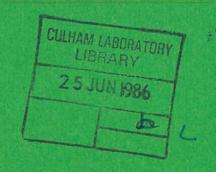
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Report



USERS MANUAL FOR THRES—F CODE

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USER MANUAL FOR THRES-F CODE

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ABSTRACT

Experimental cross-section data for neutron-induced reactions in the energy range 0–20 MeV are often incomplete or non-existent. The code described in the present manual permits the approximate calculation of the cross-sections of all the energetically possible neutron-induced reactions (except radiative capture) coupling the statistical-model theory with systematics formulae and available experimental data. Pointwise and group cross-sections for energies up to 20 MeV can be determined with only Z and A required as description of the target nucleus.

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1. Introduction

Approximately 20 reactions are possible when nuclei are bombarded by neutrons in the energy range below 20 MeV. If a target nucleus of N neutrons and Z protons is bombarded by a neutron, any of the residual nuclei shown in Fig.1 may be produced.

	N-2	N-1	N	N+1
Z	п,3п	n,2n	Original Nucleus n,n'	п,ү
Z-1	n,nt n,tn	n,t n,nd n,dn	n,d n,np n,pn	n,p
Z-2	n,αn n,nα	n,α n,He ³ n n,nHe ³	n,He ³ n,pd n,dp	

Fig.1 - Reactions produced by neutrons in the energy range up to 20 MeV.

In this energy range, the primary reaction mechanism involves the formation of a highly-excited compound nucleus consisting of both the target nucleus and the incident neutron. The energetic compound nucleus can emit a gamma ray or subsequently break up through a single or multistage process into a residual nucleus and one or more particles sharing the remaining kinetic energy.

Such was the starting point of Pearlstein [1] when he prepared the first version of the code called THRESH; the neutron cross-sections in the MeV range were analysed using an approach largely based on the statistical model, normalized to experimental data wherever possible. At higher energies direct and precompound reactions, which are not accounted for by the statistical model become important, but the input parameters to the model had been chosen to yield agreement with

experimental trends, thus extending the validity of the statistical model beyond its usual range.

Several changes have been made to the first version of the code by Pearlstein [2,7] and by Gruppelaar [3] prior to the later version described in the present manual. The basic theory and all the modifications are summarized here in order to give the user a sufficient description of the approximations and the range of validity of the results.

The calculated cross-sections do not show nuclear structure effects since discrete level information has not been included. Also, gamma emission in competition with particle emission has been ignored, an assumption that should be approximately correct except near threshold. The method emphasises simplicity and is not intended to supplant detailed nuclear model calculations but rather is intended to provide additional information on cross-sections in cases where measurements are lacking or show disagreements.

Table 1 – List of the considered cross-sections.

N°	Reaction	N°	Reaction	N°	Reaction	N°	Reaction
1	n,n'	2	n,2n	3	n,3n	4	n,p
5	n,d	6	n,t	7	n,He³	8	n,α
9	n,np	10	n,nd	11	n,nt	12	n,nHe³
13	n,nα	14	n,pn	15	n,2p	16	n,αn
17	n,αp	18	n,dn	19	n,pα		

The code calculates 19 types of neutron cross-sections for each isotope, numbered as shown in Table 1. All the fitting parameters contained in the code have a range of validity for Z between 21 and 83. The code will in fact also perform calculations for most of the isotopes out of this range in which case it prints a warning message at the beginning of the calculation. This possibility is retained for the case where the user wishes to enter his own fitting parameters (see section 2).

The next paragraphs describe in succession the input and the output of the code, the basic theoretical method, the recent systematics considered, the experimental renormalization file, the group cross-section calculations and an example of the utilization of the code.

2. INPUT of the code.

For each isotope whose cross-sections are required a set of cards has to be given in the following order:

CARD 1 - CEMSYM (format A2)

where CEMSYM=chemical symbol of the isotope

CARD 2 - IZ,IA,NOPT,NOUTPT,MATN,NORM,IREN (all integers)

(free format input, comma as separator, blank for unchanged value, slash at the end) where:

IZ=number of protons in the target nucleus. If binding energies are given, enter negative IZ value.

IA=number of nucleons in the target nucleus. If fitting constants are given, enter negative IA value.

NOPT=first option selector

- If NOPT=0 cross-sections calculated in the range
 0-20 MeV with 0.5 MeV steps (default value).
- . If NOPT=1 output in special ECN mode.
- . If NOPT=2 14 MeV and 15 MeV values only.
- . If NOPT=3 cross-section uncertainties calculated at the energy specified by the next parameter (see section 4).
- . If NOPT=4 calculation of renormalization only.
- . If NOPT=5 cross-sections calculated in the range

0-15 MeV with 0.1 MeV steps.

NOUTPT=second option selector (it can take only few values in connection with the NOPT value)

- . If NOUTPT=0 no external output (default value).
- . When NOPT=1, if NOUTPT=1 output of ENDFB formatted data [4] on file 1.
- . When NOPT=5, if NOUTPT=1 group average cross-sections will be printed and stored on file 3.
- . When NOPT=1, if NOUTPT=3 output in KEDAK format [13] on file 1 and group constants on file 2 (see section 3)
- . When NOPT=3, NOUTPT is the point energy as multiple of 0.01 MeV (i.e. 1410=14.10 MeV).

MATN=last MAT number used for previous ENDFB results (needed only for sequential calculation. Usually =0)

NORM=first renormalization option

- . If NORM=0 no renormalizations occur.
- . If NORM=1 renormalization of cross-sections to recent 14.5 MeV systematics (see section 5 default value).

IREN=second renormalization option

- . If IREN=0 no effects (default value).
- . If IREN=1 additional renormalisation of some or all cross-sections to the experimental data which have to be written in a library defined as file 8 (see section 6).

CARD 3/4/5 – (only if IZ<0) – 19 binding energy values (free format) in reaction number order.

CARD 6/7 – (only if IA<0) – 14 fitting constants (free format) in the order described in section 4.

When all the isotopes are specified insert a blank card as end of file.

2.1. Mass and binding energy default values.

In the code most of the mass excesses coming from WAPSTRA table [5] are stored in an internal array. Hence, most default binding energies are determined with a good precision.

If some data are not available a message will be printed and an alternative approximate method is used to calculate the binding energy, utilising an empirical formula, introduced by Pearlstein [1] in the original version of the code.

2.2. Fitting constants default values.

Although the meaning of these 14 constants is described in detail in section 4, their default values are given here:

$$C_1 = 1.452$$
 $C_2 = 12.0$ $C_3 = 0.25$ $C_4 = 12.0$ $C_5 = 0.10$ $C_6 = 12.0$ $C_7 = -6.5$ $C_8 = 1.8$ $C_9 = -2.5$ $C_{10} = 2.1$ $C_{11} = 1.5$ $C_{12} = 600.0$ $C_{13} = 1.5$ $C_{14} = 0.005$

3. Description of the OUTPUT.

The OUTPUT of the THRES-F code follows the options chosen in the input data and can be separated into two parts: the print output (usually defined as file 6 on IBM computers) and the output on specific other files.

In the print output for each isotope, after the identification data, some general information is printed concerning the renormalization data (if required) with the

convention of writing a positive energy value for data coming from systematics and negative for data derived from experiments. The renormalization factor for the reactions concerned is also printed.

. If NOPT=0 the binding energies and the list of the pointwise cross-sections (in barns) for 0.5 MeV energy steps are printed for all the 19 reactions and for the difference between the total cross-section and their sum.

. If NOPT=1 the data are printed in a special ECN mode which consists of:

- A. print of Q-value
- B. print of 14 and 15 MeV values
- C. print of fusion spectrum average
- D. print GAM2 group constants

The fusion spectrum has been taken as $\phi(E)=e^{-\frac{5}{kT}(\sqrt{E}-\sqrt{E_p})^2}$, where kT=0.025 MeV and $E_p=14.07$ MeV.

The GAM2 group constants are six group cross-sections weighted with the fusion spectrum starting from the pointwise cross-section values, for the first six groups of the GAM2 group structure, for which the energy boundaries are shown in App.I.

. If NOPT=3 for each reaction and at the point energy entered by the NOUTPT parameter, the uncertainties (in barns) on the cross-section values before renormalization are printed.

. If NOPT=4 only the values of the cross-sections at the renormalization point energy are calculated and printed.

. If NOPT=5 the same output format of the case NOPT=0 is printed with the energy step of 0.1 MeV.

The remaining output is controlled by the second parameter (NOUTPT).

. If NOUTPT=1 and NOPT=0 ENDFB formatted cross-sections are written on file 1 for 10 reactions only, indicated with the ENDFB number MT of which value and definition are stated as follows:

MT=106 – corresponds to (n,He³) or N=7

MT=107 – corresponds to (n,α) or N=8

. If NOUTPT=1 and NOPT=5 group cross-sections are printed. The UKCTR activation library format [6] and the GAM2 group structure are utilized. Between each set of group values, information about threshold energy and renormalization point energy (if any) are written. In the comment space of the headline of the group cross-section sets, the origin of the data of renormalization are printed (SYS=systematics; EXP=experimental).

The group cross-sections are also written on file 3; they are identified by 8 numbers (IN) which have the following meaning:

IN=1 - (n,2n) or MT=16
IN=3 - (n,p) or MT=103
IN=4 - (n,
$$\alpha$$
) or MT=107
IN=5 - (n,n'p)+(n,d) or MT=104
IN=6 - (n,n' α)+(n, α n') or MT=22
IN=7 - (n,n'pn)+(n,n'd)+(n,dn')+(n,nt) or MT=105
IN=8 - (n,3n)
IN=9 - (n,He³) or MT=106

. If NOUTPT=3 and NOPT=1 cross-sections in KEDAK format are written on file 1, and GAM2 group constants are written on file 2.

4. Basic theoretical model.

This paragraph is largely based on the work of Pearlstein [1,2,7] since the theoretical model used in the code has been kept essentially unchanged.

Nevertheless, the formulae utilised in the code are summarized here in order to give the user a self-contained description of the approximations made and the physical meanings of the fitting constants given in section 2.2.

4.1 Total non-elastic cross-section.

The total non-elastic cross-section is assumed to be constant with energy and equal to that determined by a fit of experimental data at 14 MeV, given by the following formula:

$$\sigma_{ne} = \pi (0.12 A^{\frac{1}{3}} + 0.21)^2$$
 barns, (1)

where A is the number of nucleons of the nucleus.

The sum of all partial reaction cross-sections must not exceed this value. All reaction cross-sections considered here have a threshold behaviour determined by binding energy and Coulomb barrier characteristic rising towards an apparent maximum with increasing incident neutron energy. At higher energies the cross-section falls as secondary emission takes place.

Experimental data for nuclides ranging from beryllium to plutonium show that the non-elastic cross-section varies only 20% in the energy range 5-20 MeV. That

approximately fixes the energy limits of the THRES-F code in the MeV energy range up to 20 MeV.

4.2 Neutron multiplication.

An apparent limiting cross-section applies for processes where only neutrons are emitted, this is denoted by $\sigma_{n,N}$. The ratio of the cross-section limit $\sigma_{n,N}$ to the cross-section σ_{ne} has been assumed to be described by the following energy-independent formula:

$$\frac{\sigma_{n,N}}{\sigma_{ne}} = 1 - C_1 e^{-C_2 s} , \qquad (2)$$

where s = neutron excess parameter (= $\frac{N-Z}{N+Z}$),

N = number of neutrons of the target nucleus,

Z = number of protons of the target nucleus.

The constants C_1 and C_2 are the first two fitting constants whose assumed values are given in section 2.2. C_1 is related to C_2 by the equation:

$$C_1 = e^{-0.031C_2}$$
.

The energy dependence of the fraction of the neutron emitting processes that lead to the emission of two neutrons is described by the statistical-model formula [8]:

$$\frac{\sigma_{n,2n}}{\sigma_{n,N}} = \frac{\int\limits_{0}^{E-B_{n}} \varepsilon \sigma_{c} e^{\sqrt{4a(E-\varepsilon)}} d\varepsilon}{\int\limits_{0}^{E} \varepsilon \sigma_{c} e^{\sqrt{4a(E-\varepsilon)}} d\varepsilon} , \qquad (3)$$

where:

E = the excitation energy above the ground state (MeV) in the centre of mass system (CMS),

 $a = \text{level density parameter } (\text{MeV}^{-1}),$

 σ_c = cross-section for formation of the compound nucleus by the emitted particle and excited target (assumed to be energy independent),

 B_n = energy required in the CMS to unbind one neutron (MeV),

 ε = energy carried away by the emitted neutron (MeV),

The level density parameter a is calculated from the following formula [9]:

$$a = 0.095 (j_Z + j_N + 1) A^{\frac{2}{3}} [MeV^{-1}],$$
 (4)

where j_Z = effective spin value for Z protons,

 j_N = effective spin value for N neutrons,

A = atomic mass of the nucleus.

Values for j_Z and j_N are taken from [9] and stored as an array in the code.

The energy-dependent (n,2n) cross-section is then calculated as:

$$\sigma_{n,2n}(E) = \sigma_{ne} \frac{\sigma_{n,N}}{\sigma_{ne}} \frac{\sigma_{n,2n}}{\sigma_{n,N}}(E) . \tag{5}$$

The energy dependence of the (n,3n) cross-section can be similarly obtained by substituting in eq.(3) the total binding energy required to emit two neutrons and the level-density parameter of the excited nucleus that has already emitted one neutron; (n,2n) competition has been included.

4.3 Proton and alpha emission.

Consistent with the definition of $\sigma_{n,N}$ a cross-section $\sigma_{n,C}$ is defined to include all

reactions where at least one charged particle is emitted. From eq.(2) the following energy-independent formula may be derived:

$$\frac{\sigma_{n,C}}{\sigma_{ne}} = C_1 e^{-C_2 s} . \tag{6}$$

It is assumed that the peak values of the cross-sections for (n,p) and (n,d) reactions follow similar laws:

$$\frac{\sigma_{n,p}}{\sigma_{ne}} = C_3 e^{-C_4 s} , \qquad (7)$$

$$\frac{\sigma_{n,\alpha'}}{\sigma_{ne}} = C_5 e^{-C_6 s} , \qquad (8)$$

where C_3, C_4, C_5, C_6 are fitting constants.

The excitation curve for charged-particle emission is strongly influenced by the Coulomb barrier and only incidentally by the level density. Here an empirically determined excitation curve is used. It has been found experimentally that the available energy above threshold can be simply related to the residual nuclear charge Z through the following equation [3]:

$$E_F - E_T = C_7 + C_8 \frac{Z}{A^{\frac{1}{3}}} \quad [\text{MeV}] \quad \text{for protons}, \tag{9}$$

$$E_F - E_T = C_9 + C_{10} \frac{Z}{A^{\frac{1}{3}}} [\text{MeV}] \text{ for alphas,}$$
 (10)

where E_F = energy at which the half maximum of the cross-section limit is reached,

 E_T = threshold energy,

 C_7, C_8, C_9, C_{10} are fitting constants.

For analytical convenience the following form for the energy dependence of the excitation function was assumed:

$$X(E) = \frac{1}{\frac{E_F - E}{C_{11}}} , \qquad (11)$$

where C_{11} represents the width of the excitation function in the region of maximum cross-section change. At kinetic energies less than half the potential barrier height a quantum mechanical transmission factor [10] is used for X(E); this involves the use of another fitting constant C_{14} which controls the value of the transmission factor $[X(E) \sim e^{-C_{14} f(E)}]$.

The energy dependent cross-section for charged particle emission is described by the following three-factor formula:

$$\sigma_{n,x}(E) = \sigma_{ne} \frac{\sigma_{n,x}}{\sigma_{ne}} X(E)$$
, with $x = p \text{ or } \alpha$. (12)

4.4 Inelastic neutron scattering.

At high energy $\sigma_{n,n'}$ has been obtained from the equation:

$$\sigma_{n,n'} = \sigma_{n,N} - (\sigma_{n,2n} + \sigma_{n,3n})$$
 (13)

At low energy, instead of a statistical-model calculation requiring detailed energy-level information, the following formula is used to describe the approximate energy dependence of the (n,n') cross-section:

$$\frac{\sigma_{n,n'}}{\sigma_{n,N}} = \frac{\int\limits_{0}^{E} \varepsilon \, e^{\sqrt{4a(E-\varepsilon)}} \, d\varepsilon}{\int\limits_{0}^{E'} \varepsilon \, e^{\sqrt{4a(E-\varepsilon)}} \, d\varepsilon} \quad , \tag{14}$$

where
$$E' = E + \frac{C_{12}}{a} e^{-C_{13}aE}$$
.

4.5 Other components of the non-elastic cross-section.

The remaining components of the total non-elastic cross-section caculated by THRES-F code (see Table 1) do not require input of any new parameters.

Each cross-section for the reactions where a second particle is emitted has been determined considering the two emissions as separate processes, in which the probability of the first emission is calculated from the formulae of the previous sections and the probability of the second emission from the same kind of formulae but applied to the remaining nucleus with recalculated parameters. Existing data are not sufficent to fix rigorously the (n,d), (n,t), and the (n,He^3) cross-sections relative to σ_{ne} , but the following formula can be assumed:

$$\frac{\sigma_{n,d}}{\sigma_{ne}} + \frac{\sigma_{n,l}}{\sigma_{ne}} + \frac{\sigma_{n,He^3}}{\sigma_{ne}} = \frac{\sigma_{n,C}}{\sigma_{ne}} - \left(\frac{\sigma_{n,p}}{\sigma_{ne}} + \frac{\sigma_{n,\alpha}}{\sigma_{ne}}\right) , \qquad (15)$$

The penetration of charged particles through the Coulomb barrier of the nucleus is primarily determined by their charge, although there is a slight dependence on their mass which has been neglected here. Therefore, in eq.(15), the (n,d) and the (n,t) terms have been taken proportional to the ratio defined in eq.(7) for protons, and the (n,He^3) term to the ratio defined in eq.(8) for alpha particles. Thus:

$$\frac{\sigma_{n,d}}{\sigma_{ne}} = \frac{\sigma_{n,t}}{\sigma_{ne}} = \frac{\sigma_{n,p}}{2 \sigma_{n,p} + \sigma_{n,\alpha}} \left(\frac{\sigma_{n,C}}{\sigma_{ne}} - \frac{\sigma_{n,p}}{\sigma_{ne}} - \frac{\sigma_{n,\alpha}}{\sigma_{ne}} \right). \tag{16-a}$$

$$\frac{\sigma_{n,He^3}}{\sigma_{ne}} = \frac{\sigma_{n,\alpha}}{2 \sigma_{n,p} + \sigma_{n,\alpha}} \left(\frac{\sigma_{n,C}}{\sigma_{ne}} - \frac{\sigma_{n,p}}{\sigma_{ne}} - \frac{\sigma_{n,\alpha}}{\sigma_{ne}} \right) . \tag{16-b}$$

The corresponding energy dependence follows similar formulae to those for protons and alphas.

4.6 Uncertainty calculations.

Using the Pearlstein formalism [2], cross-sections at energy \boldsymbol{E}_n can be described as:

$$\sigma_n(E_n) = f(C_1, C_2, \dots, C_M, E_n) ,$$
 (17)

where the C_i are the 14 parameters defined in section 2.2.

The uncertainties in the cross-sections can be represented by the following formula:

$$(d\sigma_n)^2 = \sum_{k=1}^M \sum_{l=1}^M \left(\frac{\partial \sigma_n}{\partial C_k}\right) \left(\frac{\partial \sigma_n}{\partial C_l}\right) S_{kl} \ dC_k \ dC_l \ ,$$
 (18)

where S_{kl} = correlation matrix,

 dC_i = increment of the C_i parameter.

The correlation matrix and increments can be determined from a least-squares fit of the above parameters to experimental cross-section values.

Such a fitting was performed by Pearlstein [2] for nuclei in the Z-range 20-83, leading to the correlation matrix and increments stored in internal arrays of the code.

The code calculates the uncertainty for each cross-section (in barns) as the square-root of the variance defined in eq.(18).

5. Systematics included in THRES-F code.

If the choice of renormalization to the systematics formulae is required, the charged-particle emission cross-sections are renormalized using the formulae implemented in the code by Gruppelaar [3] and described below.

The (n,t) and the (n,He^3) cross-sections are renormalized at 14.5 MeV to the following value, given in [12]:

$$\sigma_{n,He^3} = 0.54 \left(A^{\frac{1}{3}} + 1\right)^2 e^{-10.0 s} \left[\mu b\right],$$
 (22)

$$\sigma_{n,t} = 4.52 \left(A^{\frac{1}{3}} + 1\right)^2 e^{-10.0 s} \left[\mu b\right] \cdot$$
 (23-a)

For odd-mass nuclei it was recently found [16,17] that the (n,t) cross-sections are systematically much higher. This can be approximated by:

$$\sigma_{n,t} = 4400 \ e^{-20.5 \ s} \quad [\mu b] \cdot$$
 (23-b)

In the above formulae $\sigma_{n,t}$ is the sum of the cross-section for (n,t),(n,nd),(n,dn), and (n,npn) reactions.

The $(n,n\alpha)+(n,\alpha n)$ reaction cross-sections are renormalized at 14.5 MeV to:

$$\sigma_{n,n\alpha} = 0.125 \ \sigma_{n,\alpha} \ \cdot \tag{24}$$

The $\sigma_{n,\alpha n}$ cross-section, already included in eq.(24), is renormalized to a low value (10⁻¹⁰ mb).

6. Experimental renormalization file.

If the option of renormalization of some or all reaction cross-sections to experimental data is chosen, a file containing the available values has to be read (from FT08 on the IBM computer).

The data file has to be written in the following format:

for each isotope:

```
CARD 1 – IDEN,NAME (15,8A4)

where IDEN = Z \times 1000 + A

NAME = any alphanumeric string for identification data.

FOLLOWING CARDS – (free format) – series of values of

(K,ECAL(K),SIGCAL(K)) separated by a comma, finishing with /.

where K = reaction number (see Table 1)

ECAL(K) = point energy of the datum (MeV)

SIGCAL(K) = cross-section value ( mb ).
```

Only the cross-sections with available data have to be written.

EOF: the last card of the file has to be of the format of CARD 1 with IDEN = any negative integer.

An experimental data file is available with the code. Most of the data contained in such a file come from the compilation performed by Qaim [14] based on experimental data recently published. They cover most of the activation cross-sections for the formation of radioactive products from 14.5 MeV neutron-induced nuclear reactions.

7. The group cross-section calculation.

If the option of the group average cross-section is chosen, the code calculates group cross-section values using the GAM2 group structure (App.I) with low-energy limit of 0.1 MeV (50th group) which represents the reasonable energy range of validity of the THRES-F code. The format of the output is the UKCTR-III-A library format (App.II).

The pointwise cross-section values in 0.1 MeV energy steps are interpolated with a logarithmic-logarithmic approximation and weighted with the inverse energy function.



For the Al^{27} , being out of the Z-range for which the default values of the fitting constants C_i are calculated, a negative A value was entered in order to read a new set of fitting constants. The unchanged values have been left blank. This new set of values has no physical meaning, and does not correspond to any fitting of experimental data.

In order to utilize again the default C_i constant values, those which have been changed have to be reassigned for the successive isotope, $Nb^{\,93}$ in the present example.

In App.IV some parts of the output listing of such a calculation are shown. The meaning of the symbols used is given in section 3.

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APPENDIX I

GAM-II multigroup energy structure: definition of the first 50 groups

_	Energy Range (eV) 1.3499E+07 to 1.4918E+07 1.2214E+07 to 1.3499E+07 1.1052E+07 to 1.2214E+07 1.0000E+07 to 1.1052E+07 9.0484E+06 to 1.0000E+07	Y YY YY
Group	Energy Range (eV)	Lethargy Width
1	1.3499E+07 to 1.4918E+07	0.100
2	1.2214E+07 to 1.3499E+07	0.100
2 3 4	1.1052E+07 to 1.2214E+07	0.100
4	1.0000E+07 to 1.1052E+07	0.100
5	9.0484E+06 to 1.0000E+07	0.100
6	8.1873E+06 to 9.0484E+06	0.100
ž	7.4082E+06 to 8.1873E+06	0.100
8	6.7032E+06 to 7.4082E+06	0.100
9	6.0653E+06 to 6.7032E+06	0.100
10	5.4881E+06 to 6.0653E+06	0.100
11	4.9659E+06 to 5.4881E+06	0.100
12	4.4933E+06 to 4.9659E+06	0.100
13	4.0657E+06 to 4.4933E+06	0.100
14	3.6788E+06 to 4.0657E+06	0.100
15	3.3287E+06 to 3.6788E+06	0.100
16	3.0119E+06 to 3.3287E+06	0.100
17	2.7253E+06 to 3.0119E+06	0.100
18	2.4660E+06 to 2.7253E+06	0.100
19	2.2313E+06 to 2.4660E+06	0.100
20	2.0190E+06 to 2.2313E+06	0.100
21	1.8268E+06 to 2.0190E+06	0.100
22	1.6530E+06 to 1.8268E+06	0.100
23	1.4957E+06 to 1.6530E+06	0.100
24	1.3534E+06 to 1.4957E+06	0.100
25	1.2246E+06 to 1.3534E+06	0.100
26	1.1080E+06 to 1.2246E+06	0.100
27	1.0026E+06 to 1.1080E+06	0.100
28	9.0718E+05 to 1.0026E+06	0.100
29	8.2085E+05 to 9.0718E+05	0.100
30	7.4274E+05 to 8.2085E+05	0.100
31	6.7206E+05 to 7.4274E+05	0.100
32	6.0810E+05 to 6.7206E+05	0.100
33	5.5023E+05 to 6.0810E+05	0.100
34	4.9787E+05 to 5.5023E+05	0.100
35	4.5049E+05 to 4.9787E+05	0.100
36	4.0762E+05 to 4.5049E+05	0.100
37	3.6883E+05 to 4.0762E+05	0.100
38	3.3373E+05 to 3.6883E+05	0.100
39	3.0197E+05 to 3.3373E+05	0.100
40	2.7324E+05 to 3.0197E+05	0.100
41	2.4724E+05 to 2.7324E+05	0.100
42	2.2371E+05 to 2.4724E+05	0.100
43	2.0242E+05 to 2.2371E+05	0.100
44	1.8316E+05 to 2.0242E+05	0.100
45	1.6573E+05 to 1.8316E+05	0.100
46	1.4996E+05 to 1.6573E+05	0.100
47	1.3569E+05 to 1.4996E+05	0.100
48	1.2277E+05 to 1.3569E+05	0.100
49	1.1109E+05 to 1.2277E+05	0.100
50	8.6517E+04 to 1.1109E+05	0.250
50	0.0317ET04 to 1.1109ET03	0.230

APPENDIX II

<u>UKCTR-III-A Format</u> A Segment of a Data Retrivial Routine [6]

```
C INPUT data on Stream INP.
C IABC(I): ARRAY FOR REACTION DESCRIPTION
C NUCL: PARENT NUCLIDE DESCRIPTOR
C (NOTE ABBREVIATED FORM = 5022 = 50 SN122)
C NAME: PARENT NUCLIDE DESCRIPTOR
C (NOTE EXPANDED FORM = 50122 = 50 SN122)
C IR: REACTION TYPE
C NGP: NUMBER OF NON-ZERO CROSS-SECTIONS
C CROSS(I): GROUP REACTION CROSS-SECTION VALUES
C DIMENSION IABC(14),CROSS(100)
READ(INP,9000,END=1000) NUCL,IR,NGP,IABC
CALL TRNSLT (NAME,NUCL)
READ(INP,9100) (CROSS(I),I=1,NGP)
NGP1=NGP+1
DO 20 I=NGP1,100
20 CROSS(I)=0.0
C INSERT REQUIRED PROCESSING ROUTINE HERE
C GOTO 10
1000 STOP
9000 FORMAT(316,10A4,A2,3A4)
9100 FORMAT(6E12.5)
END
C SUBROUTINE TRNSLT(NAME,NUCLID)
IZ=NUCLID/100
IA=NUCLID-IZ×100
IF (IA.LT.IZ) IA = IA+100
IF (IA.LT.IZ) IA = IA+100
NAME=1000×IZ+IA
RETURN
END
```

APPENDIX III

JCL and INPUT Data for the THRES-F Code Example of Group Cross-section Calculation

```
// JDB (,), 'USER KXSLGC/CULHAM', TIME= (0,39), MSGCLASS=X, NDTIFY=MPHLGI
/#JOBPARM POINT=9, LINES=10
//宝
//3
              ************* THRESF *************
1/3
                   JCL FOR RUNNIG THRESF CODE
//%
                       SAMPLE CALCULATION
1/3
       //宝
//STEP1 EXEC RUNLIB, REGION.G=512K, MEMBER=FORTCODE, PRINT=X
//STEPLIB DD DSN=MPHLGI.THRESF.LDAD, DISP=SHR
13
//G.FT06F001 DD SYSDUT=X
//G.FT01F001 DD
                 DUMMY
//G.FT02F001 DD DUMMY
//G.FT03F001 DD DSN=MPHLGI.THRESF.DATA2(SAMPLE), DISP=(OLD, KEEP)
//G.FT08F001 DD
                 DSN=MPHLGI.THRESF.DATA3 (RENDRM), DISP= (OLD, KEEP)
//G.SYSIN DD #
27, 59, 5, 1, 0, 1, 1/
SN
50,120/
AL
13, -27/
1.452, 11.0, , 13.0, 0.08, , , , -2.0, , , , 1.45, /
41, -93/
1.452, 12.0, 12.0, 0.1, ,, -2.5, ,, 1.5, /
23,51/
13
```

APPENDIX IV

Example of the OUTPUT of THRES-F Code

CG- 59 Z= 27 N= 32 NORM= 1 IREN= 1 AMMERIANHERMENHERM	家家家家家家家家家家家家家家家家家家家家家家家家家家家家家家家家家家家家	k K		k k k			K K K					
24 ,A= 59 24 ,A= 59 24 ,A= 59 THE ISOTOPE 27059 1,450000E+01 MEV 7.2102 4 1.450000E+01 MEV 7.7430 1,450000E+01 MEV 7.7430 1,450000E+01 MEV 7.7430 1,450000E+01 MEV 7.2102 1,450000E+01 MEV	65 -00	=7	27	۳	32	NORM		HPEN	H			
24 ,A= 59 OR THE ISOTOPE 27059 THE ISOTOPE 27059 A	****	××××	* *	*	****	* * *	* * * *	****	* *			
POINT, REACT.NB. = 4 1.450000E+01 MEV 7.2102	MASS NOT IN	MAPS	TRA	TABLE	FOR Z		4					
POINT, REACT.NB.= 4 1.450000E+01 MEV 7.2102 POINT, REACT.NB.= 6 1.450000E+01 MEV 7.4738 POINT, REACT.NB.= 6 1.450000E+01 MEV 7.7438 POINT, REACT.NB.= 13 1.450000E+01 MEV 7.6827 POINT, REACT.NB.= 13 1.450000E+01 MEV 7.6827 POINT, REACT.NB.= 14 1.450000E+01 MEV 7.6827 POINT, REACT.NB.= 15 1.450000E+01 MEV 7.6827 POINT, REACT.NB.= 16 1.450000E+01 MEV 7.6929 ROOM NB.: 4 RENORMALISATION FACTOR= 1.97183E+00 N NB.: 5 RENORMALISATION FACTOR= 1.97466E+00 N NB.: 6 RENORMALISATION FACTOR= 1.27446E+00 N NB.: 6 RENORMALISATION FACTOR= 1.27446E+00 N NB.: 16 RENORMALISATION FACTOR= 1.27446E+00 N NB.: 16 RENORMALISATION FACTOR= 1.27446E+00	NO RENORMA	LISAI	LON	DATA	POUND	70 P	분	SOTOPE	27059		*	
POINT, REACT.NB.= 7 1.450000E+01 MEV 5.5646 POINT, REACT.NB.= 8 1.450000E+01 MEV 3.0821 POINT, REACT.NB.= 13 1.450000E+01 MEV 3.0827 POINT, REACT.NB.= 16 1.450000E+01 MEV 3.0827 POINT, REACT.NB.= 16 1.450000E+01 MEV 3.0827 REACT.NB.= 16 1.450000E+01 MEV 9.9999 REACT.NB.= 16 1.0749E+00 9.9999 N NB.: 4 RENORMALISATION FACTOR= 1.97183E+00 N NB.: 6 RENORMALISATION FACTOR= 1.27446E+00 N NB.: 6 RENORMALISATION FACTOR= 1.27446E+00 N NB.: 13 RENORMALISATION FACTOR= 1.27446E+00 N NB.: 13 RENORMALISATION FACTOR= 1.27446E+00 N NB.: 13 RENORMALISATION FACTOR= 1.27446E+00	CALIBRATION CALIBRATION CALIBRATION		;;;	<u> </u>	EACT.NB EACT.NB	8 03 8	4100	1.45	0000E+01			
1.440 BARNS 1.440 BARNS ENORMALISATION FACTOR= 1.07496E+00 ENORMALISATION FACTOR= 2.45278E-02 ENORMALISATION FACTOR= 2.45278E-02 ENORMALISATION FACTOR= 3.45278E-02 ENORMALISATION FACTOR= 3.45278E-02 ENORMALISATION FACTOR= 7.2446E+00 ENORMALISATION FACTOR= 7.4541E+00 ENORMALISATION FACTOR= 7.4541E+00	CALIBRATION CALIBRATION		<u> </u>	œ 0x 0	EACT.NB		N 0 F	444	000000000000000000000000000000000000000			
1.440 BARNS ENORMALISATION FACTOR= 1.07498E+00 ENORMALISATION FACTOR= 2.45278E-02 ENORMALISATION FACTOR= 6.4523E-02 ENORMALISATION FACTOR= 1.27446E+00 ENORMALISATION FACTOR= 1.27446E+00 ENORMALISATION FACTOR= 1.27446E+00	CALIBRATION		Ļ	~	EACT. NB		1 40	1.4.	000000			
NB.: 4 RENORMALISATION FACTOR= NB.: 5 RENORMALISATION FACTOR= NB.: 6 RENORMALISATION FACTOR= NB.: 6 RENORMALISATION FACTOR= NB.: 15 RENORMALISATION FACTOR= NB.: 15 RENORMALISATION FACTOR= NB.: 16 RENORMALISATION FACTOR=	NONELASTIC	CROSS	S	HION		60 BA	S				0-15 MEV XSECTS	CALCULATED
	REACTIO REACTIO REACTIO REACTIO REACTIO REACTIO		m m		R R R R R R R R R R R R R R R R R R R	LISAT LISAT LISAT LISAT LISAT LISAT		A A C C C C C C C C C C C C C C C C C C	1.97163 2.452163 0.6732163 7.67446	10000000000000000000000000000000000000		

CO- 50 NI DA NI DA NORTH LA LORDINA DE LE LORDINA LORD

	DELTA SIGMA	4403E+	.4403E+0	- 4400E+	.4327E+0	.3929E+	.1429E+	.329	.2296E-	.7818E-0	.6143	.5602E-0	1	Ė	.5419E-	SOA7F.	4740E	.4412E-	.4092E-	80E-	3476E-	79E	2890E-	.2608E-	332E-	.2063E-	BOIE-	.1343E	.1292E-	.1045E-		566	E-0	.0103E-	-9876E-	9653E-	.9432E-	.9214
-0.330	OKN, HE&	+ 0.0			0	- 66	.12-	.36-	- 62-	-68.	.18-	- 6	!	.12-	.16-	.19-	. 21-	. 23-	.25-	- 56-	. 56-	.27-	.27-	3.26- 2	. 52-	. 24-	. 23-	. 51.	61.	.17-	.14-	-11-	-00-	.05-	.02-	-86-	.95-	0.
11.590	7×N, HE3	0.0				•	•	+	÷ •	÷ 0.	÷ •	÷ •	1	-09.	.71-	.83-	-26	-80.	. 22-	.38-	- 24-	-17.	- 68 -	6	- 90	.52-	- 9/ .	-10.	9 1	.57-	- 88 -		. 26 -	- 56.	-34-		. 23-	.72-
6.922	L'N×9	+ + 0 0				* ·	+	+	+	+ 0.	+	+	l i	-90.	. 54-	.45-		-19.	-10.	. 53-	-45-	-69	. 63.	5.17- 4	-64	. 60				. 63.	. 13-	.43-	- 56-	-90.	-38-	-02-	.03-	
5.134	O'N×5	++					•	+	•	•	÷ 0.	+	;	.14-	-91.	.18-	- 50-	. 23-	. 54-	. 56.	. 29	-00	.35-	1.33- 1		000	0 0			75		- 55	- 45-	-95.	-47-	- 69-	-65.	. 20-
0.761	4*N*4	++							•	- 65	- 66.	-96-	1	-90.	1.	.02-	-00.	- 98 -	- 67-		.30.	- 27	. 76	8.75- 2				1 1				.37-	-12	.03-	-06.		-19.	
19.007	NE 'NXE	++		+						•		+	!	÷ 0.	÷ •	•	÷ 0.	•	•	• •		• •	• •	0 6								•		•	÷ •	+ •	+	÷
10.441	2*N, 2N	++	+	+						•	•	+	1	- 58	. 72-	.00	- 03-	. 10	- 22.		0 0	2/4	9 10	1.40	0 5		1 7 7	14		1 4		0 0	. 77	- 52	-92-	-16.	. 96.	.01-
0.0	Z X X	0.0 + 0	2.22. 6	7.53- 3	6 71- 9	0 0	7	2.07	1	6.61-1	1 -0/.0	6.81-1	1	3.30- 1	13	2.96-1	0	2.65- 1	7 !	7.37.0	* .	1 1 2 1 2 1 2	3 6	1 .00.1		0 0	2	3		1	3 :	1,	1	1.05-1	2 -06.6	9.33- 2	8.79- 2	8.26- 2
BE:	E(MEV)	0.0 + 0	- 00	-00				0 0	0 1		- 0	+ 00	1	~	.27+	- 58	+ 50	+ 000		144	100	7 2 2		101	4 6	000	+04	414	467	417				000	+/4.	404	+ -	+04.

96:	7.357	15.177	16.564	20.241	6.928	7.357	12.515	6.928	9.746	15.177	9.746
E(MEV)	dw.N×6	10*N, ND	11*N,NT	12*N, NHE3	J3KN, NHE4	14*N, PN	15*N,2P	16×N, HE4N	17*N, HE&P	18KN, DN	19×N, PHE4
1.00-1	* *	* *	**	0 · · ·	0.0	0.0	0.0	•	÷		÷
-00.	÷ 0.	+	+	+	• •		• •	÷ ·			÷ 0.
-00.	÷ •	÷ 0.	÷ 0.		+			• •	• •	• •	
-00	÷ 0.	÷ •	* 0.	*	+	•	- 4				•
-00.	÷ •	+	÷ 0.	+ 0.	+					÷ •	
-00.	÷ 0.	÷ 0.	* 0.	*	*						÷
-00.	÷ •	÷ ••	+ 0.	+	+	•		- 4	• •	•	
-00.	÷ ••	÷ 0.	+ 0.	+ 0.	+ 0	•					•
-00	÷	÷ 0.	* 0.	.0	+	+	+		• •	• •	• •
• 00 •	÷	•	÷	÷ •	÷ •	.0	÷ •		0 + 0 0	0.0	* *
j t	1	1	0	9	0	0	1	1	1	8	
1.26+ 1	.68-	•	÷ 0.	*	.23-	-69-	*		6	•	
4/2.	- 9/	÷	÷ • •	÷ 0.	.30-	-20.	+	.62-1	. 95		90
. 20	-92		÷ •	+	.38-	.25-	.18-	0.4-1	70.		
. 29	- 63-		÷ •	+ 0.	. 47-	.43-	.36-	. 24-1	- 90		100
	- 20.			÷	- 95.	-19.	- 41-	.56-1	.35.	*	0
	177.			*	-99.	- 20-	- 69-	1-06.	-65-	*	. 69
124		• •			- 26 -	-96-	- 54-	.24-1	-96.	0.	-00
1 7					.67-	.16-	.61-	.59-1	- 53-	.0	.75-
35+	52-		• •	• •	- 96 -	. 77	-69-	.95-1	.63-	÷ •	.03-
.36+	.65-	•				. 25.	. 76.	.31-1	-66.	÷ •	-01.
.37+	.73-	+	+	*	196	88-	900	.67-1	190	÷ ·	-16-
.38+	.85-	÷ 0.	÷ •	÷ 0.	.52-	- 50	.02-	1 - 1 - 1	14.	• •	. 24.
• 30	-96-	+	÷ 0.	÷ 0.	.69.	.22-	12-	79-1	57-	• •	. 27.
404	3.08-2	+ +	• • •	÷ •	95	5.39- 2	3.23- 4	0.16-14	8.00- 4	0.0	0
404					20.	- 20-	.34-	.53-1	.45-	÷ •	.57-
424	- 46-	•	. +		-12.	.72-	- 45-	1-06.	-16.	÷ 0.	-62-
+99.	.58-	+	*		7 1	000	1001	. 27-1	-39-		-22-
.454	.72-	+ 0.	+	+	.05	101	92. 4	1000		• •	-99-
+94.	.85-	÷ 0.	+	+ 0.	-60	146-	4	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	2 0		-00
.474	-96.	+	÷ •	÷ •	.35-	-65	.15-	.07-1	14.	• •	12.
+00.	-15-		+	÷	.62-	-63-	.32-	.11-1	- 10-	+	10
	- 02.	•		÷ •	- 16.	- 94.	-69.	14-1	.25-	+	-54-
*05.	- 00	÷	÷	÷ •	.21-	ċ	,	1.17-13	.30-	÷ •	- 20-

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THE LAST BY ON THE PARTY AND T	TMP.ENERGY LIMIT = 0.1061637E+08	EV CAL.EN.E O.O MEV
2759 27059 1 4 CO	39 (M,2N) CO S6	7-80GH
S.4726672E-01 3.9050251E-01 1.557	1.55780972-01 5.38604712-03	
京学 医迪德耳巴丁 医克耳耳耳耳耳耳耳耳耳		
BH JAE 27059 KN= 4 NP= 144 THR.ENE	THP.ENERGY LIMIT = 0.7938042E+06	EV CAL.EN.=14.50 MEV
2789 27089 3 30 CO	3 59 (N.P) PE 59	TWRES-P MSYS
7.7183425E-02 1.0120231E-01 1.191 9.0670347E-02 7.5455129E-02 6.0200 2.2366996E-02 1.7811500E-03 1.4345 7.0344221E-03 6.1297156E-03 5.3937 3.3912916E-03 3.3170027E-03 3.0868	1.1915779E-01 1.2422878E-01 6.0200350E-02 4,7114565E-02 1.4345579E-02 1.1699997E-02 5.3937621E-03 4,8002899E-03 3.0868468E-03 2.8908926E-03	1.1846077E-01 1.0635078E-01 3.6607429E-02 2.8501242E-02 9.7370185E-03 8.2284771E-03 4.3178534E-03 3.9434037E-04
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une Jas 27059 KNz 8 NP= 151 TWP.ENE	TMP.EMERGY LIMIT = 0.0	EV CAL.EN.=14.50 MEV
£759 £7059 & 50 CO	59 (N,A) MN 56	THRES-P ASYS
3.1445406E-02 3.1674389E-02 8.574 3.923463E-03 2.4636495E-03 1.6153 4.0175626E-04 3.0723005E-04 8.4084 1.179867E-04 3.0723005E-04 8.4084 3.4791261E-05 3.625286E-05 4.6580 3.4399670E-05 3.4661774E-05 3.3117 2.6513634E-05 2.7670627E-05 2.6853 2.426198E-05 2.3003871E-05 2.0828	2.5749698E-03 1.7317060E-02 1.6155331E-03 1.0712417E-03 2.4054926E-04 1.9312868E-04 6.4076668E-05 7.432944E-05 3.3117321E-03 3.1764124E-05 2.695592E-03 2.6650929E-03	1.0769900E-02 6.4486079E-03 7.4806786E-04 5.4002670E-04 6.462904E-05 6.002428E-04 4.0730794E-05 5.949399E-03 3.0565949E-05 2.9493604E-03 2.5487447E-05 2.4868306E-03 1.7059429E-05 1.5430283E-05

CAL. EN. = 14.70 MEV
0.5220661E+07 EV
LIMIT =
THR. ENERGY
66
N NP
N N
** JA= 27059

S	2.3933448E-02
THRES-F *SYS	3.8794063E-02 1.0040447E-03
CO 59 (N,D) FE 58.	6.9659393E-02 6.1086748E-02 6.2314495E-03 6.2232648E-03
11	1.1897701E-01 9.4836764E-03
2759 27059	1.4117497E-01 1.4690548E-02

		CAL.EN.=14.50 MEV	ø	7.0640817E-04 3.8164575E-04 2.2998024E-04 1.5521297E-04
		E Z	× ×	90
			THRES-F *SYS	2998024E-
		7		ณ
		THR.ENERGY LIMIT = 0.7045801E+07 EV	រវា	164575E-04
		.,	Σ	ω.
		LIMIT	CO 59 (N,NA) MN 55	2-04
		RGY	60	0817
	M.	THR. ENE	8	
-	×			50.0
	京京京京京京京京京京京京京京京京京京京京京京京京京京京京京京京京京京京京	. 160	Φ.	1.4622519E-03 3.9418650E-05
	×	S.		1665
	X X		•0	3.94
	*	ä	59	
		7059	270	8E-0
		*** JAz 27059 KN= 13 NP: 61	2759 27059	3.3184558E-03
		*	Q	170
		×		. H

r ev CAL.EN.=14.50 MEV	THRES-F *SYS	4.4570261E-05
0.9073208E÷07	E 37	9804555E-03
*** JA= 27059 KN= 6 NP= 61 THR.ENERGY LIMIT = 0.9073208E+07 EV	CO 39 (N,T) PE 37	6.8871304E-04 3.5678176E-04 1.7668353E-04 8.9804555E-05 4.4570261E-05
T 6 NP 1 61	D)	3.5678176E-04
*** JA= 27059 KN	2759 27059 7	6.8871304E-04

>		
E		
CAL.EN.=14.50 MEV	THRES-F *SYS	
™		
THR.ENERGY LIMIT = 0.1178605E+08 EV	57	
•	Z Z	
,,	9	
LIMII	CO 59(N, HE3) MN 57	2-07
SG.	ę,	7886
- HE NEW - EN NEW - E	8	4.7465974E-06 1.9454437E-06 3.4847886E-07
đ	m	37E-06
II D. Z		544
~	٥	1.94
II Z ¥	•	
60/	2759 27059	4E-06
N T	759	5897
r t	N	.74
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		5.973320E-03 BARNS 1.420760E-03 BARNS 3.004537E-05 BARNS 3.60544E-06 BARNS 4.409998E-03 BARNS 4.409998E-04 BARNS 2.009159E-04 BARNS 9.999998E-14 BARNS	0-15 MEV XSECTS CALCULATED	
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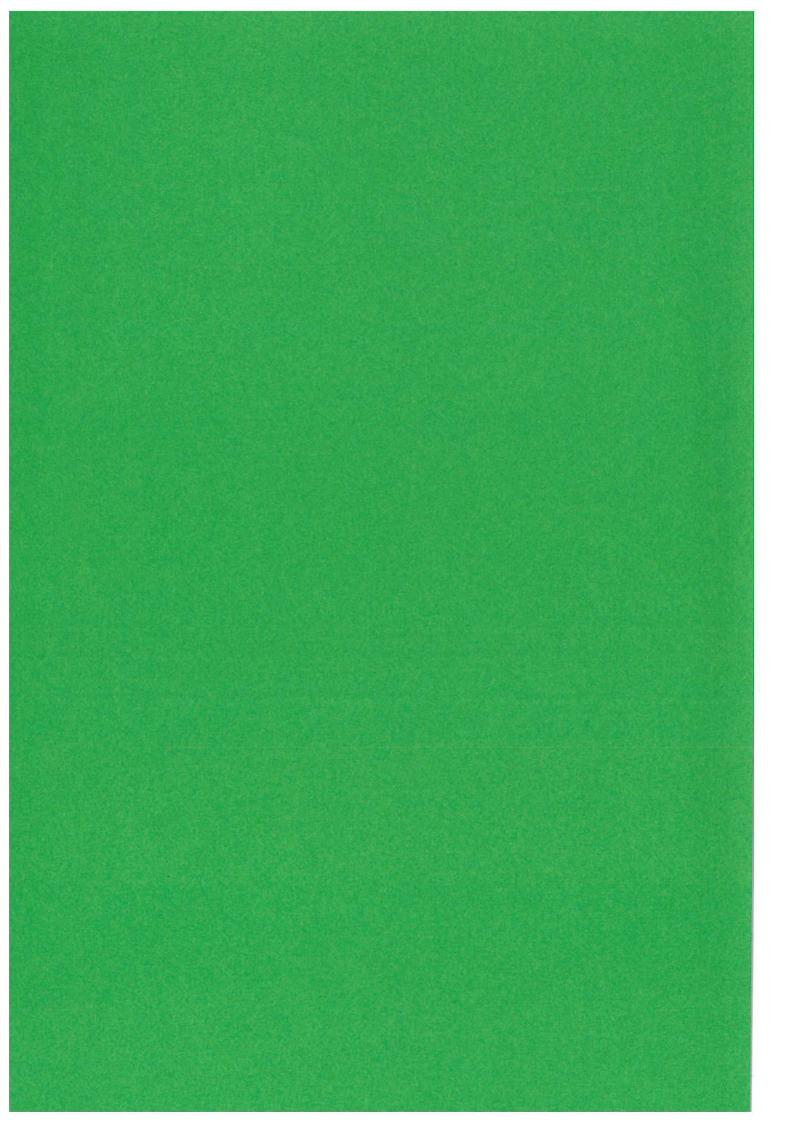
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S= 0.0980



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