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COMPUTER PROGRAMS FOR CALCULATING GROUP CROSS-SECTION COVARIANCES FROM UNCERTAINTY PARAMETERS IN THE ENDF/B-V FORMAT – UNC 32/33 –

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SUMMARY

Cross-section libraries in the ENDF/B-V format contain uncertainty information for a number of cross-section sets.
The programs UNC 32/33 read this information and convert it to a group structure of interest for further calculations. The output of the programs becomes available in the form of a set of covariance matrices.
These programs are useful for estimating the role of covariances in the calculation of reaction rates and adjusted neutron spectra, since the programs provide a convenient tool for deriving covariance matrices of cross-sections in a selected coarse group structure directly from libraries in the ENDF/B-V format.

KEYWORDS

U CODES
CROSS-SECTIONS
DATA COVARIANCES
MULTIGROUP THEORY
CORRELATIONS

CONTENTS page

1. INTRODUCTION

For multigroup calculations in neutron metrology uncertainties of cross-section values may give valuable and sometimes indispensable extra information.
Such uncertainties need to be available in the form of covariance matrices.
The cross-section libraries of interest for neutron metrology are often available in the ENDF/B-V format [1]. Examples of libraries in this format are the ENDF/B-V dosimetry file (TAPE531) [2] and the international reactor dosimetry file (IRDF-85) [3].
For the retrieval of cross-section and uncertainty data from a library in the ENDF/B-V format special conversion programs are needed.
In these programs extrapolation procedures are carried out as prescribed by the library, for collecting the relevant information from different parts of the library (i.e. resonance parameters are stored separately from the continuous cross-section contribution) and for the calculation of coarse group cross-section or uncertainty values.
In the calculation of the coarse group cross-section values a weighting neutron spectrum has to be applied. In the case that several weighting spectra and/or group structures have to be applied, the working method described above leads to a series of complicated computer calculations. The calculations can be simplified by the introduction of a 640 groups user library for the reactions of interest. The group structure of this library [4] is considered to be fine enough to assume that the group cross-section is independent of the shape of the weighting spectrum inside a fine group. According to this assumption the user library has to be calculated only once from the original library.
A program which is used to calculate a user library of this type is ENTOSAN [5]. A user library of this type can be made available for further calculations and some documentation is available [6]. This library can be used, for instance, in combination with the SAND-II program for calculations with neutron spectra, in combination with the program FITOCO [7] to calculate coarse group cross-sections, etc.

In a cross-section library with the ENDF/B-V format the uncertainty information for a particular cross-section may in principle be found in different parts of the library. The information of these parts has to be combined to obtain the cross-section covariance matrix. The parts mentioned refer to:

- the uncertainties in the resonance parameters stored in FILE 32 of the library;
- the uncertainties in the "flat" cross-section distribution in FILE 33 of the library.

The working method which is applied in the derivation of the cross-section covariances from the library data consists of two steps:

- First a user library is made which contains the cross-section uncertainty in the resonance parameter region in a fine group structure. These data are calculated from the uncertainties of resonance parameters which are stored in FILE 32. The fine group structure is the 640 groups SAND-II structure for the region of interest. This user library can be made with the program UNC32 and it needs to be made only once for each original library.
- Secondly, the calculation of a cross-section covariance matrix for a coarse group structure of interest and a selected weighting neutron spectrum is performed. This calculation comprises the combination of all uncertainty information (FILE 32 + FILE 33). The neutron spectrum applied in the weighting has to be available in the 640 groups of the SAND-II structure. The calculations for this second step can be performed with the program UNC33.

The output of the program is written on a file in the form of a relative covariance matrix.
In most cases an utility program will be needed for the conversion of the format of the output file to a file which is needed in the neutron spectrum adjustment program or a program to calculate uncertainties in reaction rates, etc.
Cross-section covariances between different types of cross-sections which may be present in the library cannot be converted by the program UNC33.

2. CALCULATION PROCEDURE UNC32

The basic definition for the covariance of two random variables (x,y) is

$$\mathrm{cov}(x,y) = \sum_{m=1}^{n} (x_m - \bar{x}).(y_m - \bar{y}) \;/\; (n-1),$$

or $$\mathrm{cov}(x,y) = \sum_{m=1}^{n} \Delta x_m . \Delta y_m \;/\; (n-1),$$

where n is the number of measurements "m", and $\bar{x}$ and $\bar{y}$ are the average values for x_m and y_m, respectively.

In this case we are interested in the covariances of fine group cross-section values due to the variance and covariance of resonance parameters. The cross-section value for the fine group i, denoted by σ_i, is a function of the resonance parameters $p_1 \ldots p_5$ (each resonance is described by five parameters). In most cases more than one resonance contributes to the cross-section. So for σ_i we may write

$$\sigma_i = \sum_{r=1}^{NRES} f_{i,r}(p_a) \quad \text{for a=1...5,}$$

where $f_{i,r}$ denotes the value for the i-th group of the shape function of the cross-section due to the r-th resonance.

For fine group j for the same reaction we obtain an analogous expression:

$$\sigma_j = \sum_{s=1}^{NRES} f_{j,s}(p_b) \quad \text{for b=1...5.}$$

According to the Taylor expansion, truncated after the first-order terms, the changes in the fine group cross-sections due to the uncertainties in the parameters (for small changes) can be written as

$$\sigma_{i,m} = \sum_{r=1}^{NRES} \sum_{a=1}^{5} \frac{\delta\sigma_i}{\delta p_{r,a}} \cdot \Delta p_{m,r,a}.$$

For the fine group j we obtain

$$\sigma_{j,m} = \sum_{s=1}^{NRES} \sum_{b=1}^{5} \frac{\delta\sigma_j}{\delta p_{s,b}} \cdot \Delta p_{m,s,b}.$$

Substitution of these relations in the definition of the covariance yields the covariance between the cross-section values σ_i and σ_j:

$$\mathrm{cov}(\sigma_i,\sigma_j) = \sum_{m=1}^{n} \Delta\sigma_{i,m}.\Delta\sigma_{j,m}/(n-1)$$

$$= \sum_{m=1}^{n} \sum_{r=1}^{NRES} \sum_{a=1}^{5} \frac{\delta\sigma_i}{\delta p_{r,a}} . \Delta p_{m,r,a} \sum_{s=1}^{NRES} \sum_{b=1}^{5} \frac{\delta\sigma_j}{\delta p_{s,b}} . \Delta p_{m,s,b}/(n-1).$$

We assume that the various resonances are independent, so that the quantities $\Delta p_{m,r,a}$ and $\Delta p_{m,s,b}$ are uncorrelated with respect to the resonances present.

We therefore may write

$$\mathrm{cov}(\sigma_i,\sigma_j) = \sum_{m=1}^{n} \sum_{r=1}^{NRES} \sum_{a=1}^{5} \frac{\delta\sigma_i}{\delta p_{r,a}} . \Delta p_{m,r,a} \sum_{b=1}^{5} \frac{\delta\sigma_j}{\delta p_{r,b}} . \Delta p_{m,r,b}/(n-1)$$

$$= \underbrace{\sum_{r=1}^{NRES} \sum_{a=1}^{5} \frac{\delta\sigma_i}{\delta p_{r,a}} . \underbrace{\sum_{b=1}^{5} \frac{\delta\sigma_j}{\delta p_{r,b}} \mathrm{cov}(p_{r,a},p_{r,b})}_{\text{VMULSF}}}_{\text{VIPA}}.$$

Below this expression for the propagation of covariances it is indicated which subroutines are applied in the program.

This calculation is performed for all σ_i,σ_j combinations.

3. CALCULATION PROCEDURE UNC33

In principle, the conversion which is applied in the program UNC33 is rather simple. The basic relation is presented below for the relative covariance CMUSER for the rough output groups i and j

$$\mathrm{CMUSER}_{i,j} = \Big(\sum_{l\in U} \sum_{k\in U} \Big[\underbrace{\Big(\sum_{x\in l} \sigma_x.\phi_x\Big)}_{\text{WLSUM}} * \mathrm{CFIJN}_{k,l} * \underbrace{\Big(\sum_{x\in k} \sigma_x.\phi_x\Big)}_{\text{WKSUM}}\Big]\Big)/\mathrm{REUSER}_i * \mathrm{REUSER}_j.$$

Notation:

$\sum_{a\in b}$ means a summation over all energy groups, each separate group noted by a, lying inside (totally or partly) the b-th energy group;

l = l^{th} ENDF energy group;

k = k^{th} ENDF energy group;

U = U^{th} output energy group;

x = x^{th} SAND-II energy group;

σ_x = fine group cross-section value for reaction of interest, for group x;

ϕ_x = fine group weighting spectrum value, for group x;

$CFIJN_{k,l}$ = relative covariance value from library for groups k and l;
$REUSER_i$ = response in i-th output group.

In case also uncertainty information from FILE 32 is present for the reaction of interest, this relative covariance information is read from the output file of the progam UNC32 and added to the results from FILE 33 obtained by the relation given above.
In the calculations a fine group cross-section library of the SAND-II type is applied. In order to reduce the input of the program a modification was made in the library. Instead of the decay constant, the ENDF/B-V (or IRDF) material number and the reaction type number are now introduced.

4. DESCRIPTION OF SOME ENDF/B-V CODES

Some symbolic names which are used in the following part of the report are explained with a few words. A complete description can be found in [1].

MAT	material number in the library
FILE	part of the library
SECTION	part of a FILE (here FILE 33) identified by MAT and MT
SUBSECTION	part of a SECTION which describes a single covariance matrix
MT	reaction type number
NL	number of SUBSECTIONS within a SECTION
NC	number of NC type "SUB-SUBSECTIONS" This type of SUB-SUBSECTIONS may be used to describe that the covariance matrix for a certain energy range of the reaction of interest has to be found as part of data for another reaction (MAT- and MT-number) in the library with the ENDF/B-V format.
NI	number of NI type "SUB-SUBSECTIONS" to describe explicitly the various components of the covariance matrix given in the SUBSECTION
LTY	indication on evaluation method of NC type "SUB-SUBSECTIONS" (independent on other reactions or correlated).

5. THE PROGRAMS

The programs are written in FORTRAN-V for a CDC computer with operating system NOSBE.

5.1. The program UNC32

In the program a few SUBROUTINES from special libraries are applied. The basic idea of the program is the same as that applied in the program ENTOSAN [5]. This means, that the calculation sequence is completed for each energy group separately.
For the calculation of the uncertainty in the cross-section the law of propagation of uncertainties is applied, which converts the uncertainties of the resonance parameters into uncertainties of the fine group cross-section values. In this conversion the derivative of the resonance function has to be determined. For a few parameters this can be done analytically, but for other parameters a numerical procedure had to be applied.
The program calculates the uncertainties for (n,γ) and (n,f) reactions. For the calculation of the cross-section contribution for a set of resonance parameters the procedure described for the single-level Breit-Wigner in [1] is applied.
The channel radius is calculated as $a=0.123*(1.008665.AWRI)^{1/3}+0.08$.
In the calculation of the derivatives also the single-level Breit-Wigner procedure is applied.
The derivatives of this relation to the resonance energy and to the neutron width are calculated numerically for each resonance in the energy range of interest. Corresponding data are also calculated directly for the other resonance parameters. See also App. 1.
The computer program needs 41,000 words in the memory.

5.2. The program UNC33

Figures 2 to 6 show the flow charts of the major parts of the program, while figure 1 shows the link with files. The subroutine SELREC searches for the data for the MAT number, as specified in the input by the user, in the ENDF/B-V format file. These data are copied on a scratch file (tape 1).

The part selected in this way is called a section [1], which is handled further by the subroutine SECTION (figure 3). Each section is divided into NL SUBSECTIONS, while each subsection in turn is subdivided into NC SUB-SUBSECTIONS of the NC type and NI SUB-SUBSECTIONS of the NI type.

Subroutine SUBNC reads and handles an NC type SUB-SUBSECTION, while the subroutine SUBNI interprets an NI type SUB-SUBSECTION. The route in the subroutine SUBNC depends on the value of the LTY parameter [1] (see also figure 4). If this LTY parameter is equal to unity, the cross-section of current interest is derived in the energy range E(1) to E(2), in a special way, i.e. through the evaluation of ratio measurements using a so called standard material characterized by MATS and MTS.

The routine INTERV, taken from [8], was used to determine accurately the position of E(1) and E(2) in the SAND-II energy grid, for calculating the uncertainty contribution of the standard material MATS. The uncertainty information of this standard material for this energy range has to be incorporated also.

For this reason, when LTY equals 1 we enter the subroutine SELREC to search for the standard material MATS (see figure 4), and store the data, if present, on scratch file tape 2, for later use. If the standard material is not available on the ENDF/B-V tape, the contribution is ignored.

After all NC type SUB-SUBSECTIONS have been passed, the subroutine SUBNI is passed NI times (see figures 3 and 5).

Within this subroutine the subroutine STRUC will be activated. The subroutine STRUC converts the ENDF/B-V format uncertainty data into uncertainty information for the output energy group structure (see fig. 6).

Finally, the subroutine STRUCRS is entered to search for resonance uncertainty information for MAT and to add this information if present. The complete route is followed again for the standard material MATS if LTY is equal to 1.

The computer program needs 50,000 words in the memory for execution.

6. OUTPUT OF THE PROGRAM UNC32

The output of the program comprises a review of the uncertainty data for each resonance present in the uncertainty FILE 32 for the reaction which is treated. The reaction code and also the MAT number are printed. The calculated results are printed together with some additional information, like the size of the output matrix (i.e. the number of groups with the SAND-II group structure).
The output comprises the relative standard deviation in per cent for the fine group cross-section, the lower boundary energy of the fine group of interest and the covariance information. The covariance information is given in the form of the upper triangle of the correlation matrix. An example of this output is given in table 2.
The output of the program comprises also the file which is required to calculate the uncertainty for the complete energy region of the reaction of interest. For this reason the file should be handled as a library which is stored for further use.
Each run of the program gives such a library.
It seems to be convenient to make only one library for all reactions of interest. For this reason all reactions of interest at this moment were treated in one run.
For four MAT numbers and five reactions a user library was made. In these calculations the cross-section library DOSCROS84 [6] was used. Some data of this user library are given in the following list:

MAT	reaction code	size
6311	NA23G5	132*132
6337	NP237G5	120*120
6337	NP237F5	120*120
6432	FE58G5	383*383
6435	CU63G5	144*144

It is not yet possible to combine libraries from different runs or to extend a library from one run with new data from another run.
The output file (COVF32) is written unformatted on a "direct access file".

7. OUTPUT OF THE PROGRAM UNC33

The output of the program comprises a review of the uncertainty data for the reaction of interest, partly specified by uncertainties in point-wise specified cross-section data (FILE 33), and partly by uncertainties in resonance parameters (FILE 32), if available. The output covariance information is in a coarse group structure relative to the response, and weighted with a fine group spectrum. The reaction code and also the MAT number is printed. The calculated results consist of response, standard deviation and correlation data.
The relative covariance data are printed in the form of the upper triangle of the correlation matrix.
An example of part of this output is given in table 3.
The output of the program comprises also the file with the relative uncertainties for the selected coarse-group structure and for the selected reactions. The latter file (COVF33) is written unformatted on a "direct access file".

8. APPLICATIONS OF THE PROGRAMS

The cross-section libraries which could be used in the input of the program were the second version of the ENDF/B-V dosimetry file (TAPE531) and the IRDF-85 dosimetry file. These files contain resonance-parameter uncertainties for four materials and five reactions. A library with relative covariance information (COVF32) in the fine-group structure was made with the program UNC32 for these five reactions.
The running time per reaction on our CDC computer is about 20 s (CPU). It has to be remarked that, due to the actual uncertainty information present in this library, the running time could be reduced by about 40% if a few extra statements were added in the program to check the uncertainty and thus the need to calculate derivatives. In these cross-section libraries no uncertainty data are supplied for the fission channel width GF and for the spin, or total angular momentum of the resonance AJ.

It should also be remarked that in this version of the libraries the three uncertainty parameters which are supplied for each resonance are independent.

In the line-printer output of the program which gives the standard deviations and the correlation matrices some unexpected values can be found. The standard deviations which are expressed relative to the fine-group cross-section values have for some groups very large values. For the ^{23}Na(n,γ) reaction a few values larger than 100% are found (maximum 282% at E=1.8x10^{5} eV). A similar effect can be observed for the reactions ^{58}Fe(n,γ) and ^{237}Np(n,f) (maximum 732% at E=2.3x10^{2} eV for Fe and >1000% for Np at E=5.5 and 5.7 eV).

The reason of these large uncertainties in small energy regions is not completely clear, but from the absolute uncertainties in the same region it can be observed that they give a much more smooth distribution. Probably the large values are partly due to the more detailed structure in the DOSCROS84 library. This DOSCROS84 library was calculated from the same libraries in the ENDF/B-V format, but from FILE 2 and 3 data. Thus for the evaluation of the cross-section another set of resonance parameters is used than the set applied to give the uncertainties.

With this user library COVF32 the calculations for a selected coarse group structure for a particular weighting spectrum and selected reactions can be performed with the program UNC33. In table 5 a summary is given for the coefficients of variation and correlations for three characteristic neutron spectra. The required cross-section uncertainty data from the library with the ENDF/B-V format were converted to the required group structure with the programs described. In figure 7 a plot is given of a part of the user library COVF32 data for the reaction ^{23}Na(n,γ). The part refers to a reduction in the number of groups in connection with the possibilities of the plotting program. The energy group at the highest energy is plotted too broad due to a shortcoming in the plotting program. In figure 8 the covariance data are shown in more detail. The results obtained with UNC33 for the relative covariances for a certain weighting spectrum and selected group structure are plotted in figure 9. Table 6 gives the numerical data for the same reaction, but another group structure, also calculated by UNC33.

The central processor time needed for a run with UNC33 is strongly dependent on the complexity of the uncertainty data. For the calculation of the relative cross-section covariance for the reaction ^{239}Pu(n,f) about 60 s were needed on a CDC 855/175 computer system.

9. INPUT FOR THE PROGRAMS

The programs can be used for several reactions in one run. In this case it is advantageous to define the input in the same sequence as the reactions are present on the library, to diminish the search time. This means that in the input the MAT numbers should be in increasing order.

9.1. Input of the program UNC32

The first record (80 characters) is used for the identification of the output covariance information.
For each MAT number four records.*)

- MAT number in the ENDF/B-V for which uncertainty data have to be calculated;
- The word GAMMA or FISSION.*) With this word it is indicated whether data for a (n,γ) or for a (n,f) cross-section covariances have to be calculated;
- The reaction code as used in the cross-section library in the SAND-II format;
- The word ENDEND.

*) In some cases it might be necessary to calculate for one MAT number both the (n,γ) and the (n,f) cross-section covariances. This can be achieved with six records, i.e.
  - MAT number;
  - GAMMA;
  - The reaction code from the cross-section library in the SAND-II format for the (n,γ) reaction;
  - FISSION;
  - The reaction code from the cross-section library in the SAND-II format for the (n,f) reaction;
  - ENDEND.

For a run with UNC32 the following library and output files are used.

file	name in program	library
1	ENDFB	ENDF/B-V TAPE531, IRDF-85
15	SANDLIB	DOSCROS in unformatted form (1984 or later version!)
16	COVFIL	output file with relative covariances (640 groups structure); direct access file

An example of the application of the program is given in table 1.
In this table the input with the instruction cards is shown.

9.2. Input of the program UNC33

The first record (80 characters) is used for the identification of the output covariance information.
The next record contains the number of user-defined energy groups N.
The next record(s) contains the lower energy values in MeV, N+1 values, in increasing order. The values are read free formatted.
The next record must contain the word "TABULAR" !
The next record (80 characters) is used for the identification of the weighting neutron spectrum.
The next 93 records contain the group fluence rate values in 640 groups; each separate record has the following format: FLUX, 7E10.3.
The next record(s) (One for each output cross-section covariance which has to be calculated) contains 3 items, namely MAT number, MT number, and the short reaction code (between apostrophes!) of the corresponding cross-section set on a DOSCROS library, not older than the 1984 version [6].
The records are read in free formatted form.
It is emphasized here that the user should specify these records by increasing MAT and MT number, to reduce searching time on the huge ENDF/B-V files.
For a run with the program the following libraries/files are required (see also figure 1).

file	name in program	library
3	ENDFB	ENDF/B-V TAPE531, IRDF-85
15	SANDLIB	DOSCROS in unformatted form (1984 or later version!)
16	COVF32	uncertainty information in fine group cross-section values, calculated from the resonance parameters (file 32), direct access file
4	COVF33	output file with relative covariances in the coarse users group structure; direct access file

An example of the application of the program is given in table 4.

10. ACKNOWLEDGEMENT

This report describes updated versions of the programs UNC32 and UNC33. The original versions of the programs were written by H.Ch. Rieffe and G.C.H.M. Verhaag. Thanks are due to them for their contribution to this work.
An earlier version of the program UNC33 was used in the REAL84 exercise. A few participants to this exercise commented on shortcomings and errors in the program; especially the detailed contribution of Dr. M. Matzke (PTB, Braunschweig) was highly appreciated. The latter comments stimulated the documentation of this version of the program.

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Table 1. Input for the program UNC32.

```
XX,T200,IO200,CL140000.
ACCOUNT,XXXXXXXX,XX,XXX.
COMMENT.
COMMENT.  UNC32 JOB
COMMENT.
REQUEST,COVFIL,PF.
ATTACH,PR,XXX,ID=XX.                  PROGRAM UNC32 (SOURCE )
ATTACH,SANDLIB,DOSCROS84,ID=XX    .   CROSS-SECTION LIBRARY (640)
ATTACH,ENDFB,XXX,ID=XX.               ENDF/B-V LIBRARY
ATTACH,NUMRCN.                        SUBROUTINE LIBRARY
LIBRARY,NUMRCN.
FTN5,I=PR,LO=A/M/R.
LGO.
CATALOG,COVFIL,ID=XX.                 PROGRAM OUTPUT FILE
REWIND,INPUT.                         ==
SKIPF,INPUT,1.00,C.                   == PRINT INPUT
COPYSBF,INPUT.                        ==
*EOR
 INPUT FOR UNC32 AND THE ENDF/B-V LIBRARY
6311
GAMMA
NA23G52
ENDEND
6337
GAMMA
NP237G5
FISSION
NP237F5
ENDEND
6432
GAMMA
FE58G5
ENDEND
6435
GAMMA
CU63G5
ENDEND
```

++++++ FOR XX ETC. THE CORRECT IDENTIFICATION HAS TO BE USED ++++

Table 2. Example of output of UNC32.

```
LIBRARY : DOSIMETRY TAPE ENDF/B V.2

COMMENT WRITTEN IN COV LIBRARY :
 TEST OF UNC32
 INPUT   MAT=  6311

REL. SDEV OF ER :  1.42 PERCENT  , ( RESONANCE NO.:  1 ) ER=  2

                PARAMETER CORRELATION MATRIX
  SDEV (PC)       GF          GG          GN          AJ

   UND           UND         UND         UND         UND
 14.16                       100           0         UND
  3.99                                   100         UND
   UND                                               UND

                      UND=UNDEFINED!

REL. SDEV OF ER :   .01 PERCENT  , ( RESONANCE NO.:  2 ) ER=  2

                PARAMETER CORRELATION MATRIX
  SDEV (PC)       GF          GG          GN          AJ

   UND           UND         UND         UND         UND
 16.47                       100           0         UND

  INPUT WORD = GAMMA
  INPUT REACTION NAME = NA23G52
  RESONANCE   1 HANDLED
  RESONANCE   2 HANDLED
  RESONANCE   3 HANDLED
                .
                .
                .
  RESONANCE  17 HANDLED
  RESONANCE  18 HANDLED

   REACTION: NA23G52 , MAT-NUMBER: 6311

X-SECTION CORRELATION MATRIX (132 X 132)

    GROUP    REL.SDEV       ENERGY     X-SECTION
     NO        (PT)          (EV)       (BARNS)
 *    1       15.26       6.000E+02   5.599E-03

100 100 100 100  99  99  99  99  98  98  97  95  94  92  89  8(
 90  91  91  92  93  93  93  82   2  94  94  95  95  95  95  9!
 63  53  42  35  26  18  10   0   3   4   2   1   1   0   0   (
  2   0   0   1   1   0   0   1   0   0   0   0   0   0   0   (
 *    2       15.27       6.300E+02   5.619E-03

100 100 100 100 100  99  99  99  99  98  97  96  94  92  90  8/
 90  91  91  92  92  93  93  82   2  94  94  95  95  95  95  9'
```

Table 3. Part of the line printer output of UNC33.

```
COMMENT CARD TO IDENTIFY TAPE4                          : UNC33-V.1 , GR.STR.: 55 , W.SPEC: AN4, ENDF/B-V.2: T.531  ,
NUMBER OF USER GROUPS (NGUSER)                          :  55
COMMENT CARD TO IDENTIFY THE WEIGHTING SPECTRUM USED    :        REACTOR CAVITY   FILE AN4

--- WEIGHTING SPECTRUM ---

4.870E+14 5.100E+14 5.340E+14 5.580E+14 5.870E+14 6.230E+14 6.580E+14 6.930E+14 7.350E+14 7.820E+14 8.290E+14 8.760E+14   12
9.230E+14 9.700E+14 1.020E+15 1.080E+15 1.110E+15 1.170E+15 1.240E+15 1.300E+15 1.370E+15 1.460E+15 1.550E+15 1.650E+15   24
          .10E+15 1.830E+15 1.940E+15 2.050E+15 2.170E+15 2.280E+15 2.390E+15 2.510E+15 2.620E+15 2.740E+15 2.860E+15 3.000E+15   36
          .170E+15 3.430E+15 3.610E+15 3.790E+15 3.960E+15 4.140E+15 4.320E+15 4.500E+15 4.690E+15 4.910E+15 5.130E+15          48
          .940E+15 6.260E+15 6.580E+15 6.950E+15 7.370E+15 7.790E+15 8.200E+15 8.610E+15 9.010E+15 9.420E+15                    60
          .1.130E+16 1.180E+16 1.230E+16 1.310E+16 1.380E+16 1.450E+16 1.520E+16 1.590E+16 1.670E+16                           72
          .16 2.070E+16 2.150E+16 2.220E+16 2.300E+16 2.380E+16 2.470E+16 2.540E+16 2.630E+16                                  84
          .00E+16 3.17GE+16 3.26UE+16 3.350E+16 3.440E+16 3.520E+16 3.620E+16 3.730E+16                                        96
          .250E+16 4.300E+16 4.350E+16 4.380E+16 4.410E+16 4.430E+16 4.440E+16                                                 108
---------- ENDF/B-V .090E+16 3.980E+16 3.850E+16 3.700E+16 3.540E+16 3.340E+16                                               120
Z          :  11                .16 2.070E+16 1.890E+16 1.700E+16 1.530E+16 1.370E+16                                        132
A          :  23                .0E+15 3.500E+15 2.750E+15 2.160E+15 1.620E+15                                               144
-----------                      .60E+14 3.010E+14 2.88UE+14 2.730E+14                                                        156
NUMBER OF SUB-SECTIONS  :  1     .500E+14 1.430E+14 1.360E+14                                                                168
-----------

---------- SUB-SECTION NO.:  1
MAT,MT,MAT1,MT1         : 6311 102 6311 102
NUMBER OF NC-TYPE SUB-SUBSECTIONS  :  0
NUMBER OF NI-TYPE SUB-SUBSECTIONS  :  1
-------------------------------------------------------------------

---------- NI-S.S.:  1----------

ENERGY BOUNDARIES (IN EV)
1.0000E-05 5.0000E+01 6.0000E+02 5.0000E+05 5.0000E+06 2.0000E+07

COVARIANCE MATRIX
4.0000E-04  .0000E+00  .0000E+00  .0000E+00  .0000E+00
 .0000E+00 2.2500E-03  .0000E+00  .0000E+00  .0000E+00
 .0000E+00  .0000E+00 1.0000E-02  .0000E+00  .0000E+00
 .0000E+00  .0000E+00  .0000E+00 4.0000E-02  .0000E+00
 .0000E+00  .0000E+00  .0000E+00  .0000E+00 6.2500E-02
---------- EOF S.S.:  1----------

E(1): 1.000E-04 EV, E(2): 2.000E+07 EV

--- UNC33-V.1 RESPONSE CALCULATIONS, MAT: 6311, MT: 102 ---

  GROUP-NUMBER      ENERGY-BOUNDARIES (EV)          RESPONSE (BQ)

         1          4.140E-01 -  1.068E+01            1.637E-17
         2          1.068E+01 -  1.013E+02            3.804E-18
                    1.013E+02 -  1.585E+03            2.564E-18
                    .485E+03 -  2.612E+03             3.329E-18
                               3.355E+03              4.559E-18
                                                      7.134E-19
                                                      4.201E-20
```

```
SEARCH FOR COVARIANCE DATA OF:        6311      NA23G52

COVARIANCE FILE:  COVFIL GENERATED BY UNC32, ENDF/B-V.2,FILE=531,MF=32,MT=151

SEARCH COMPLETED, NRC=    6
-------------------------------------------- SUBP. SECRP --------

CROSS-SECTION NAME          : NA23G52                           MAT-NUMBER     : 6311

X-SECTION CORRELATION MATRIX ( 55 X  55)                                                  UPPER TRIANGLE

 GROUP   REL.SDEV        ENERGY    X-SECTION
  NO       (PT)           (EV)      (BARNS)
   1       2.00        4.140E-01  6.371E-02
                     100  83   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0
   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0
   2       1.88        1.068E+01  1.560E-02
                         100  20   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0
   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0
   3       7.99        1.013E+02  6.822E-03
                             100  86  86  71  86  21  89  85  71  61  10   9  1
   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0
   4      23.42        1.585E+03  3.664E-02
                                 100  70  44  69  17  75  7
   0   0   0   0   0   0   0   0   0   0   0   0   0   0
   5      17.85        2.612E+03  1.766E-01
                                     100
   0   0   0   0   0   0   0   0
   6      19.34        3.35
   0   0   0
   7      20.00

  44      20.00        3.679E+06  1.613E-04

  45      20.00        4.066E+06  1.604E-04
                                                                       100   3   0   .
  46      24.11        4.966E+06  1.634E-04
                                                                           100 100 100 100 100 100 100 100 ...
  47      25.00        6.065E+06  1.664E-04
                                                                               100 100 100 100 100 100 100 100 100
  48      25.00        7.047E+06  1.682E-04
                                                                                   100 100 100 100 100 100 100 100
  49      25.00        7.408E+06  1.695E-04
                                                                                       100 100 100 100 100 100 100
  50      25.00        8.187E+06  1.713E-04
                                                                                           100 100 100 100 100 100
  51      25.00        8.607E+06  1.739E-04
                                                                                               100 100 100 100 100
  52      25.00        1.000E+07  1.773E-04
                                                                                                   100 100 100 100
  53      25.00        1.105E+07  1.817E-04
                                                                                                       100 100 100
  54      25.00        1.222E+07  1.982E-04
                                                                                                           100 100
  55      25.00        1.419E+07  2.259E-04
                                                                                                               100
```

Table 3 (continued).

Table 4. Input of the program UNC33.

```
XX,T500,IO200,CL200000.
ACCOUNT,XXXXXXXX,XX,XXX.
COMMENT.
COMMENT.  UNC33 JOB
COMMENT.
REQUEST,COVF33,PF.
ATTACH,PR,XXX,ID=XX.                PROGRAM UNC33 (SOURCE )
ATTACH,ENDFB,XXX,ID=XX.             ENDF/B-V LIBRARY
ATTACH,COVF32,XXX,ID=XX.            USERS LIBRARY FROM UNC32
ATTACH,SANDLIB,DOSCROS84,ID=XX.     CROSS-SECTION LIBRARY (640)
FTN5,I=PR,L=0.
LGO,*PL=15000.
CATALOG,COVF33,N31,ID=XX.           PROGRAM OUTPUT FILE
*EOR
UNC3303 , GR.STR.: 37 , W.SPEC: XX , ENDF/V-V2  :T531.
 37
 .1000E-09 .1265E-06 .4140E-06 .1068E-04 .1013E-03
 .1585E-02 .2612E-02 .3355E-02 .5531E-02 .7102E-02
 .1171E-01 .1503E-01 .2188E-01 .2418E-01 .2606E-01
 .3431E-01 .4087E-01 .6738E-01 .8652E-01 .9804E-01
 .1832E+00 .3020E+00 .6081E+00 .8209E+00 .1003E+01
 .1353E+01 .1496E+01 .1827E+01 .2123E+01 .2466E+01
 .2725E+01 .4066E+01 .6065E+01 .7408E+01 .1000E+02
 .1221E+02 .1733E+02 .2000E+02
'TABULAR'
HFR-SPECTRUM: POSITION XX
FLUX 1.636E+19 1.715E+19 1.795E+19 1.874E+19 1.973E+19 . . . . .
FLUX 2.330E+19 2.468E+19 2.627E+19 2.785E+19 2.943E+19 . . . . .
FLUX 3.416E+19 3.573E+19 3.731E+19 3.927E+19 4.163E+19 . . . . .
FLUX 4.907E+19 5.219E+19 5.531E+19 5.842E+19 6.153E+19 . . . . .
          .         .         .         .         .
          .         .         .         .         .
          .         .         .         .         .
          .         .         .         .         .
FLUX 7.977E+08 7.407E+08 6.878E+08 6.386E+08 5.930E+08 . . . . .
FLUX 4.747E+08 4.408E+08 4.093E+08 3.800E+08 3.529E+08 . . . . .
FLUX 2.825E+08 2.623E+08 2.436E+08 2.262E+08 2.101E+08 . . . . .
FLUX 1.682E+08 1.561E+08 1.450E+08 0.
6395    18  'U235F52'
6398    18  'U238F52'
6398   102  'U238G52'
6399    18  'PU239F52'
```

++++++ FOR XX ETC. THE CORRECT IDENTIFICATION HAS TO BE USED ++++

Table 5. Coefficients of variation and correlation for three characteristic neutron spectra. (coefficient of variation given in per cent).

Reaction	coefficient of variation in cross-section averaged over spectrum:			coefficient of correlation in cross-section between spectrum:		
	(Maxwell) (1)	(1/E) (2)	(Watt)a) (3)	(1)-(2)	(1)-(3)	(2)-(3)
6Li(n,a)	.40	.40	3.21	1.00	.02	.05
10B(n,a)	.22	.22	6.39	1.00	.00	.00
19F(n,2n)			2.79			
23Na(n,g)	2.00	4.88	13.06	.95	.00	.00
24Mg(n,p)			4.08			
27Al(n,a)			5.47			
27Al(n,p)			5.86			
32S(n,p)			8.15			
45Sc(n,g)	.89	1.14	3.20	.95	.00	.00
46Ti(n,p)			12.61			
47Ti(n,np)			30.00			
47Ti(n,p)		11.31	11.26			
48Ti(n,np)			30.00			
48Ti(n,p)			10.30			
55Mn(n,2n)			12.95			
54Fe(n,p)		7.31	3.53			
56Fe(n,p)			4.48			
58Fe(n,g)	5.96	14.34	30.71	.34	.00	-.03
59Co(n,2n)			10.92			
59Co(n,g)	.67	.77	4.61	.95	.00	.00
59Co(n,a)			4.29			
58Ni(n,2n)			10.92			
58Ni(n,p)		9.57	6.51			
60Ni(n,p)			7.47			
63Cu(n,a)			5.27			
63Cu(n,g)	2.00	2.76	19.01	.06	.00	.25
63Cu(n,2n)			1.74			
64Zn(n,p)		12.81	7.45			.57
65Cu(n,2n)			7.31			
93Nb(n,n')		46.89	18.91			.88
103Rh(n,n')		5.24	3.02			.87
115In(n,g)	6.00	5.99	4.29	1.00	.00	.00
115In(n,n')		12.87	11.99			
127I(n,2n)			17.22			
197Au(n,g)	.78	3.05	8.36	.27	.00	.00
232Th(n,f)		6.56	5.09			
232Th(n,g)	5.08	10.95	11.70	.01	.00	.11
235U(n,f)	.32	2.14	1.97	.14	.00	.01
238U(n,f)	25.04	6.29	2.02	.01	.04	.55
238U(n,g)	.74	3.45	5.81	.00	.00	.01
237Np(n,f)	46.59	16.22	9.32	.00	.00	.93
239Pu(n,f)	.72	4.10	3.02	.04	.00	.29

a) 235U fission spectrum from ENDF/B-V version 2.

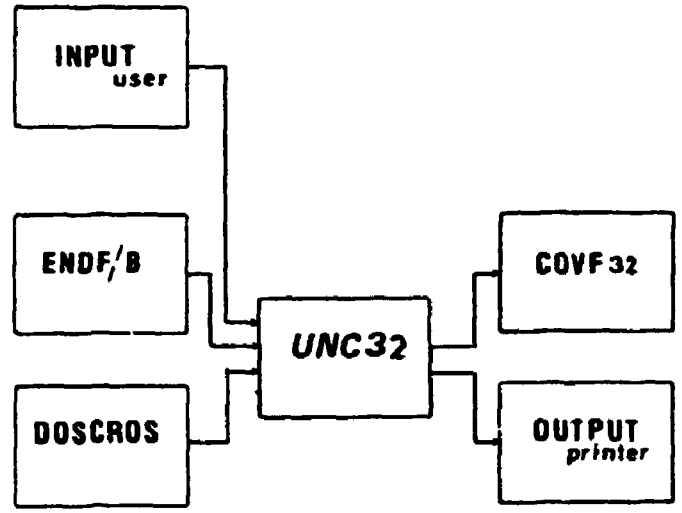
Remark 1: The following computer programs,operational at ECN, have been used:UNC33,STAYNL and FITOCO.
Remark 2: The weighting spectrum for UNC33 and FITOCO was determined in the FLUX81 experiment and refers to HFR pos.C3.
Remark 3: The 1/E spectrum originated from SAND-2.

Table 6. Uncertainty matrix for $^{23}Na(n,\gamma)$.

CROSS-SECTION NAME : NA23G52 MAT-NUMBER : 6311

X-SECTION CORRELATION MATRIX (27 X 27) UPPER TRIANGLE

GROUP NO	REL.SDEV (PCT)	ENERGY (EV)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27
1	2.00	1.000E-04	100	100	100	100	100	100	100	100	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2.00	2.150E-01		100	100	100	100	100	100	100	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	2.00	4.650E-01			100	100	100	100	100	100	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	2.00	1.000E+00				100	100	100	100	100	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	2.00	2.150E+00					100	100	100	100	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	2.00	4.650E+00						100	100	100	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	2.00	1.000E+01							100	100	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	2.00	2.150E+01								100	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	4.26	4.650E+01									100	100	100	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	4.74	1.000E+02										100	100	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	4.74	2.150E+02											100	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	12.77	4.650E+02												100	98	98	61	95	10	15	21	38	12	0	0	0	0	0	0
13	19.52	1.000E+03													100	95	56	90	9	14	20	36	11	0	0	0	0	0	0
14	17.86	2.150E+03														100	64	99	10	16	22	39	12	0	0	0	0	0	0
15	21.33	4.650E+03															100	66	9	13	18	33	10	0	0	0	0	0	0
16	15.77	1.000E+04																100	12	27	25	45	14	0	0	0	0	0	0
17	54.69	2.150E+04																	100	6	7	13	4	0	0	0	0	0	0
18	35.57	4.650E+04																		100	11	20	6	0	0	0	0	0	0
19	25.55	1.000E+05																			100	28	9	0	0	0	0	0	0
20	14.19	2.000E+05																				100	17	0	0	0	0	0	0
21	14.43	4.000E+05																					100	95	95	95	74	0	0
22	20.00	8.000E+05																						100	100	100	78	0	0
23	20.00	1.400E+06																							100	100	78	0	0
24	20.00	2.500E+06																								100	78	0	0
25	15.62	4.000E+06																									100	62	62
26	25.00	6.500E+06																										100	100
27	25.00	1.050E+07																											100



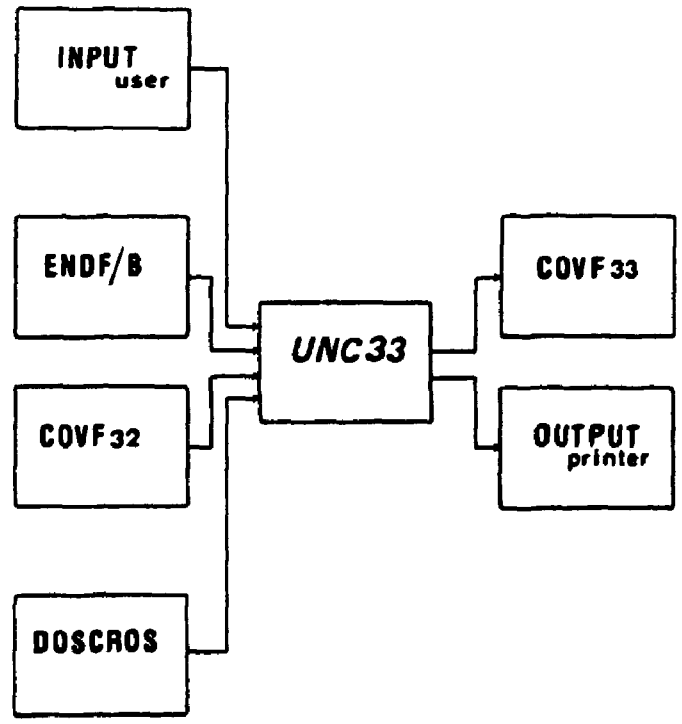


Fig. 1. Link of UNC32 and UNC33 programs with libraries/files.

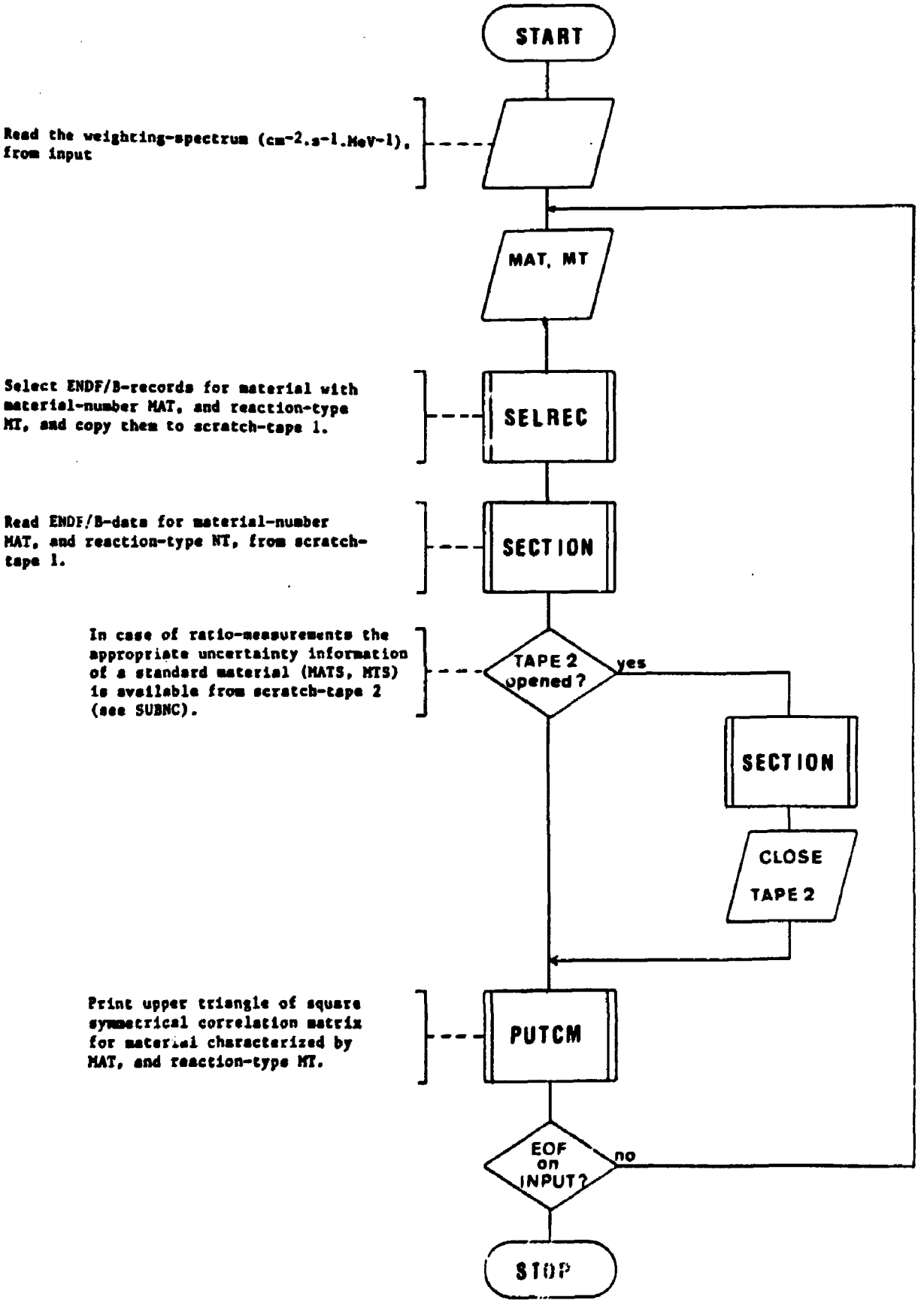


Fig. 2. Flow-chart of the program UNC33

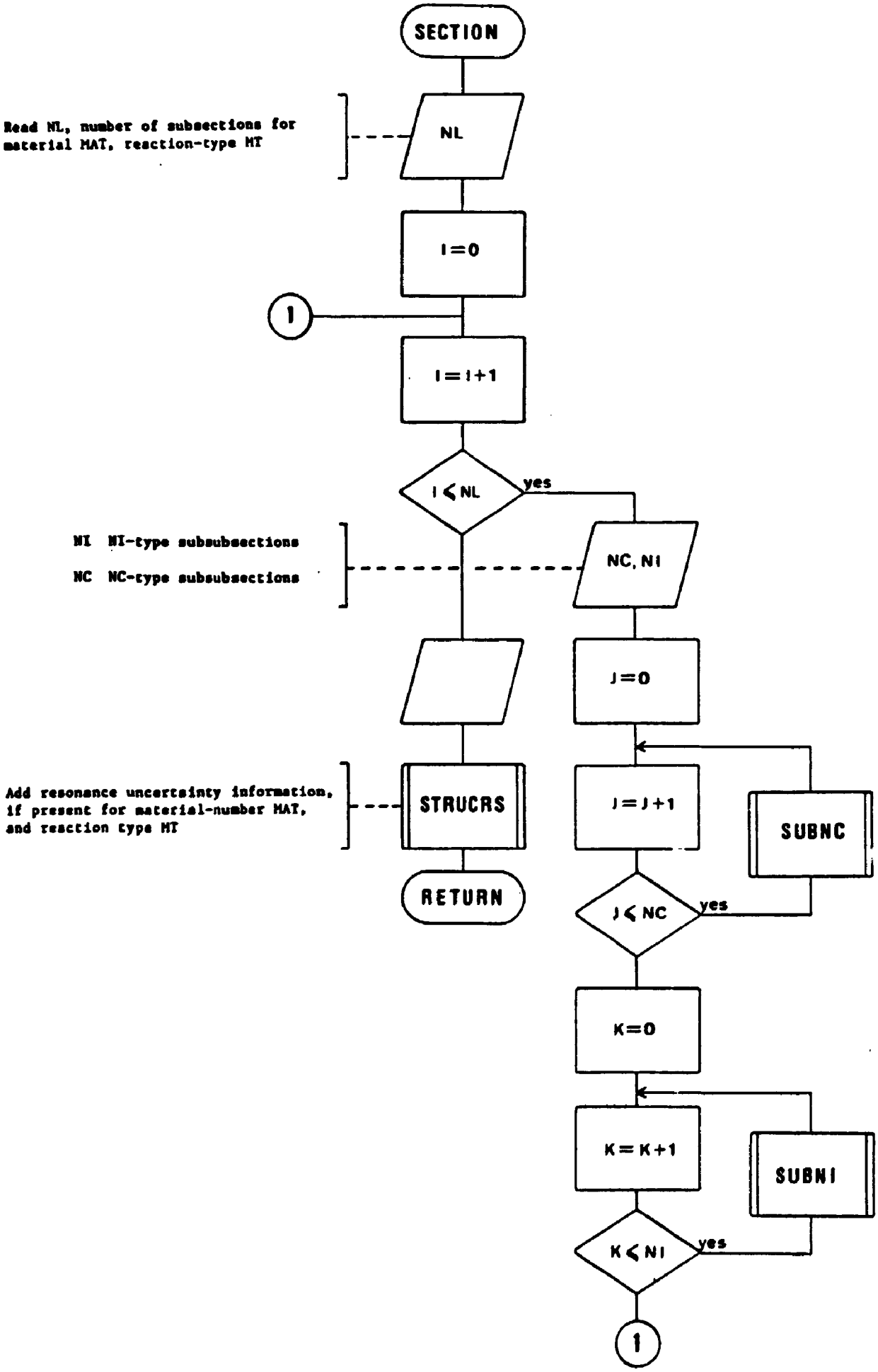


Fig. 3. Flow-chart of subroutine SECTION

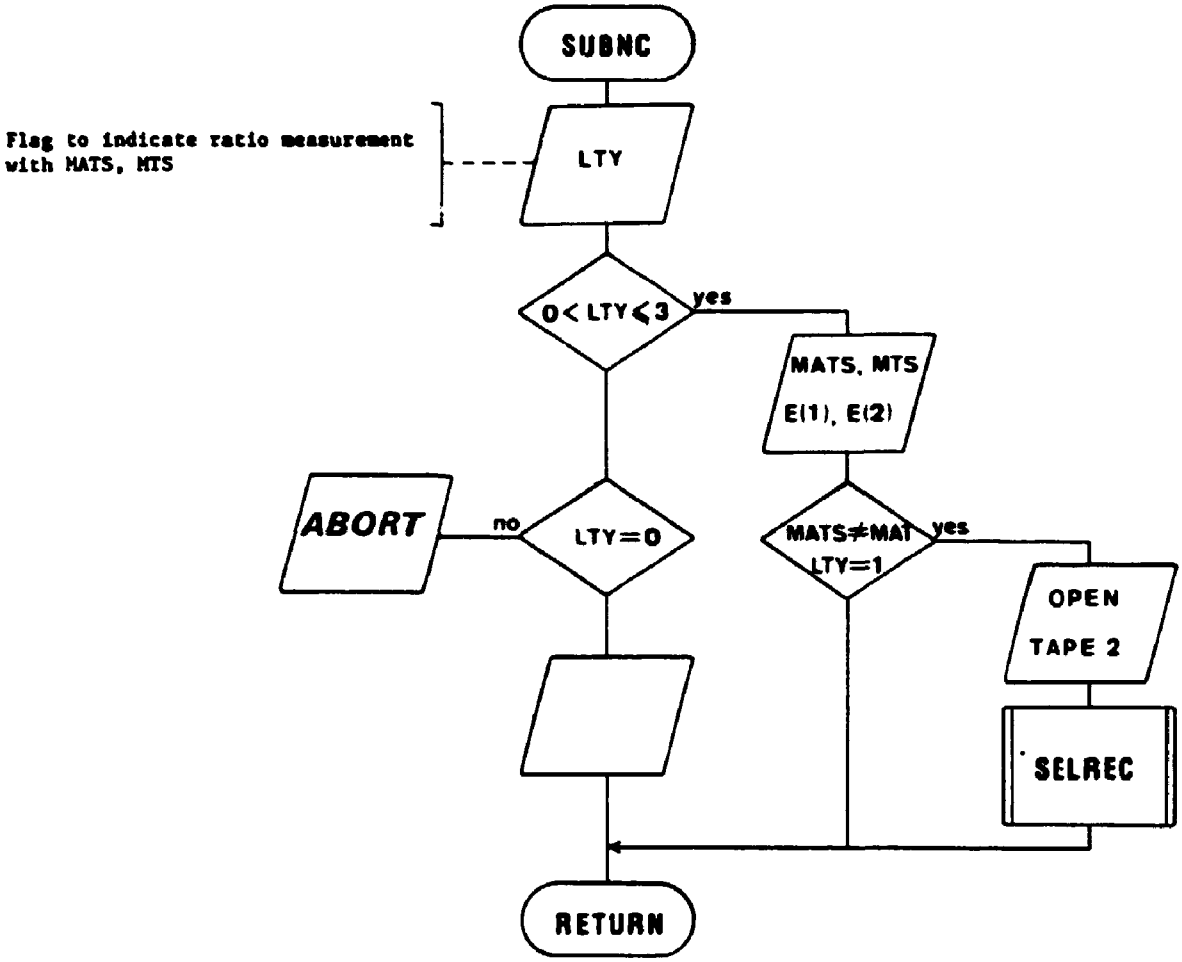


Fig. 4. Flow-chart of subroutine SUBNC

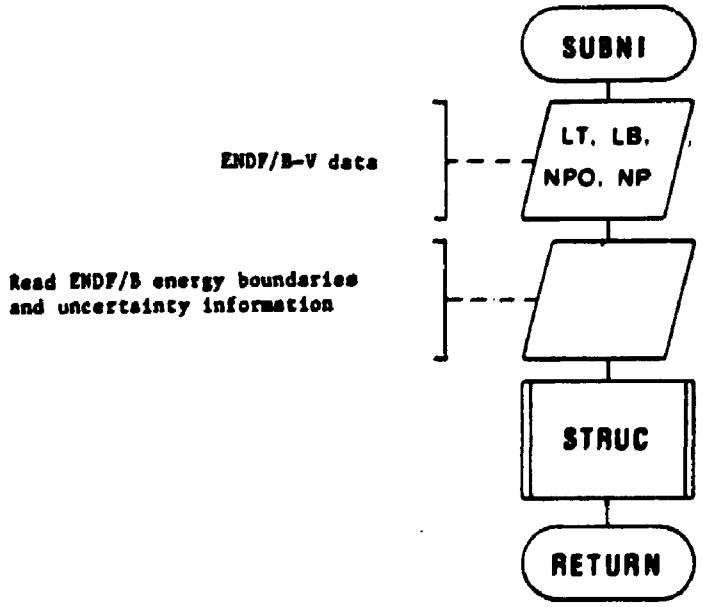


Fig. 5. Flow-chart of subroutine SUBNI

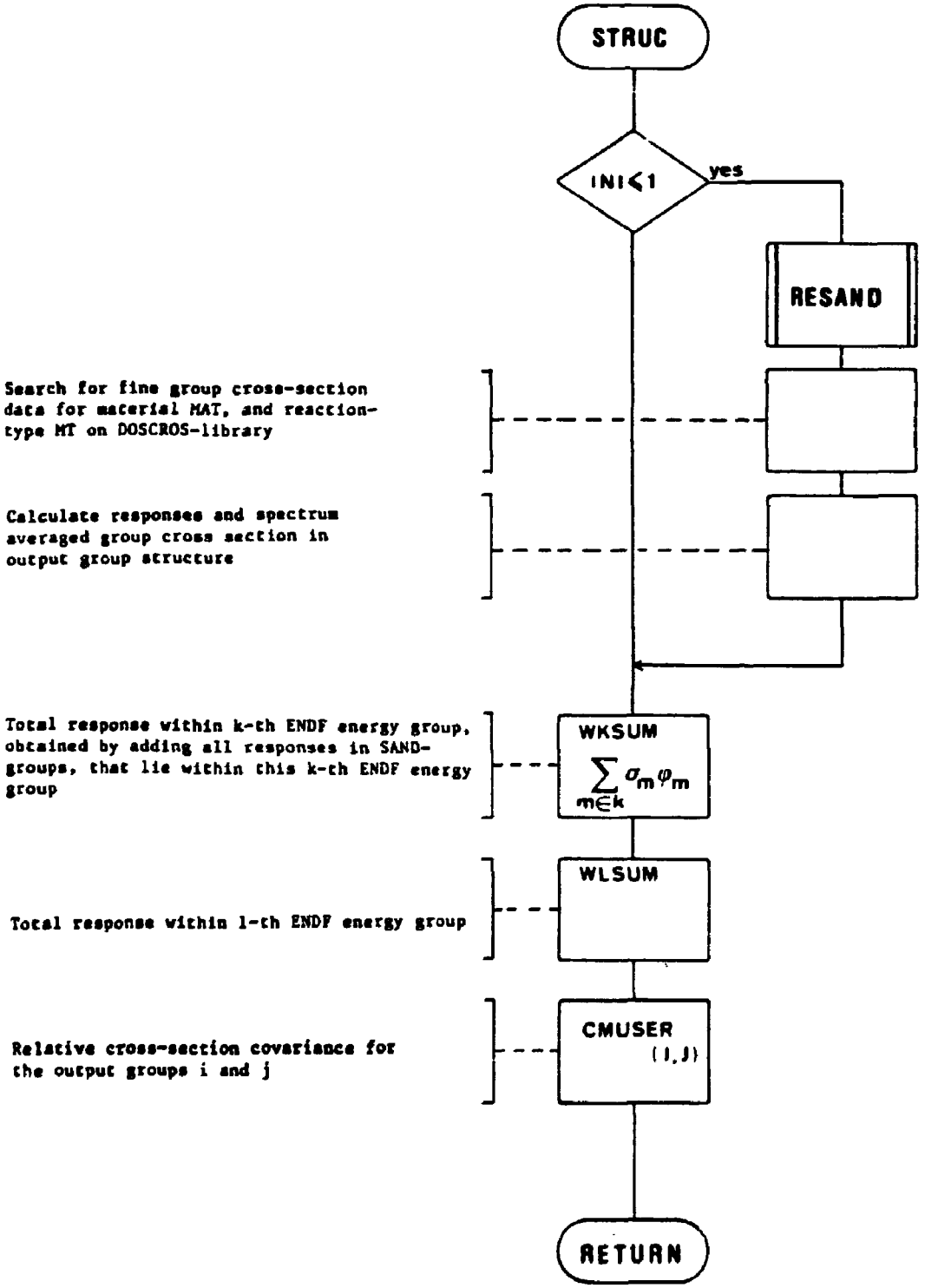
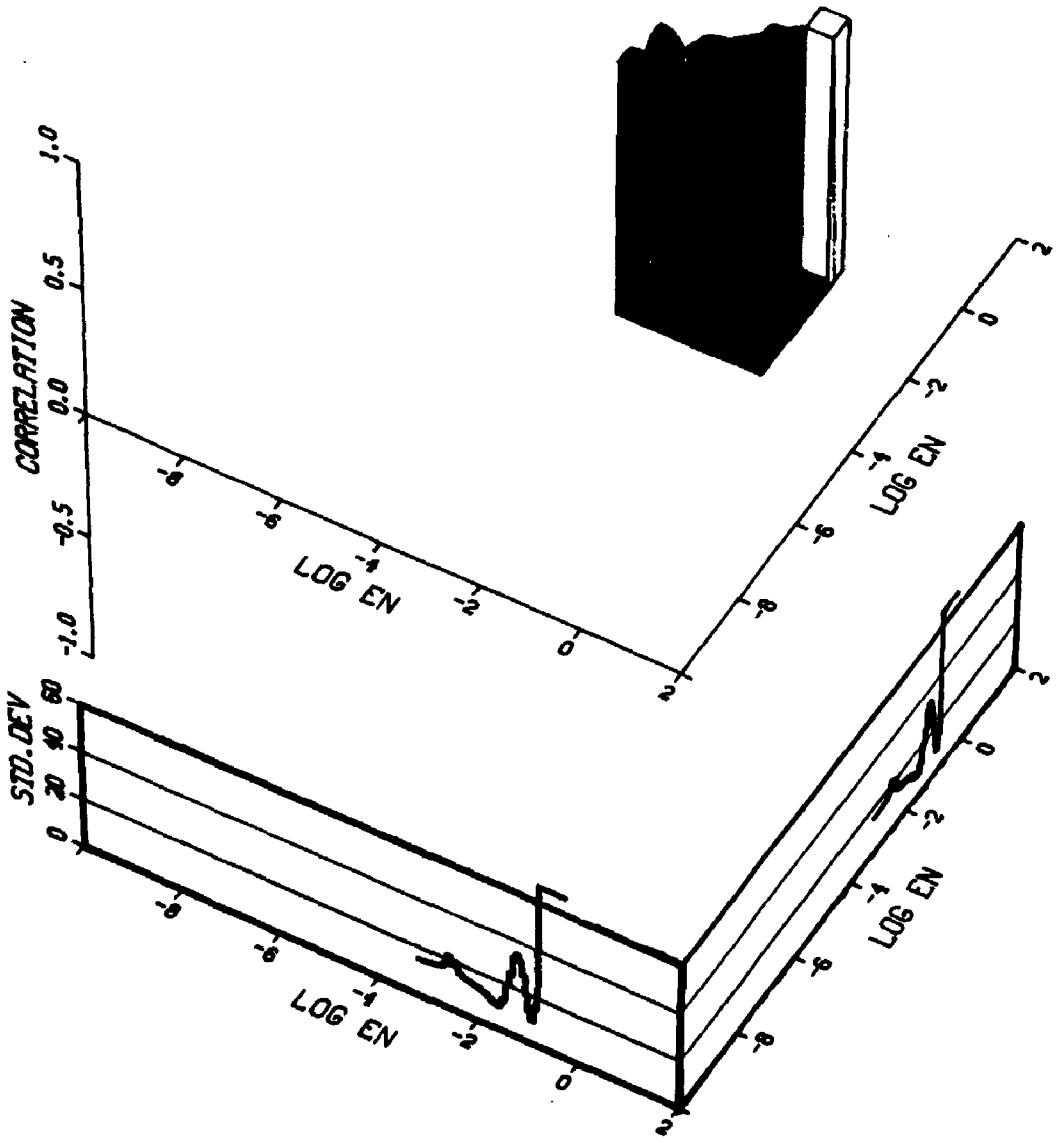


Fig. 6. Flow-chart of subroutine STRUC



CROSS SECTION COVARIANCE DATA FOR NA23G

Fig. 7. Part of users library COVF32 calculated by UNC32.

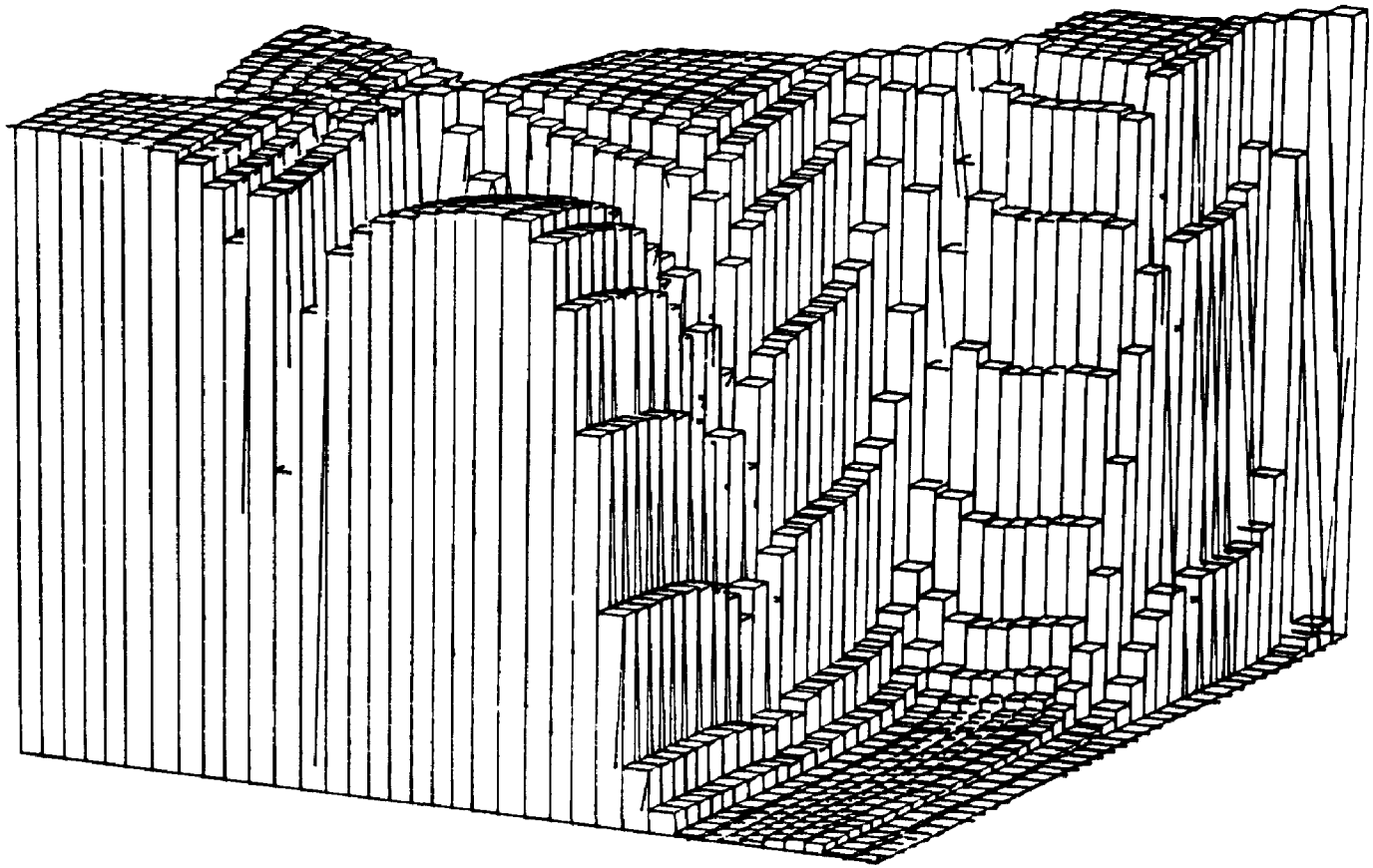


Fig. 8. The covariance data from fig. 7 in more detail (last point corrected).

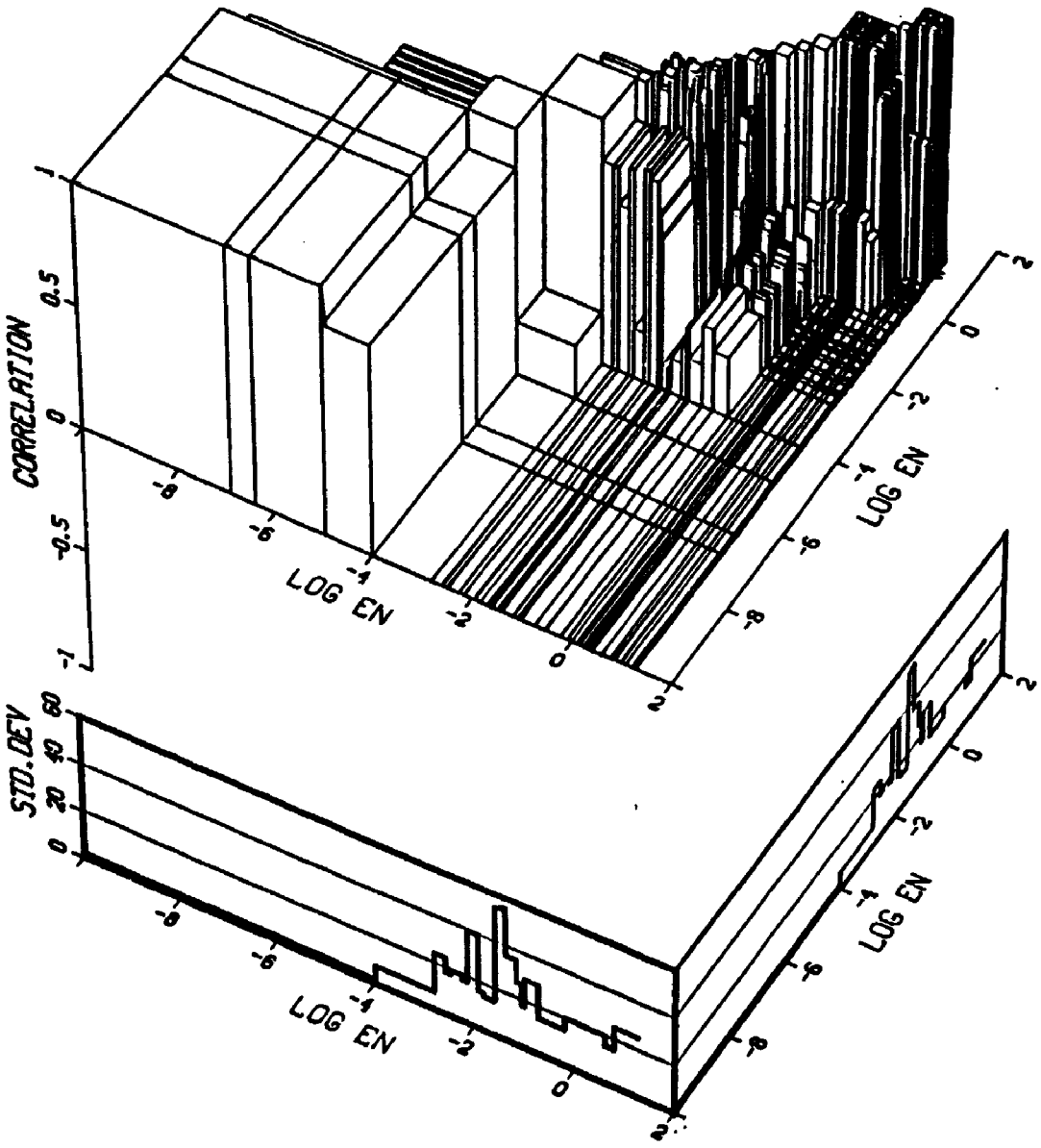


Fig. 9. Results obtained with the program UNC33.

CROSS SECTION COVARIANCE DATA FOR NA23G

Appendix 1. Calculation of derivatives.

In the vicinity of a resonance at energy E_r^+, the cross-section for a neutron of energy E undergoing an (n,γ) or (n,f) reaction is given by the single level Breit-Wigner formula

$$\sigma_{n,x}(E) = \frac{4\pi}{k^2} g_j \frac{\Gamma_n \Gamma_x}{(2\Delta E_r)^2 + \Gamma_t^2}$$

with $x = \gamma$ resp. f;

$\Delta E = E - E_r^+$;

$k^2 = \left(\frac{0.0022\ A}{A+1}\right)^2 \frac{1}{E}$

$g_j = \frac{2J+1}{2(2I+1)}$, with I = target spin and J = resonance spin;

$\Gamma_t = \Gamma_n + \Gamma_f + \Gamma_\gamma$;

Γ_t = total resonance width;

Γ_n = neutron width;

Γ_f = fission width;

Γ_γ = gamma width.

For group cross-sections one has

$$\sigma_g = \int_{E_g}^{E_{g+1}} \frac{4\pi}{k^2} g_j \frac{\Gamma_n \Gamma_x}{(2\Delta E)^2 + \Gamma_t^2}\, dE .$$

which gives

$$\sigma_{n,x}(E) = \frac{4\pi}{k^2} \frac{J+0,5}{2I+1} \frac{\Gamma_n \Gamma_x}{(2\Delta E)^2 + (\Gamma_n+\Gamma_x+\Gamma_\gamma)^2}$$

It can be proven that

$$\frac{\partial \sigma_g}{\partial p} = \int_{E_g}^{E_{g+1}} \frac{\partial \sigma(x,p)}{\partial p}\, dE .$$

Proof:

Let $F(p) = \int_{x_1}^{x_2} f(x,p)\, dx$,

then $$\frac{\partial F}{\partial p} = \lim_{\Delta p \to 0} \frac{F(p+\Delta p) - F(p)}{\Delta p} = \lim_{\Delta p \to 0} \frac{\int f(x,p+\Delta p)dx - \int f(x,p)dx}{\Delta p}$$

According to the Taylor expression one has

$$f(x,p+\Delta p) = f(x,p) + \frac{\partial f(x,p)}{\partial p} \Delta p .$$

This gives

$$\frac{\partial F}{\partial p} = \lim_{\Delta p \to 0} \frac{\int_{x_1}^{x_2} f(x,p+\Delta p)dx - \int_{x_1}^{x_2} f(x,p)dx}{\Delta p} =$$

$$= \lim_{\Delta p \to 0} \frac{\int f(x,p) + \frac{\partial f(x,p)}{\partial p} \Delta p\, dx - \int f(x,p)dx}{\Delta p} =$$

$$= \lim_{\Delta p \to 0} \frac{\int_{x_1}^{x_2} f(x,p)dx - \int_{x_1}^{x_2} f(x,p)dx + \int_{x_1}^{x_2} \frac{\partial f(x,p)}{\partial p} \Delta p\, dx}{\Delta p} =$$

$$= \lim_{\Delta p \to 0} \frac{\int_{x_1}^{x_2} \frac{\partial f(x,p)}{\partial p} \Delta p\, dx}{\Delta p} = \int_{x_1}^{x_2} \frac{\partial f(x,p)}{\partial p}\, dx .$$

This gives that it is enough to determine the derivatives to the parameters of the Breit-Wigner formula.

$$\frac{\partial \sigma_x(E)}{\partial \Gamma_x} = \frac{4\pi}{k^2} \frac{J+0,5}{2I+1} \left[\frac{\Gamma_n\{(2\Delta E)^2 + (\Gamma_t)^2) - 2\Gamma_n\Gamma_x(\Gamma_t)\}}{\{(2\Delta E)^2 + \Gamma_t^2)\}^2}\right] =$$

$$= \frac{4\pi}{k^2} \frac{J+0,5}{2I+1} \left[\frac{\Gamma_n}{(2\Delta E)^2 + \Gamma_t^2} - \frac{2\,\Gamma_n\Gamma_x\Gamma_t}{((2\Delta E)^2 + \Gamma_t^2)^2}\right] =$$

$$= \frac{\sigma(E)}{\Gamma_x} - \frac{8\pi}{k^2} \frac{I+0,5}{2I+1} \frac{\Gamma_n\Gamma_x\Gamma_t}{((2\Delta E)^2 + \Gamma_t^2)^2} .$$

$$\frac{\partial \sigma_x(E)}{\partial \Gamma_y} = -\frac{8\pi}{k^2} \frac{J+0,5}{2I+1} \frac{\Gamma_n\Gamma_x\Gamma_t}{((2\Delta E)^2 + \Gamma_t^2)^2} , \quad y = f \text{ resp. } \gamma.$$

$$\frac{\partial \sigma_x(E)}{\partial J} = \frac{\sigma_x(E)}{J+0,5} .$$

Hence the E_R and Γ_n are dependent of the neutron energy E it is difficult to give the exact formulas for $\frac{\partial \sigma(E)}{\partial E_r}$ and $\frac{\partial \sigma(E)}{\partial \Gamma_n}$.

So it is used

$$\frac{\partial \sigma_g}{\partial \Gamma_n} = \frac{\int \sigma(E,\Gamma_n+\Delta\Gamma_n)dE - \int \sigma(E,\Gamma_n-\Delta\Gamma_n)dE}{2\Delta\Gamma_n}$$

and

$$\frac{\partial \sigma_g}{\partial E_r} = \frac{\int \sigma(E,E_r+\Delta E_r)dE - \int \sigma(E,E_r-\Delta E_r)dE}{2\Delta E_r} .$$