent description of the material contents.

Table 1

Names of the materials contained in KEDAK

Material	Material name	Material name on internal KEDAK
H	0010001	Hbbb1
H bound in H_2	0011001	HbbH1
H bound in H_2O	0012001	Hbbø1
$H^2 = D$	0010002	Hbbb2
He^3	0020003	HEbb3
He^4	0020004	HEbb4
C^{12}	0060012	Cbb12
N	0070000	Nbbbb
O^{16}	0080016	øbb16
Na^{23}	0110023	NAb23
Al^{27}	0130027	Alb27
Cr	0240000	CRbbb
Cr^{50}	0240050	CRb50
Cr^{52}	0240052	CRb52
Cr^{53}	0240053	CRb53
Cr^{54}	0240054	CRb54
Fe	0260000	FEbbb
Fe^{54}	0260054	FEb54
Fe^{56}	0260056	FEb56
Fe^{57}	0260057	FEb57
Fe^{58}	0260058	FEb58
Ni	0280000	NIbbb
Ni^{58}	0280058	NIb58
Ni^{60}	0280060	NIb60
Ni^{61}	0280061	NIb61

Table 1 (cont.)

Material	Material name	Material name on internal KEDAK
Ni^{62}	0280062	NIb62
Ni^{64}	0280064	NIb64
Mo	0420000	MØbbb
Mo^{92}	0420092	MØb92
Mo^{94}	0420094	MØb94
Mo^{95}	0420095	MØb95
Mo^{96}	0420096	MØb96
Mo^{97}	0420097	MØb97
Mo^{98}	0420098	MØb98
Mo^{100}	0420100	MØ100
U^{235}	0920235	Ub235
U^{238}	0920238	Ub238
Pu^{239}	0940239	PU239
Pu^{240}	0940240	PU240
Pu^{241}	0940241	PU241
Pu^{242}	0940242	PU242

Table II: Names of the data types foreseen on KEDAK

Name of data type K G S	Name as in ENDF/B* ?	Name of data type on internal KEDAK	Further names	Arguments	Functional values
1 458 0	n	ISØT1	-	-	1. Atomic weight (A) 2. Atomic number (Z) 3. Nuclear spin of ground state (I)
1 459 0	n	ISØT2	-	-	1. $ƛ\sqrt{E} = \hbar/\sqrt{2m_n} \cdot \frac{A+1}{A}$ = reduced neutron wave length [$eV^{1/2} b^{1/2}$] 2. R = nuclear radius [$b^{1/2}$] 3. E_B = binding energy of the last neutron in compound nucleus
1 460 0	n	ISØT3	-	Isotope atomic weight	Isotopic abundance (%)
1 457 0	n	PLNUE	-	-	1. ν_o 2. ν_1 3. ν_2 4. ν_3 where $\nu = \sum_{i=o}^{3} \nu_i E^i$ = average total number of fission neutrons
1 456 0	n	CHICR	-	1. Neutron incident energy	1. A 2. B 3. C Parameters of the Cranberg fission spectrum
2 152 0	n	RES	-	1. Resonance energy 2. Neutron orbital angular momentum (l)	1. $g_J = (2J+1)/(2(2I+1))$ 2. total half width Γ 3. neutron half width Γ_n

Name of data type K G S	Name as in ENDF/B* ?	Name of data type on internal KEDAK	Further names	Arguments	Functional values
				3. Compound nucleus spin (J)	4. capture half width Γ_γ 5. fission half width Γ_f 6. (n,p)-half width Γ_p 7. (n,α)-half width Γ_α 8. (n,n')-half width $\Gamma_{n'}$
2 153 0	n	ST	-	1. l 2. J	1. average capture width $\overline{\Gamma_\gamma}$ 2. average level spacing $\overline{D}$ 3. average reduced neutron width $\overline{\Gamma_n^{(o)}}$ 4. strength function $\overline{\Gamma_n^{(o)}}/\overline{D}$ 5. number of exit channels in fission ν_f 6. number of exit channels in neutron elastic scattering (ν_n)
2 154 0	n	STD	-	-	1. average observed level spacing 2. a } parameters of the statistical 3. 2 σ^2 } theory
2 155 0	n	STGF	-	1. neutron incident energy 2. l 3. J	1. number of exit channels in fission ν_f 2. average fission width $\overline{\Gamma_f}$ for the number of exit channels ν_f 3. average capture width $\overline{\Gamma_\gamma}$ 4. average neutron width $\overline{\Gamma_n}$

Name of data type K G S	Name as in ENDF/B* ?	Name of data type on internal KEDAK	Further names	Arguments	Functional values
					5. S_f 6. S_γ 7. R_f 8. R_γ } statistical fluctuation factors***
3 001 0	y	SGT	-	neutron incident energy	total cross section
3 002 0	y	SGN	-	"	elastic scattering cross section
3 003 0	y	SGX	-	"	non-elastic cross section
3 004 0	y	SGI	-	"	total inelastic cross section
3 005 0	y	SGI	E_i	"	inelastic cross section for excitation of rest nucleus level E_i
3 016 0	y	SG2N	-	"	cross section for the (n,2n)-process
3 017 0	y	SG3N	-	"	cross section for the (n,3n)-process
3 019 0	y	SGF	-	"	fission cross section
3 022 0	y	SGIA	-	"	cross section for the (n,n'α)-process
3 023 0	y	SGI3A	-	"	" " " " (n,n'3α)- "
3 024 0	y	SG2NA	-	"	" " " " (n,2nα)- "
3 025 0	y	SG3NA	-	"	" " " " (n,3nα)- "
3 027 0	y	SGA	-	"	absorption cross section
3 028 0	y	SGIP	-	"	cross section for the (n,n'p)-process
3 029 0	y	SGNI	-	"	" " " " sum of σ_n and $\sigma_{n'}$
3 102 0	y	SGG	-	"	" " " " (n,γ) - process
3 103 0	y	SGP	-	"	" " " " (n,p) - "
3 104 0	y	SGD	-	"	" " " " (n,d) - "

Name of data type K G S	Name as in ENDF/B* ?	Name of data type on internal KEDAK	Further names	Arguments	Functional values
3 105 0	y	SGH3	-	neutron incident energy	cross section for the (n,H^3) - process
3 106 0	y	SGHE3	-	"	" " " " (n,He^3) - "
3 107 0	y	SGALP	-	"	" " " " (n,α) - "
3 108 0	y	SG2HE	-	"	" " " " $(n,2\alpha)$ - "
3 201 0	n	SGTR	-	"	transport cross section
3 206 0	n	ETA	-	"	average number of fission neutrons per neutron absorption
3 207 0	n	ALPHA	-	"	ratio of capture to fission cross section
3 251 0	y	MUEL	-	"	average cosine of the elastic scattering angle in the laboratory system $\overline{\cos\Theta_L} = \overline{\mu_L}$
3 452 0	y	NUE	-	"	average number of fission neutrons
3 455 0	n	NUEP	-	"	average number of prompt fission neutrons
3 461 0	n	CHIF	-	neutron outgoing energy	energy spectrum of prompt fission neutrons (thermal fission)
3 462 0	n	CHIFD	-	"	energy spectrum of delayed fission neutrons (thermal fission)
4 002 1	n	SGNL	E_o **	cosine of scattering angle	differential elastic scattering cross section at the neutron incident energy E_o in the laboratory system
4 002 2	n	SGNC	E_o **	"	differential elastic scattering cross section at the neutron incident energy E_o in the center-of-mass system
4 004 1	n	SGIL	E_o	"	differential inelastic scattering cross section at the neutron incident energy E_o in the laboratory system

Name of data type K G S	Name as in ENDF/B * ?	Name of data type on internal KEDAK	Further names	Arguments	Functional values
4 004 2	n	SGIC	E_o	cosine of scattering angle	differential inelastic scattering cross section at the neutron incident energy E_o in the center-of-mass system
4 005 1	n	SGIL	1. E_i 2. E_o	" "	differential inelastic scattering cross section for excitation of the rest nucleus level E_i at the neutron incident energy E_o in the laboratory system
4 005 2	n	SGIC	1. E_i 2. E_o	"	differential inelastic cross section for **excitation** of the rest nucleus level E_i at the neutron incident energy E_o in the center-of-mass system
4 029 1	n	SGNIL	1. E_2 2. E_o	"	differential cross section for elastic and inelastic scattering at the neutron incident energy E_o to neutron outgoing energies between E_o and E_2 in the laboratory system
4 029 2	n	SGNIC	1. E_2 2. E_o	"	differential cross section for elastic and inelastic scattering at the neutron incident energy E_o to neutron outgoing energies between E_o and E_2 in the center-of-mass system

Name of data type K G S	Name as in ENDF/B*?	Name of data type on internal KEDAK	Further Names	Arguments	Functional values
4 463 1	n	LEGNL	1. E_o 2. order L_m	L	coefficient f_L in the Legrende-polynomial expansion of the differential elastic scattering cross section $\sigma_n(\Theta)=\frac{\sigma_n}{4\pi}\sum_{L=o}^{L_m}(2L+1)\ f_L(E)\ P_L\ (\cos\Theta)$ in the laboratory system
4 463 2	n	LEGNC	1. E_o 2. order L_m	L	coefficent f_L in the Legrende-polynomial expansion of the differential elastic scattering cross section $\sigma_n(\Theta)=\frac{\sigma_n}{4\pi}\sum_{L=o}^{L_m}(2L+1)\ f_L(E)\ P_L\ (\cos\Theta)$ in the center-of-mass system
4 464 1	n	LEGIL	1. E_o 2. order L_m	L	coefficient f_L' in the Legrende-polynomial expansion of the differential inelastic scattering cross section $\sigma_{n'}(\Theta)=\frac{\sigma_{n'}}{4\pi}\sum_{L=o}^{L_m}(2L+1)\ f_L'\ (E)\ P_L\ (\cos\Theta)$ in the laboratory system

Name of data type K G S	Name as in ENDF/B* ?	Name of data type on internal KEDAK	Further names	Arguments	Functional values
4 464 2	n	LEGIC	1. E_o 2. order L_m	L	coefficient f_L' in the Legrende-polynomial expansion of the differential inelastic scattering cross section $\sigma_{n'}(\Theta) = \frac{\sigma_{n'}}{4\pi} \sum_{L=o}^{L_m} (2L+1)\, f_L'(E)\, P_L(\cos\Theta)$ in the center-of-mass system
4 465 1	n	LEGIL	1. E_i 2. E_o 3. order L_m	L	coefficient f_L^i in the Legrende-polynomial expansion of the differential inelastic cross section for excitation of the rest nucleus level E_i $\sigma_{n'}^{E_i}(\Theta) = \frac{\sigma_{n'}}{4\pi} \sum_{L=o}^{L_m} (2L+1)\, f_L^i(E)\, P_L(\cos\Theta)$ in the laboratory system
4 465 2	n	LEGIC	1. E_i 2. E_o 3. order L_m		coefficient f_L^i in the Legrende-polynomial expansion of the differential inelastic cross section for excitation of the rest nucleus level E_i $\sigma_{n'}^{E_i}(\Theta) = \frac{\sigma_{n'}}{4\pi} \sum_{L=o}^{L_m} (2L+1)\, f_L^i(E)\, P_L(\cos\Theta)$ in the center-of-mass system

Name of data type K G S	Name as in ENDF/B*?	Name of data type on internal KEDAK	Further names	Arguments	Functional values
4 466 1	n	LGNIL	1. E_2 2. E_o 3. order L_m	L	coefficient f_L^{02} in the Legrende-polynomial expansion of the differential cross section for elastic and inelastic scattering at the neutron incident energy E_o to neutron outgoing energies between E_o and E_2 $\sigma^{02}_{n+n'}(\Theta) = \frac{\sigma^{02}_{n+n'}}{4\pi} \sum_{L=o}^{L_m} (2L+1)\, f_L^{02}(E) P_L(\cos\Theta)$ in the laboratory system
4 466 2	n	LGNIC	1. E_2 2. E_o 3. order L_m	L	coefficient f_L^{02} in the Legrende-polynomial expansion of the differential cross section for elastic and inelastic scattering at the neutron incident energy E_o and E_2 $\sigma^{02}_{n+n'}(\Theta) = \frac{\sigma^{02}_{n+n'}}{4\pi} \sum_{L=o}^{L_m} (2L+1)\, f_L^{02}(E) P_L(\cos\Theta)$ in the center-of-mass system

Name of data type K G S	Name as in ENDF/B ^{x}?	Name of data type on internal KEDAK	Further names	Arguments	Functional values
5 461 0	n	CHIF	E_o	neutron outgoing energy	energy spectrum of prompt fission neutrons at the neutron incident energy E_o
5 462 0	n	CHIFD	E_o	"	energy spectrum of delayed fission neutrons at the neutron incident energy E_o
5 004 0	y	CHII	E_o	"	energy spectrum of inelastically scattered neutrons at the neutron incident energy E_o
5 016 0	y	CHI2N	E_o	"	1.) 2.) energy spectrum of the two neutrons emitted in the (n,2n) process at the neutron incident energy E_o

x K always corresponds to the ENDF/B format. If also NG corresponds to the ENDF/B format, then the second column contains "yes", otherwise "no".

xx E_o for this and all pertinent further data types in the laboratory system. This is also true for E_2.

xxx $S_f = \frac{\bar{\Gamma}_\gamma}{\bar{\Gamma}_n \bar{\Gamma}_f} \left\langle \frac{\Gamma_n \Gamma_f}{\Gamma} \right\rangle$; $S_\gamma = \frac{\bar{\Gamma}_\gamma}{\bar{\Gamma}_n} \left\langle \frac{\Gamma_n}{\Gamma} \right\rangle$; $R_f = \frac{\bar{\Gamma}_\gamma}{\bar{\Gamma}_n^2 \, \bar{\Gamma}_f} \left\langle \frac{\Gamma_n^2 \Gamma_f}{\Gamma} \right\rangle$; $R_\gamma = \frac{\bar{\Gamma}_\gamma}{\bar{\Gamma}_n^2} \left\langle \frac{\Gamma_n^2}{\Gamma} \right\rangle$