

JAERI - M  
84-192

NEANDC(J) 107/AU

INDC(JPN) 93/GL

PROGRAM RESEDD (VERSION 84-07) : A PROGRAM  
FOR RECONSTRUCTION OF RESONANCE CROSS  
SECTIONS FROM EVALUATED NUCLEAR DATA  
IN THE ENDF/B FORMAT  
(MODIFIED VERSION OF RESEND)

October 1984

Tsuneo NAKAGAWA

日本原子力研究所  
Japan Atomic Energy Research Institute

JAERI-Mレポートは、日本原子力研究所が不定期に公刊している研究報告書です。  
入手の間合わせは、日本原子力研究所技術情報部情報資料課（〒319-11茨城県那珂郡東海村）あて、お申しこしてください。なお、このほかに財団法人原子力弘済会資料センター（〒319-11茨城県那珂郡東海村日本原子力研究所内）で複写による実費頒布をおこなっております。

JAERI-M reports are issued irregularly.

Inquiries about availability of the reports should be addressed to Information Section, Division of Technical Information, Japan Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki-ken 319-11, Japan.

©Japan Atomic Energy Research Institute, 1984

編集兼発行 日本原子力研究所  
印刷 株高野高速印刷

Program RESEND (Version 84-07) :

A Program for Reconstruction of Resonance Cross Sections  
from Evaluated Nuclear Data in the ENDF/B Format  
(Modified Version of RESEND)

Tsuneo NAKAGAWA

Department of Physics, Tokai Research Establishment, JAERI

( Received September 25, 1984 )

RESEND is a computer program to calculate resonance cross sections from evaluated resonance parameters in the ENDF/B format. This program was improved from RESEND by modifying the multi-level Breit-Wigner formula, adding a function of Doppler broadening, and so on. This report explains functions of RESEND and describes input data. Some examples are also given.

Keywords : Computer Program, Resonance, Neutron Cross Section, Evaluated Data, ENDF/B format, Doppler Broadening.

プログラムRESEND (84-07版)

ENDF/Bフォーマットの評価済みデータから共鳴断面面積を求めるためのプログラム (RESENDの改良版)

日本原子力研究所東海研究所物理部

中川庸雄

(1984年9月25日受理)

RESENDはENDF/Bフォーマットの評価済み共鳴パラメータから共鳴断面面積を計算するための計算機プログラムである。このプログラムはRESENDを改善したもので、Breit-Wigner多準位公式の改良、ドップラー効果の計算機能の追加などが行われた。本報告はRESENDの機能および入力データの説明を行うものである。いくつかの使用例も同時に示される。

## Contents

1. Introduction .....	1
2. Calculation of Cross Sections at Zero Kelvin .....	3
2.1 Resonance Formulas .....	3
2.2 Effective Scattering Radius .....	7
2.3 Energy Points and Accuracy of Calculated Curves .....	10
2.4 Approximation of Distant Resonances .....	13
2.5 Interpolation in Unresolved Resonance Region .....	13
2.6 Lowest Value of Calculated Cross Sections .....	14
3. Calculation of Doppler Broadened Cross Sections .....	14
3.1 Numerical Integration .....	15
3.2 Data Handling in RESEDD .....	18
4. Input Data .....	20
4.1 JCL for JAERI FACOM-M 380 Computer System .....	20
4.2 Input Data .....	21
5. Examples .....	24
Acknowledgments .....	27
References .....	27
Appendix .....	45

## 目 次

1. 緒 言	1
2. 0 Kでの断面積の計算	3
2.1 共鳴公式	3
2.2 実効散乱半径	7
2.3 エネルギー点と計算結果の精度	10
2.4 遠方レベルの近似	13
2.5 非分離共鳴領域における内挿	13
2.6 計算された断面積の最小値	14
3. ドップラー効果を考慮した断面積の計算	14
3.1 数値積分	15
3.2 RESENDDDでのデータ処理	18
4. 入力データ	20
4.1 原研FACOM-M 380 計算機のJCL	20
4.2 入力データ	21
5. 使用例	24
謝 辞	27
参考文献	27
付 録	45

## 1. Introduction

In the ENDF/B format<sup>1,2)</sup>, evaluated neutron cross sections in a resonance region are stored as a set of resonance parameters and so called background cross sections. This method is very effective to reduce a size of evaluated data files. On the other hand, a computer program is needed to reconstruct cross sections in the whole neutron energy region. For this purpose, the program RESEND<sup>3)</sup> was made by Ozer. We introduced RESEND from BNL and used it for reconstruction of resonance cross sections and for evaluation work of the Japanese Evaluated Nuclear Data Library (JENDL). However, it was found that RESEND had the following inconvenience;

- (1) It takes a long CPU time in treating the multi-level Breit-Wigner formula.
- (2) RESEND cannot treat the Reich-Moore formula.
- (3) RESEND reconstructs cross sections only at zero Kelvin.

In addition to them, some minor errors were found. Therefore the modification of RESEND was made, and finally the program RESENDDD was developed.

The work of RESENDDD is separated into two steps, that is, 1) calculation of zero-Kelvin cross sections and 2) calculation of the Doppler broadened cross sections. In the first step, RESENDDD has the following new functions.

- (1) Both ENDF/B-IV and ENDF/B-V formats are available for an input file.
- (2) Calculation method of the multi-level Breit-Wigner formula was improved not to take a long CPU time and to permit J-unknown

resonances.

- (3) An energy dependent scattering radius can be treated.
- (4) Resonance parameters for the Reich-Moore formula can be processed.
- (5) Modification of energy selection method was made.
- (6) Option for interpolation in the unresolved resonance region was introduced.
- (7) Distant resonances can be treated approximately.

The cross sections calculated from resonance parameters are tentatively stored in a scratch disk, and then they are combined with the background cross sections and connected to cross sections outside of the resonance region. Cross sections thus obtained are the total, elastic scattering, fission and radiative capture cross sections. If the nonelastic, (n,f) (first chance fission), and/or neutron disappearance cross sections are given in an input file, the resonance contributions are also added to them. This first step will be described in Chapter 2.

If the Doppler broadening is required, broadened cross sections are calculated in the second step, by means of numerical treatment of the broadening equation. This method is almost similar to that used in the program SIGMA1<sup>4)</sup> made by Cullen. The Doppler broadening is performed by using pointwise data obtained in the first step or those in an input file. Therefore the broadening is carried out independently of resonance formulas. Chapter 3 describes the Doppler broadening process.

Finally Chapter 4 explains JCL of RESEND in the JAERI computer system, and input data. Some examples are also given in Chapter 4.



## 2. Calculation of Cross Sections at Zero Kelvin

### 2.1 Resonance Formulas

A resonance region is separated into two subregions; one is a resolved resonance region and another is an unresolved resonance region. In the ENDF/B-IV format<sup>1)</sup>, the following four formulas are allowed in the resolved resonance region,

- 1) Single-level Breit-Wigner formula,
- 2) Multi-level Breit-Wigner formula,
- 3) Reich-Moore formula, and
- 4) Adler-Adler formula.

Among them, the Reich-Moore formula is not allowed in the ENDF/B-V format<sup>2)</sup>. On the other hand, only one formula is available in the unresolved resonance region, with a few methods of representation of average resonance parameters. These formulas are precisely described in Refs. 1 and 2. RESEND also accepts almost the same formulas. A function which calculates cross sections with the Reich-Moore formula was not included in the original RESEND. In RESEND, this function was added by referring to the ENDF/B format processing program RAMP1<sup>5)</sup>.

#### Multi-level Breit-Wigner formula used in RESEND

As is well known, in the case where the single-level Breit-Wigner formula is adopted, negative values often appear in the elastic scattering and the total cross sections. In order to avoid the negative cross sections, resonance interference terms should be taken into account, that is, the multi-level Breit-Wigner formula should be used. In the

original RESEND, contributions from the interference terms are calculated as follows.

$$\frac{\pi}{k^2} \sum_J g_J \sum_{r=2s+1}^{NR} \sum_{s=1}^{r-1} \frac{2\Gamma_{nr}\Gamma_{ns} \{ (E-E_r') (E-E_s') + \Gamma_r\Gamma_s/4 \}}{\{ (E-E_r')^2 + \Gamma_r^2/4 \} \{ (E-E_s')^2 + \Gamma_s^2/4 \}} \quad (2.1)$$

However, the calculation of this takes a lot of CPU time and in the case where J values of some resonances are unknown, this calculation cannot be performed.

In RESEND, the formula was modified to accept also resonances whose J value is unknown, by applying a statistical way of distribution of their contributions to possible J states. At the same time, the CPU time for computation of the resonance interference terms was reduced very much by changing the formula as follows. Derivation of Eq. (2.2) will be shown in Appendix.

#### 1) Elastic scattering cross section

$$\begin{aligned} \sigma_{n,n}(E) = & \frac{\pi}{k^2} \sum_l^{NL} \{ 4(2l+1) \sin^2 \varphi_l + \sum_J^{NJ} g_J \{ (F_{J1})^2 + (F_{J2})^2/4 + 2\sin 2\varphi_l \times F_{J1} \\ & - (1 - \cos 2\varphi_l) F_{J2} + P_{J1} (1 - P_{J1}) f_0 \\ & - P_{J1} (1 - P_{J1}) (f_1^2 + f_2^2/4 - f_0) / (N_{Rl} - 1) \} \}, \end{aligned} \quad (2.2)$$

where

$$F_{J1} = \sum_r^{NRJ} \frac{\Gamma_{nr} (E - E_r')}{(E - E_r')^2 + \Gamma_r^2/4} + P_{J1} f_1, \quad (2.3)$$

$$F_{J2} = \sum_r^{NRJ} \frac{\Gamma_{nr} \Gamma_r}{(E - E_r')^2 + \Gamma_r^2/4} + P_{J1} f_2, \quad (2.4)$$

$$f_0 = \sum_u^{NRL} \frac{\Gamma_{nu}^2}{(E - E_u')^2 + \Gamma_u^2/4}, \quad (2.5)$$

$$f_1 = \sum_u^{NRL} \frac{\Gamma_{nu} (E - E_u')}{(E - E_u')^2 + \Gamma_u^2/4}, \quad (2.6)$$

and

$$f_2 = \sum_u^{NRL} \frac{\Gamma_{nu} \Gamma_u}{(E - E_u')^2 + \Gamma_u^2/4}. \quad (2.7)$$

In the above equations, symbols used have the following meaning.

- NL the number of  $\ell$ -states.  
 NJ the number of J-states for a particular  $\ell$ -state.  
 NRL the number of  $\ell$ -state resonances whose J value is unknown.  
 NRJ the number of  $\ell$ -state resonances whose J value is known.  
 k the neutron wave number.

$$k = 2.196771 \times 10^{-3} \frac{AWR}{AWR+1} \times \sqrt{E(\text{eV})}.$$

- $g_J = (2J+1)/2(2I+1)$ , where I is the spin of a target nuclide.  
 E an incident neutron energy in the laboratory system (eV).  
 $E_r$  the  $r$ -th resonance energy (eV).  
 $E_r'$  a shifted energy (eV) of the  $r$ -th resonance calculated as follows,

$$E_r' = E_r + \frac{S_l(|E_r|) - S_l(E)}{2P_l(|E_r|)} \times \Gamma_{nr}(|E_r|).$$

- $\Gamma_{nr}$  the neutron width (eV) of the  $r$ -th resonance, calculated at an incident energy of E (eV) as follows.

$$\Gamma_{nr} = \frac{P_l(E)}{P_l(|E_r|)} \times \Gamma_{nr}(|E_r|),$$

where  $\Gamma_{nr}(|E_r|)$  is the neutron width at the resonance energy  $E_r$  and given in an input file.

- $\Gamma_{fr}$  the fission width (eV) of the  $r$ -th resonance.  
 $\Gamma_{\gamma r}$  the radiative width (eV) of the  $r$ -th resonance.  
 $\Gamma_r$  the total width (eV) of the  $r$ -th resonance.

$$\Gamma_r = \Gamma_{nr} + \Gamma_{fr} + \Gamma_{\gamma r}.$$

$S_l(E)$  a shift factor (see Table 1).

$P_l(E)$  a penetration factor (see Table 2).

$\varphi_l$  a hard-sphere scattering phase shift (see Table 3).

$AWR$  weight of a target nuclide in the neutron mass unit.

neutron mass = 1.008665 u.

The sums in Eqs. (2.3) and (2.4) are carried out over resonances whose  $J$  value is known, and those in Eqs. from (2.5) to (2.7) over resonances whose  $J$  value is unknown. RESEND D considers that, if a given  $J$  value is an impossible value from the combination of  $\ell$  and  $I$  values, the  $J$  value of the resonance is unknown. Usually, the same  $J$  value as the spin of target nuclide,  $I$ , should be adopted for those resonances. The quantity of  $P_{Jl}$  in Eqs. (2.2), (2.3) and (2.4) stands for an occurrence probability of compound nucleus states with the total angular momentum of  $J$  in the combination of the target spin  $I$  and orbital angular momentum  $\ell$  of incident neutrons. In RESEND D, by assuming that it is proportional to  $(2J+1)$ ,  $P_{Jl}$  is calculated as

$$P_{Jl} = N_{Jl}g_J / \sum_J N_{Jl}g_J, \quad (2.8)$$

where  $N_{Jl}$  is the number of possible channel spins which generate the same total angular momentum  $J$ .

If  $J$  values of all the resonances are known, Eqs. (2.5), (2.6) and (2.7) are zero, and Eq. (2.2) is essentially the same as the equations given in Refs. 1 and 2.

## 2) Other cross sections

The fission and radiative capture cross sections are calculated

with the same equations as the single-level Breit-Wigner formula.

$$\sigma_{n,f}(E) = \frac{\pi}{k^2} \sum_l \sum_j^{NL, NJ} g_{lj} \sum_{r=1}^{NR} \frac{\Gamma_{nr} \Gamma_{fr}}{(E-E_r')^2 + \Gamma_r^2/4}, \quad (2.9)$$

$$\sigma_{n,\gamma}(E) = \frac{\pi}{k^2} \sum_l \sum_j^{NL, NJ} g_{lj} \sum_{r=1}^{NR} \frac{\Gamma_{nr} \Gamma_{\gamma r}}{(E-E_r')^2 + \Gamma_r^2/4}, \quad (2.10)$$

The total cross section is given as a sum of the elastic scattering, fission and radiative capture cross sections.

$$\sigma_{tot}(E) = \sigma_{n,n}(E) + \sigma_{n,f}(E) + \sigma_{n,\gamma}(E). \quad (2.11)$$

### Reich-Moore formula used in RESEDD

The Reich-Moore formula was tentatively modified a little to accept J-unknown resonances. The scattering matrix in the Reich-Moore formula is written as follows.

$$U_{n,c}^J = \exp(-i\varphi_n - i\varphi_c) \{ 2 [ (I-K)^{-1} ]_{n,c} - \delta_{n,c} \}, \quad (2.12)$$

where  $n$  and  $c$  stand for entrance and outgoing channels, and

$$(I-K)_{n,c} = \delta_{n,c} - \frac{i}{2} \sum_r \frac{\Gamma_{nr}^{1/2} \Gamma_{cr}^{1/2}}{E_r - E - i\Gamma_{\gamma r}/2}. \quad (2.13)$$

In RESEDD, by using the same quantity as Eq. (2.8), Eq. (2.13) is replaced with Eq. (2.14).

$$(I-K)_{n,c} = \delta_{n,c} - \frac{i}{2} \sum_r \frac{\Gamma_{nr}^{1/2} \Gamma_{cr}^{1/2}}{E_r - E - i\Gamma_{\gamma r}/2} - \frac{i}{2} P_{Jl} \sum_u \frac{\Gamma_{nu}^{1/2} \Gamma_{cu}^{1/2}}{E_u - E - i\Gamma_{\gamma u}/2}, \quad (2.14)$$

where the first sum is for the resonances whose J value is known and the second for J-unknown resonances.

## 2.2 Effective Scattering Radius

Energy dependence of an effective scattering radius cannot be treated in the ENDF/B format. In some cases, however, a resonance region goes up to a few hundred keV. In such a wide energy region, it is indicated from the optical model calculation that the effective scattering radius depends on neutron energies. It was investigated by Kikuchi<sup>6)</sup> that if an energy dependent scattering radius was taken into account, better fitting of calculated cross sections to experimental data could be obtained in the case of nickel isotopes.

By introducing a modified format, RESENDD can treat energy dependence of a scattering radius. The new format is consistent with the ENDF/B format in the case of an energy independent scattering radius.

According to the ENDF/B format, the general structure of resonance-parameter data is in the following format, by using the same notation as Refs. 1 and 2.

```
( MAT, 2, 151/ ZA,AWR, 0, 0,NIS, 0 ) HEAD
( MAT, 2, 151/ZAI,ABN, 0,LFW,NER, 0 ) CONT(isotope)
( MAT, 2, 151/ EL, EH,LRU,LRF, 0, 0 ) CONT(energy range)
  subsection for the first energy range of the first isotope
( MAT, 2, 151/ EL, EH,LRU,LRF, 0, 0 ) CONT(energy range)
  subsection for the second energy range of the first isotope
-----
-----
( MAT, 2, 151/ZAI,ABN, 0,LFW,NER, 0 ) CONT(isotope)
( MAT, 2, 151/ EL, EH,LRU,LRF, 0, 0 ) CONT(energy range)
  subsection for the first energy range of the NIS-th isotope
( MAT, 2, 151/ EL, EH,LRU,LRF, 0, 0 ) CONT(energy range)
  subsection for the second energy range of the NIS-th isotope
```

```
( MAT, 2, 0/0.0,0.0, 0, 0, 0, 0 ) SEND
```

The first record of each subsection is as follows;

```
( MAT, 2, 151/SPI, AP, 0, 0,NLS, 0 ) CONT
```

In order to represent the energy dependence of an effective scattering radius, the CONT(energy range) record and the first CONT record of a subsection were modified as follows. The new flag, NRO, was introduced in the CONT(energy range) record.

```
( MAT, 2, 151/ EL, EH,LRU,LRF,NRO, 0 ) CONT(energy range)
```

NRO = 0, the scattering radius is energy independent

In this case, the format is completely the same as the ENDF/B format.

```
( MAT, 2, 151/ EL, EH,LRU,LRF, 0, 0 ) CONT(energy range)
```

```
( MAT, 2, 151/SPI, AP, 0, 0,NLS, 0 ) CONT
```

NRO = 1, energy dependence of the scattering radius is given by a polynomial function

```
( MAT, 2, 151/ EL, EH,LRU,LRF, 1, 0 ) CONT(energy range)
```

```
( MAT, 2, 151/0.0,0.0, 0, 0,NTM, 0 /
```

```
P1, P2, - - -
```

```
- - - -, PNTM ) LIST
```

```
( MAT, 2, 151/SPI,0.0, 0, 0,NLS, 0 ) CONT
```

NTM is the number of coefficients of the polynomial function.  $P_i$  is the coefficient of the  $i$ -th term. The effective scattering radius  $R(E)$  in  $\text{cm}^{-12}$  at the neutron energy  $E(\text{eV})$  is calculated as follows:

$$R(E) = P_1 + P_2 E + \dots + P_{\text{NTM}} E^{(\text{NTM}-1)}$$

NRO = 2, energy dependence of the scattering radius is given as a TAB1 record

```
( MAT, 2, 151/ EL, EH,LRU,LRF, 2, 0 ) CONT(energy range)
( MAT, 2, 151/0.0,0.0, 0, 0, 1, NP /
      NP,INT, 0, 0, 0, 0 /
      E1, R1, E2, R2, - -
      - - , ENP, RNP      ) TAB1
( MAT, 2, 151/SPI,0.0, 0, 0,NLS, 0 ) CONT
```

It should be noted that this modified format is only for JAERI internal use and is not authorized in the ENDF/B format.

### 2.3 Energy Points and Accuracy of Calculated Curves

Cross sections are calculated at the energies automatically selected from resonance energies and accuracy specified by input data (see Section 4.2). At first, node energies are determined from resonance energies and upper and lower boundaries of resonance regions. The energy of 0.0253 eV is also included in the node energies if it is in the resonance region. Furthermore, additional node energies are determined from resonance energies and total widths as



$$E_n = E_r \pm 0.28868 \times \Gamma.$$

These energies are positions where the second derivative of the following curve has a value of zero.

$$f(E) = \frac{1}{(E-E_r)^2 + \Gamma^2/4}.$$

Then, an energy interval between successive two node energies is subdivided into very fine energy meshes in the following manner (so-called energy halving technique):

- (1) Cross sections at two node energies,  $E_i$  and  $E_{i+1}$ , are calculated.
- (2) Cross sections at the center of the two node energies are calculated.
- (3) Cross sections at the center of the two node energies are estimated from the cross sections calculated at the step (1), by applying a linear-linear interpolation.
- (4) Then, a test of the following inequality is done:

$$\left| \frac{\sigma(E_c) - \sigma^l(E_c)}{\sigma(E_c)} \right| < \varepsilon, \quad (2.15)$$

where  $E_c = (E_i + E_{i+1})/2$ ,  $\sigma^l(E_c)$  is the interpolated value at  $E_c$  from  $\sigma(E_i)$  and  $\sigma(E_{i+1})$ ,  $\sigma(E_c)$  is the cross section calculated from resonance parameters, and  $\varepsilon$  is an allowable error (accuracy given by input data, see Section 4.2).

- (5) If the tests of the inequalities (2.15) for the total, elastic scattering, fission and radiative capture cross sections are satisfied at  $E_c$ , it is assumed that the energy interval of  $E_i$  and  $E_{i+1}$  is small enough to obtain cross sections at any energies in this energy interval by linear interpolation within the accuracy of  $\varepsilon$ . The calculated cross sections at  $E_c$  are abandoned, and the same procedure is carried out in the next energy interval from  $E_{i+1}$  to  $E_{i+2}$ .

(6) If not satisfied,  $E_c$  is considered as a new node energy, and inserted into the string of node energies.

$$E_c \Rightarrow E_{i+1},$$

$$E_{i+1} \Rightarrow E_{i+2}, \text{ and so on.}$$

The calculated cross sections at  $E_c$  are stored as those at  $E_{i+1}$  and the procedure from (2) to (6) is repeated until the test (4) is satisfied.

In RESENDD, the following special care is paid for determination of  $E_c$  (the center energy of  $E_i$  and  $E_{i+1}$ ). In the ENDF/B format, floating numbers such as neutron energies are written with accuracy of 6 digits. Therefore the values of energies will be rounded to 6 digits when they are written on an output file. In order to avoid differences between energy values in a computer and those in an output file, energy values are always rounded to the output accuracy before calculation of cross sections. If rounded values of  $E_c$  is the same as  $E_i$  or  $E_{i+1}$  the halving technique cannot be continued any more. In such a case, Eq. (2.15) is assumed to be satisfied.

In the keV region, energy resolution of the ENDF/B format is in the order of meV. In order to reproduce correct shape of very narrow resonances in the high energy region, a more accurate format is needed for neutron energy values. For output of RESENDD, in addition to the 6-digit format, 7- and 9-digit formats are also available for neutron energy values. One of these formats is selected by input data.

In RESENDD, another method of energy determination is available. In the case of comparison of cross sections, it is convenient to calculate cross sections at the same set of energy points. An energy-point file can be specified for this purpose. The energy-point file must contain the total cross section, in the ENDF/B format, whose energies

are considered as energies where the cross sections are calculated.

## 2.4 Approximation of Distant Resonances

Generally, contributions from distant resonances are very small. To avoid consumption of CPU time for calculation of these small contributions, RESEND has the following option.

In an energy interval between two successive resonances, the distant resonances are classified by a criterion of  $\alpha$  given by input data (see Section 4.2). If the following inequality is satisfied, the  $k$ -th resonance is considered as a distant resonance.

$$| E_k - (E_i + E_{i+1})/2 | > \alpha \times \Gamma_k , \quad (2.16)$$

where  $E_k$  and  $\Gamma_k$  are the resonance energy and total width of the  $k$ -th resonance,  $E_i$  and  $E_{i+1}$  are the resonance energies of the  $i$ -th and  $i+1$ -th resonances. The contributions of distant resonances are calculated exactly at  $E_i$  and  $E_{i+1}$ . Then the cross sections at  $E$ , where  $E_i < E < E_{i+1}$ , are estimated as follows:

$$\sigma(E) = \sigma^N(E) + \frac{E - E_i}{E_{i+1} - E_i} \times \{ \sigma^D(E_{i+1}) - \sigma^D(E_i) \} + \sigma^D(E_i) , \quad (2.17)$$

where  $\sigma^N$  and  $\sigma^D$  are contributions from near and distant resonances, respectively. This option is available only for the case of the single-level Breit-Wigner formula.

It should be noted, however, that this option was introduced several years ago as an attempt to make CPU time shorter when the speed of computers were slow. This option should be used only in the case where small cross section is not important.

## 2.5 Interpolation in Unresolved Resonance Region

On the interpolation defined in the unresolved resonance region, there is confusion of interpreting its meaning. One considers that it means interpolation of unresolved resonance parameters, and another that it indicates interpolation of calculated cross sections. Refs. 1 and 2 say that the interpolation given in the unresolved resonance region is for calculated cross sections. However, for some cases where number of energies where parameters are given is too small, it seems to be better that parameters are interpolated. RESEND adopted both interpretations, and one of them is selected by input data (see Section 4.2).

## 2.6 Lowest Value of Calculated Cross Sections

If the single-level Breit-Wigner formula is applied in the resolved resonance region, negative values of the elastic scattering and total cross sections often appear. In such cases, to avoid difficulty of negative cross section handling, a lowest positive value can be set as one of input data (see Section 4.2). When calculated cross sections are written on an output file, they are compared with this value. If the calculated cross section is smaller than this, the cross section is replaced with the lowest value.

## 3. Calculation of Doppler Broadened Cross Sections

The Doppler broadened cross section,  $\sigma(E,T)$ , can be written in the following form,

On the interpolation defined in the unresolved resonance region, there is confusion of interpreting its meaning. One considers that it means interpolation of unresolved resonance parameters, and another that it indicates interpolation of calculated cross sections. Refs. 1 and 2 say that the interpolation given in the unresolved resonance region is for calculated cross sections. However, for some cases where number of energies where parameters are given is too small, it seems to be better that parameters are interpolated. RESENDDD adopted both interpretations, and one of them is selected by input data (see Section 4.2).

## 2.6 Lowest Value of Calculated Cross Sections

If the single-level Breit-Wigner formula is applied in the resolved resonance region, negative values of the elastic scattering and total cross sections often appear. In such cases, to avoid difficulty of negative cross section handling, a lowest positive value can be set as one of input data (see Section 4.2). When calculated cross sections are written on an output file, they are compared with this value. If the calculated cross section is smaller than this, the cross section is replaced with the lowest value.

## 3. Calculation of Doppler Broadened Cross Sections

The Doppler broadened cross section,  $\sigma(E,T)$ , can be written in the following form,

$$\sigma(E,T) = \frac{1}{2E} \sqrt{\alpha/\pi} \int_0^\infty dE' \sqrt{E'} \sigma(E',0) \times \{ \exp[-\alpha(\sqrt{E'} - \sqrt{E})^2] - \exp[-\alpha(\sqrt{E'} + \sqrt{E})^2] \}, \quad (3.1)$$

where  $T$  is temperature in Kelvin and

$$\alpha = AWR/kT \text{ (the Doppler width constant),}$$

$$= 11605.6 \times AWR/T \text{ (eV}^{-1}\text{),}$$

$AWR$  is mass of target nuclide in the neutron mass unit,  $k$  is the Boltzmann constant,

$\sigma(E',0)$  is a cross section at  $E'$  (eV) and zero Kelvin.

In RESEDD, Eq. (3.1) is calculated directly with almost the same numerical integration method as that applied in SIGMA1<sup>4)</sup>.

### 3.1 Numerical Integration

Eq. (3.1) can be rewritten as follows:

$$\sigma(y,T) = \frac{1}{\pi^{1/2} y^2} \int_0^\infty x^2 \sigma(x,0) \times \{ \exp[-(x-y)^2] - \exp[-(x+y)^2] \} dx, \quad (3.2)$$

where

$$x^2 \equiv \alpha E', \text{ and}$$

$$y^2 \equiv \alpha E.$$

We can use the cross sections calculated at 0 K as  $\sigma(x_i,0)$  and assume that  $\sigma(x,0)$  can be obtained by linear-linear interpolation of a given cross section table, with accuracy of  $\varepsilon$  (see Section 2.3). Therefore  $\sigma(x,0)$  can be written as follows in the range from  $x_i$  and  $x_{i+1}$ :

$$\sigma(x,0) = \sigma(x_i) + (x^2 - x_i^2) S_i, \quad (3.3)$$

where

$$S_i \equiv \frac{\sigma(x_{i+1}) - \sigma(x_i)}{x_{i+1}^2 - x_i^2}.$$

By using Eq. (3.3), Eq. (3.2) is rewritten as,

$$\sigma(y, T) = \sigma(y)^* - \sigma(-y)^*, \quad (3.4)$$

where

$$\begin{aligned} \sigma(y)^* &\equiv \frac{1}{\pi^{1/2} y^2} \int_0^\infty x^2 \sigma(x, 0) \exp[-(x-y)^2] dx, \\ &= \frac{1}{\pi^{1/2} y^2} \sum_i \int_{x_i}^{x_{i+1}} x^2 [\sigma(x_i) + (x^2 - x_i^2) S_i] \exp[-(x-y)^2] dx, \\ &= \frac{1}{\pi^{1/2} y^2} \sum_i \int_{x_i-y}^{x_{i+1}-y} (z+y)^2 [\sigma(x_i) - S_i x_i^2 + (z+y)^2 S_i] \exp[-z^2] dz, \\ &= \sum_i \{A_i [\sigma(x_i) - S_i x_i] + B_i S_i\}, \end{aligned} \quad (3.5)$$

where

$$A_i \equiv \frac{1}{\pi^{1/2} y^2} \int_{x_i-y}^{x_{i+1}-y} (z^2 + 2yz + y^2) \exp[-z^2] dz, \quad (3.6)$$

$$B_i \equiv \frac{1}{\pi^{1/2} y^2} \int_{x_i-y}^{x_{i+1}-y} (z^4 + 4yz^3 + 6y^2 z^2 + 4y^3 z + y^4) \exp[-z^2] dz. \quad (3.7)$$

Therefore if above  $A_i$  and  $B_i$  are calculated,  $\sigma(y, T)$  is easily obtained.

We define the following two functions  $F_n$  and  $H_n$ :

$$F_n(a) \equiv \frac{1}{\pi^{1/2}} \int_{|a|}^\infty z^n \exp[-z^2] dz, \quad (3.8)$$

$$\begin{aligned} H_n(a, b) &\equiv \frac{1}{\pi^{1/2}} \int_{|a|}^{|b|} z^n \exp[-z^2] dz, \\ &= F_n(a) - F_n(b). \end{aligned} \quad (3.9)$$

By using a recurrence formula of  $F_n$ :

$$F_n(a) = \frac{1}{2} \left\{ (n-1)F_{n-2}(a) + \frac{a^{n-1}}{\pi^{1/2}} \exp\{-a^2\} \right\},$$

and an error function erf(a) and a complimentary error function erfc(a):

$$\text{erf}(a) = \frac{2}{\pi^{1/2}} \int_0^a \exp\{-z^2\} dz,$$

$$\text{erfc}(a) = \frac{2}{\pi^{1/2}} \int_a^\infty \exp\{-z^2\} dz = 1 - \text{erf}(a),$$

we can calculate  $F_n(a)$  as follows:

$$F_0(a) = \frac{1}{2} \text{erfc}(|a|),$$

$$F_1(a) = \frac{1}{2\pi^{1/2}} \exp\{-a^2\},$$

$$F_2(a) = \frac{1}{2} \left\{ F_0(a) + \frac{a}{\pi^{1/2}} \exp\{-a^2\} \right\},$$

$$F_3(a) = \frac{1}{2} \left\{ 2F_1(a) + \frac{a^2}{\pi^{1/2}} \exp\{-a^2\} \right\},$$

$$F_4(a) = \frac{1}{2} \left\{ 3F_2(a) + \frac{a^3}{\pi^{1/2}} \exp\{-a^2\} \right\}. \tag{3.10}$$

Then the functions  $A_i$  and  $B_i$  are represented by means of  $H_n$  as follows.

For  $x_i, x_{i+1} \geq y$ ,

$$A_i = \frac{1}{y^2} H_2(a, b) + \frac{2}{y} H_1(a, b) + H_0(a, b), \tag{3.11}$$

$$B_i = \frac{1}{y^2} H_4(a, b) + \frac{4}{y} H_3(a, b) + 6H_2(a, b) + 4yH_1(a, b) + y^2H_0(a, b), \tag{3.12}$$

where  $a = x_i - y$  and  $b = x_{i+1} - y$ .

For  $x_i, x_{i+1} \leq y$ ,



$$A_i = \frac{1}{y^2} H_2(a, b) - \frac{2}{y} H_1(a, b) + H_0(a, b), \quad (3.13)$$

$$B_i = \frac{1}{y^2} H_4(a, b) - \frac{4}{y} H_3(a, b) + 6H_2(a, b) - 4yH_1(a, b) + y^2 H_0(a, b), \quad (3.14)$$

where  $a = y - x_{i+1}$  and  $b = y - x_i$ .

In RESEND, the summation of Eq. (3.5) is carried out over the range of  $x$  described below. For  $\sigma(y)^*$ , the range of  $x$  is as follows:

$$y-4 < x < y+4, \text{ and } 0 < x, \quad (3.15)$$

namely,

$$\sqrt{E} - \frac{4}{\alpha^{1/2}} < \sqrt{E'} < \sqrt{E} + \frac{4}{\alpha^{1/2}}, \text{ and } 0 < E'.$$

At the boundaries of  $x$ ,  $\exp[-(x-y)^2]$  in the integration is  $1.13 \times 10^{-7}$  which is small enough. For  $\sigma(-y)^*$ ,

$$0 < x < 4-y, \quad (3.16)$$

namely,

$$0 < \sqrt{E'} < \frac{4}{\alpha^{1/2}} - \sqrt{E}.$$

Only  $\sigma(y)^*$ , therefore, contributes to the Doppler broadened cross section in the range of  $y \geq 4$ ; in other words  $E \geq 16/\alpha$ .

### 3.2 Data Handling in RESEND

Cross sections to be Doppler broadened have to be given in a form of energy vs. cross section and their interpolation scheme should be linear-linear in order to apply the above mentioned technique. Therefore if interpolation scheme of data is not linear-linear, it is changed to linear-linear interpolation by adding some energies to represent the original curve within accuracy of  $\epsilon$ . This method is very similar to the

energy halving technique described in Section 2.3. In this case, an energy  $E_c$  in an energy interval from  $E_i$  and  $E_{i+1}$  is chosen as an energy where the largest difference between the original curve and straight line is occurred. The value of  $E_c$  for each interpolation scheme is calculated as follows:

For INT=3 (linear-log),

$$E_c = (E_i - E_{i+1}) / \ln(E_i / E_{i+1}), \quad (3.17)$$

For INT=4 (log-linear),

$$E_c = \frac{1}{B} \left\{ \ln \left( \frac{\sigma_i - \sigma_{i+1}}{E_i - E_{i+1}} \times \frac{1}{B} \right) - A \right\}, \quad (3.18)$$

$$B \equiv \ln(\sigma_i / \sigma_{i+1}) / (E_i - E_{i+1}), \quad A \equiv \ln(\sigma_{i+1}) - B \times E_{i+1},$$

For INT=5 (log-log),

$$E_c = \exp \left\{ \frac{1}{B-1} \ln \frac{E_i^B (\sigma_i - \sigma_{i+1})}{B (E_i - E_{i+1}) \sigma_i} \right\}, \quad \text{for } B < 3.0, \quad (3.19)$$

$$E_c = \exp \left\{ \frac{1}{B-1} \ln \left( \frac{\sigma_i - \sigma_{i+1}}{E_i - E_{i+1}} \times \frac{1}{B} \right) - [\ln \sigma_{i+1} \ln E_i - \ln \sigma_i \ln E_{i+1}] / \ln(E_i / E_{i+1}) \right\}, \quad \text{for } B \geq 3.0, \quad (3.19')$$

$$B \equiv \ln(\sigma_i / \sigma_{i+1}) / \ln(E_i / E_{i+1}),$$

Then, the following inequality is used in place of Eq. (2.15),

$$\left| \frac{\sigma^L(E_c) - \sigma^G(E_c)}{\sigma^G(E_c)} \right| < \varepsilon, \quad (3.20)$$

where  $\sigma^L(E_c)$  and  $\sigma^G(E_c)$  are the cross sections interpolated with linear-linear interpolation and with originally given interpolation, respectively, and  $\varepsilon$  is accuracy which is assumed to be the same as the value of  $\varepsilon$  in Eq. (2.15).

The Doppler broadening is performed only for the total, elastic scattering, fission and capture cross sections, at all the energies given in their cross section data. In order to avoid meaningless calcu-

lation in higher energy region, an energy range where the broadening is performed can be specified by input data (see Section 4.2).

## 4. Input Data

### 4.1 JCL for JAERI FACOM-M 380 Computer System

In JAERI, RESEDD has been compiled by FORTRAN 77 compiler of FACOM-M 380. The size of program is about 640 K bytes. An AUTODOUBLE option was applied to use the 7- and 9-digit formats described in Section 2.3.

RESEDD needs five scratch files to tentatively store calculated cross sections or other quantities in the binary form. Their data set reference numbers are set by input data as will be described in the next section.

For the convenience of users, a catalogued procedure was made to set scratch disks and load the program. By using this catalogued procedure, the JCL cards are simplified as follows:

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER .....
    C.O .....
    OPTP
//*PROC=J2608.PROCLIB.CNTL
// EXEC RESEDD
// (DD cards for input and output files)
//SYSIN DD *
    (input data)
++
//
```

DD cards for the five scratch files are automatically given by this

lation in higher energy region, an energy range where the broadening is performed can be specified by input data (see Section 4.2).

## 4. Input Data

### 4.1 JCL for JAERI FACOM-M 380 Computer System

In JAERI, RESEDD has been compiled by FORTRAN 77 compiler of FACOM-M 380. The size of program is about 640 K bytes. An AUTODOUBLE option was applied to use the 7- and 9-digit formats described in Section 2.3.

RESEDD needs five scratch files to tentatively store calculated cross sections or other quantities in the binary form. Their data set reference numbers are set by input data as will be described in the next section.

For the convenience of users, a catalogued procedure was made to set scratch disks and load the program. By using this catalogued procedure, the JCL cards are simplified as follows:

```
//JCLG JOB
// EXEC JCLG
//SYSIN DD DATA,DLM='++'
// JUSER .....
//   C.O .....
//   OPTP .....
//*PROC=J2608.PROCLIB.CNTL
// EXEC RESEDD
// (DD cards for input and output files)
//SYSIN DD *
//   (input data)
++
//
```

DD cards for the five scratch files are automatically given by this

catalogued procedure as the data set reference numbers from 95 to 99.

## 4.2 Input Data

Here, described are the input data which control a RESEND job. A free format was applied for the input data. Columns of 1 to 72, in a card image, are used. Input data are classified into several kinds as follows.

### a) Job condition

The following parameters determine a RESEND-job condition. They are given in a form of 'parameter name = value'. As many pairs of input data as needed can be entered on an input card or separate cards. A value in parenthesis is a built-in value of the parameter. Once values of parameters are entered, they are kept until new values are specified.

INF = (1) Data set reference number of an input file in the ENDF/B format.

OUTF = (6) Data set reference number of an output file. In the case of OUTF=6, output will be written on a line printer.

EINF = (0) Data set reference number of an energy-point specification file. This file should consist of the total cross section data with the MAT number of MATE whose energies are used as energy points where the present calculation is performed (see Section 2.3). If EINF=0, energies are determined with the energy halving technique.

FORM = (4) Format of an input file. FORM=4 and =5 are available, and they stand for the ENDF/B-IV and ENDF/B-V format, respectively.

OFORM = (0) Format of an output file. OFORM=4 and =5 are available like the parameter FORM. If OFORM is not specified or OFORM=0, OFORM is assumed to be equivalent to FORM (format of input data). The format of only the first two or three records of MF=1, MT=451 is modified according to OFORM.

MAT = (0) MAT number of input data.

MATO = (0) MAT number of output data. If MATO is zero or not specified, the same MAT number as input data is used as MATO.

MATE = (0) MAT number of energy-point data. In the case where EINF is not zero, calculation is made at energy points of the total cross section of MATE in the input file of EINF. If MATE is zero, the same MAT number as MAT is assumed.

ERR = (0.01) Accuracy of calculation ( $\epsilon$  in Eq. (2.15), see Section 2.3).

DIGIT = (7) Format of energy values in an output file (see Section 2.3).

DIGIT= 6 ; Six-digit format.

DIGIT= 7 ; Seven-digit format.

DIGIT= 9 ; Nine-digit format.

OPT = (0) Output option.

OPT = 0 ; Only the total, elastic scattering, fission and capture cross sections are written on an output file.

OPT = 1 ; All cross sections given in an input file are written.

OPT = 2 ; All data in an input file are written.

POUT = (1) Print-out option for resonance parameters.

POUT = 0 ; Resonance parameters are not written on a line-printer.

POUT = 1 ; Resonance parameters are written on a line-printer.

APP = (0) Control of distant resonances (see Section 2.4).

APP = 0 ; The approximation is not applied.

APP  $\neq$  0 ; The value of  $\alpha$  in Eq. (2.16) is assumed to be equal to APP.

INTER = (1) Interpolation option for unresolved resonance region (see Section 2.5).

INTER = 0 ; Unresolved resonance parameters are interpolated.

INTER = 1 ; Cross sections are interpolated.

LSIG = (-1.0) Option on negative cross sections (see Section 2.6).

LSIG  $\geq$  0.0 ; If calculated cross section is less than LSIG, it is replaced with a given value as LSIG (barns).

LSIG < 0.0 ; This replacement is not done.

PRINT = (1) Print-out option for negative cross sections.

PRINT = 0 ; Even if negative cross sections are obtained, no error message is written on a line-printer.

PRINT = 1 ; If negative cross sections are obtained, error message is written on a line-printer.

TEMP = (0.0) Temperature in Kelvin. If TEMP is greater than 0.0, the Doppler broadening is performed at this temperature.

E = ( $10^{-5}, 20 \times 10^6$ ) An energy range of the Doppler broadening. The lower and upper boundaries are given in the form of

E = E<sub>1</sub>, E<sub>2</sub>. (in eV).

SCRR = (99) Data set reference number of a scratch file-1.

SCRS = (98) Data set reference number of a scratch file-2.

SCRD = (97) Data set reference number of a scratch file-3.

SCRL = (96) Data set reference number of a scratch file-4.

SCRE = (95) Data set reference number of a scratch file-5.

b) LABEL card

A literal record, the first record of an output file in the ENDF/B format, is written on the file defined by the OUTF parameter. A literal input record in the following format must follow the LABEL card.

columns	format	meaning
1 - 66	66A1	Literal data
67 - 70	I4	Tape identification number

c) GO card

A calculation starts when a GO card is read. Therefore all input data for job-condition parameters must have been specified until this card.

d) EOF card

This card means an end of output to the current output file defined by the OUTF parameter. If this card is entered, a TEND record is written on the last of the output file, and the output file is rewound.

d) STOP card

The current RESEND job will be terminated by this card.

## 5. Examples



SCRE = (95) Data set reference number of a scratch file-5.

b) LABEL card

A literal record, the first record of an output file in the ENDF/B format, is written on the file defined by the OUTF parameter. A literal input record in the following format must follow the LABEL card.

columns	format	meaning
1 - 66	66A1	Literal data
67 - 70	I4	Tape identification number

c) GO card

A calculation starts when a GO card is read. Therefore all input data for job-condition parameters must have been specified until this card.

d) EOF card

This card means an end of output to the current output file defined by the OUTF parameter. If this card is entered, a TEND record is written on the last of the output file, and the output file is rewound.

d) STOP card

The current RESEND job will be terminated by this card.

## 5. Examples

**Example 1** Calculation of zero-Kelvin cross sections

The following is an example of the simplest form of input data for calculation of zero-Kelvin cross sections.

	Card No.
//SYSIN DD *	
OUTF=2	1
LABEL	2
EXAMPLE OF RESEDD	3
MAT=2291	4
GO	5
EOF	6
STOP	7
/*	

In this example, the 1-st card defines a data set reference number of an output file. The literal record, EXAMPLE OF RESEDD, is written on the output file by the second card. The MAT number of 2291 is specified by the 4-th card. Other values of job-condition parameters are assumed to be equivalent to initial values. The calculation is started by the next GO card. Figure 1 shows the output written on a line-printer. The resonance parameters used are listed there together with shift factors and penetration factors. In this example, the total angular momentum is unknown for the resonances whose J values are listed as 1.50. A first few hundred records of output to a magnetic disk are given in Fig. 2. Calculated cross sections are shown in Figs. from 3 to 5.

If other calculations are needed, additional pairs of MAT and GO cards should be entered as follows.

	Card No.
MAT=2291	4
GO	5
MAT=2300	added-1
GO	added-2
MAT=2312	added-3
GO	added-4
EOF	6

By this input, cross sections of three materials are calculated. It should be noted that the calculated cross sections have to be written on the output file in increasing order of MAT numbers.

**Example 2** Accuracy and CPU time.

In this example, relation of accuracy and CPU time is shown. The cross sections were calculated from the  $^{63}\text{Cu}$  data of JENDL-2<sup>7)</sup> by applying various values of accuracy. Table 4 lists number of energy points generated to reproduce cross section curves within the required accuracy  $\epsilon$ , and spent CPU time. Calculated curves are shown in Figs. 6 and 7. It is seen that ERR of 0.01 gives satisfactory accuracy.

**Example 3** Output to a line-printer.

In the case of OUTF=6, output is written on a line-printer. Figure 8 shows such an example.

**Example 4** Calculation of Doppler broadened cross sections.

Doppler broadened cross sections at 300 K are calculated by changing the 4-th card of Example 1 as follows.

MAT=2291,TEMP=300	Card No.
GO	4
	5

**Example 5** Temperature and CPU time.

The Doppler broadened cross sections were calculated at 300, 1000, 2000 and 3000 K. Spent CPU time is listed in Table 5. Obtained cross sections are shown in Figs. from 9 to 13.

## Acknowledgments

This program was modified on the basis of RESEND. Many people, in particular members of JNDC and the Nuclear Data Center of JAERI, contributed to this improvement. Recently, international comparison of energy dependent cross-section generation programs was organized by Dr. Cullen, IAEA, and RESEND was used by Dr. Hasegawa, JAERI, to participate in the comparison. Some errors of RESEND could be found through this comparison, and they have been corrected. The author acknowledges all of these valuable contributions.

## References

- 1) Revised by D. Garber, C. Dunford, and S. Pearlstein : " ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF ", BNL-NCS-50496 (1975).
- 2) Edited by R. Kinsey : " ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF/B-V ", BNL-NCS-50496 (1979), and revised by B.A. Magurno (1983).
- 3) O. Ozer : " Program RESEND ", BNL-17134 (1972).
- 4) D.E. Cullen : " Program SIGMA1 (version 79-1): Doppler broaden evaluated cross sections in the evaluated nuclear data file/version B (ENDF/B) format ", UCRL-50400 Vol. 17, Part B, Rev. 2. (1979).
- 5) M.R. Bhat : " ENDF/B Processing Codes for the Resonance Region ", BNL 50296 (1971).
- 6) Y. Kikuchi : submitted to J. Nucl. Sci. Technol. (1984).
- 7) Edited by T. Nakagawa : " Summary of JENDL-2 General Purpose File ", JAERI-M 84-103 (1984).

## Acknowledgments

This program was modified on the basis of RESEND. Many people, in particular members of JNDC and the Nuclear Data Center of JAERI, contributed to this improvement. Recently, international comparison of energy dependent cross-section generation programs was organized by Dr. Cullen, IAEA, and RESEND was used by Dr. Hasegawa, JAERI, to participate in the comparison. Some errors of RESEND could be found through this comparison, and they have been corrected. The author acknowledges all of these valuable contributions.

## References

- 1) Revised by D. Garber, C. Dunford, and S. Pearlstein : " ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF ", BNL-NCS-50496 (1975).
- 2) Edited by R. Kinsey : " ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF/B-V ", BNL-NCS-50496 (1979), and revised by B.A. Magurno (1983).
- 3) O. Ozer : " Program RESEND ", BNL-17134 (1972).
- 4) D.E. Cullen : " Program SIGMA1 (version 79-1): Doppler broaden evaluated cross sections in the evaluated nuclear data file/version B (ENDF/B) format ", UCRL-50400 Vol. 17, Part B, Rev. 2. (1979).
- 5) M.R. Bhat : " ENDF/B Processing Codes for the Resonance Region ", BNL 50296 (1971).
- 6) Y. Kikuchi : submitted to J. Nucl. Sci. Technol. (1984).
- 7) Edited by T. Nakagawa : " Summary of JENDL-2 General Purpose File ", JAERI-M 84-103 (1984).

Table 1 Shift factors

$l$	$S_l$
0	0
1	$-1 / ( 1 + \rho^2 )$
2	$-( 18 + 3\rho^2 ) / ( 9 + 3\rho^2 + \rho^4 )$
3	$-( 675 + 90\rho^2 + 6\rho^4 ) / ( 225 + 45\rho^2 + 6\rho^4 + \rho^6 )$
4	$-( 44100 + 4725\rho^2 + 270\rho^4 + 10\rho^6 )$ $/( 11025 + 1575\rho^2 + 135\rho^4 + 10\rho^6 + \rho^8 )$

$$\rho \equiv ka,$$

where  $a$  is the channel radius defined as

$$a = [1.23\sqrt{AWR} + 0.8] \times 0.1 \text{ cm}^{-12}.$$

Table 2 Penetration factors

$l$	$P_l$
0	$\rho$
1	$\rho^3 / ( 1 + \rho^2 )$
2	$\rho^5 / ( 9 + 3\rho^2 + \rho^4 )$
3	$\rho^7 / ( 225 + 45\rho^2 + 6\rho^4 + \rho^6 )$
4	$\rho^9 / ( 11025 + 1575\rho^2 + 135\rho^4 + 10\rho^6 + \rho^8 )$

$$\rho \equiv ka,$$

where  $a$  is the channel radius defined as

$$a = [1.23\sqrt{AWR} + 0.8] \times 0.1 \text{ cm}^{-12}.$$

Table 3 Hard-sphere scattering phase shifts

Hard-sphere scattering phase shifts are calculated as shown in this table, by using the effective scattering radius given in an input file.

Here,  $\hat{\rho} = kR$ .

$l$	$\varphi_l$
0	$\hat{\rho}$
1	$\hat{\rho} - \tan^{-1}\hat{\rho}$
2	$\hat{\rho} - \tan^{-1} \{ 3\hat{\rho} / (3 - \hat{\rho}^2) \}$
3	$\hat{\rho} - \tan^{-1} \{ (15 - \hat{\rho}^3) / (15 - \hat{\rho}^2) \}$
4	$\hat{\rho} - \tan^{-1} \{ (105\hat{\rho} - 10\hat{\rho}^3) / (105 - 45\hat{\rho}^2 + \hat{\rho}^4) \}$

Table 4 Accuracy and CPU time

Resonance cross sections were calculated from the Cu-63 data of JENDL-2 with several kinds of accuracy. The number of energy points obtained in the resonance region and spent CPU time of FACOM-M 380 are compared.

$\epsilon$	energy points	CPU time (sec)
0.5	602	1.1
0.1	1156	1.9
0.05	1641	2.5
0.01	3565	5.1
0.005	5057	7.2
0.001	11263	15.5
0.0005	15922	21.8

Table 5 CPU time for Doppler broadening

Doppler broadened cross sections of the Cu-63 data of JENDL-2 were calculated at 300, 1000, 2000 and 3000 K. CPU time spent are compared. The calculation accuracy of 0.01 was used for all cases.

temperature (K)	CPU time (sec)
0	5.1
300	11.0
1000	13.2
2000	14.6
3000	15.2



LABEL

EXAMPLE OF RESEND

60

SCRR# 99 SCRS= 98 SCRD= 97 SCRE= 95 2 EINF= 0 MATE= 2291  
 MAT = 2291 MATD= 2291 INF = 1 OUTF= 2  
 ERR = 1.0000D-02 LSIG=-1.0000D+00 TEMP= 0.0 E = 0.0 TO 2.0000D+07  
 OPT = 0 DIGIT= 7 INTERPOLATION OPTION = 1  
 FORM= 4 OFOR= 4

MATERIAL NUMBER = 2291

Z\*1000 + A = 29063.  
 WEGHT(Neutron Unit) = 62.38920  
 LRP = 1  
 LFI = 0  
 MAT NUMBER (OUTPUT) = 2291

ISOTOPE NUMBER ..... 1  
 ISOTOPE ..... 29(CU) 63  
 ABUNDANCE ..... 1.0000D+00  
 NUMBER OF ENERGY RANGES ..... 1

RANGE 1

\*\*\* RESOLVED RESONANCE / MULTILEVEL BREIT-WIGNER \*\*\*

LOWER ENERGY LIMIT ..... 1.0000D-05 NUCLEAR SPIN..... 1.5000D+00  
 UPPER ENERGY LIMIT ..... 3.5000D+04 EFFECTIVE SCATTERING RADIUS(A+) 6.7000D-01  
 NUMBER OF L STATES ..... 2  
 L VALUE ..... 0 EFFECTIVE SCATTERING RADIUS(A-) 0.0  
 NUMBER OF RESONANCES ..... 33

INDEX	RESONANCE ENERGY(EV)	J	TOTAL	NEUTRON CAPTURE	FISSION	SHIFT FACTOR	PENETRATION FACTOR
1	-3.0690D+02	2.00	5.1030D+00	4.5530D+00	5.5000D-01	0.0	2.1508D-02
2	5.7700D+02	2.00	1.3840D+00	8.6400D-01	5.2000D-01	0.0	2.9491D-02
3	2.0380D+03	1.00	4.3103D+01	4.2533D+01	5.7000D-01	0.0	5.5425D-02
4	2.6420D+03	2.00	4.6600D+00	4.0800D+00	5.8000D-01	0.0	6.3106D-02
5	4.3930D+03	1.00	5.8533D+00	5.1733D+00	6.8000D-01	0.0	8.1374D-02
6	4.8520D+03	1.00	1.4620D+01	1.4000D+01	6.2000D-01	0.0	8.5519D-02
7	5.3870D+03	2.00	3.6120D+01	3.5680D+01	4.4000D-01	0.0	9.0111D-02
8	5.8190D+03	2.00	9.8200D+00	9.3600D+00	4.6000D-01	0.0	9.3654D-02
9	7.0860D+03	1.00	1.7067D+00	1.3067D+00	4.0000D-01	0.0	1.0335D-01
10	7.5650D+03	1.00	1.6577D+01	1.6000D+01	5.7700D-01	0.0	1.0678D-01
11	7.9300D+03	2.00	8.8577D+01	8.8000D+01	5.7700D-01	0.0	1.0933D-01

Fig. 1 Output on a line-printer by Example 1.

INDEX	RESONANCE ENERGY(EV)	J	TOTAL	RESONANCE WIDTH NEUTRON	CAPTURE	FISSION	SHIFT FACTOR	PENETRATION FACTOR
12	8.3500D+03	1.00	6.7333D+00	6.0533D+00	6.8000D-01	0.0	0.0	1.1219D-01
13	9.1900D+03	2.00	4.6820D+01	4.6400D+01	4.2000D-01	0.0	0.0	1.1770D-01
14	9.9300D+03	1.00	9.6577D+01	9.6000D+01	5.7700D-01	0.0	0.0	1.2234D-01
15	1.0840D+04	2.00	5.6577D+01	5.6000D+01	5.7700D-01	0.0	0.0	1.2783D-01
16	1.2530D+04	1.00	1.5417D+01	1.4667D+01	7.5000D-01	0.0	0.0	1.3743D-01
17	1.3170D+04	2.00	7.4497D+01	7.3920D+01	5.7700D-01	0.0	0.0	1.4090D-01
18	1.3170D+04	1.00	3.3733D+01	3.3333D+01	4.0000D-01	0.0	0.0	1.4090D-01
19	1.5090D+04	2.00	1.2110D+01	1.1600D+01	5.1000D-01	0.0	0.0	1.5082D-01
20	1.5820D+04	2.00	1.4730D+01	1.4160D+01	5.7000D-01	0.0	0.0	1.5442D-01
21	1.6320D+04	1.00	1.9093D+01	1.8533D+01	5.6000D-01	0.0	0.0	1.5684D-01
22	1.7880D+04	1.00	8.0577D+01	8.0000D+01	5.7700D-01	0.0	0.0	1.6417D-01
23	1.8035D+04	2.00	3.0337D+01	2.9760D+01	5.7700D-01	0.0	0.0	1.6488D-01
24	2.0900D+04	2.00	7.1297D+01	7.0720D+01	5.7700D-01	0.0	0.0	1.7749D-01
25	2.1124D+04	1.00	1.0258D+02	1.0200D+02	5.7700D-01	0.0	0.0	1.7844D-01
26	2.2672D+04	2.00	9.6577D+01	9.6000D+01	5.7700D-01	0.0	0.0	1.8486D-01
27	2.4765D+04	2.00	7.5777D+01	7.5200D+01	5.7700D-01	0.0	0.0	1.9321D-01
28	2.5618D+04	1.00	3.1124D+02	3.1067D+02	5.7700D-01	0.0	0.0	1.9651D-01
29	2.6447D+04	1.00	1.2058D+02	1.2000D+02	5.7700D-01	0.0	0.0	1.9966D-01
30	2.9359D+04	2.00	3.0871D+02	3.0813D+02	5.7700D-01	0.0	0.0	2.1036D-01
31	3.1205D+04	2.00	3.8977D+01	3.8400D+01	5.7700D-01	0.0	0.0	2.1688D-01
32	3.3400D+04	1.50	3.2558D+02	3.2500D+02	5.7700D-01	0.0	0.0	2.2438D-01
33	5.6200D+04	1.50	3.0858D+02	3.0800D+02	5.7700D-01	0.0	0.0	2.3359D-01

L VALUE ..... 1 EFFECTIVE SCATTERING RADIUS(A-) 0.0  
 NUMBER OF RESONANCES .... 11

INDEX	RESONANCE ENERGY(EV)	J	TOTAL	RESONANCE WIDTH NEUTRON	CAPTURE	FISSION	SHIFT FACTOR	PENETRATION FACTOR
1	6.5000D+02	1.00	3.6640D-01	1.6400D-02	3.5000D-01	0.0	-9.9902D-01	3.0637D-05
2	8.0600D+02	1.50	5.8200D-01	5.0000D-03	5.7700D-01	0.0	-9.9879D-01	4.2294D-05
3	9.9600D+02	1.50	5.9360D-01	1.6600D-02	5.7700D-01	0.0	-9.9850D-01	5.8083D-05
4	6.8400D+03	1.50	7.1700D-01	1.4000D-01	5.7700D-01	0.0	-9.8980D-01	1.0362D-03
5	2.0806D+04	1.50	2.0770D+00	1.5000D+00	5.7700D-01	0.0	-9.6959D-01	5.3849D-03
6	2.1050D+04	1.50	4.1770D+00	3.6000D+00	5.7700D-01	0.0	-9.6925D-01	5.4780D-03
7	2.1619D+04	1.50	5.7770D+00	5.2000D+00	5.7700D-01	0.0	-9.6844D-01	5.6969D-03
8	2.3204D+04	1.50	1.9770D+00	1.4000D+00	5.7700D-01	0.0	-9.6621D-01	6.3201D-03
9	2.3487D+04	1.50	2.9770D+00	2.4000D+00	5.7700D-01	0.0	-9.6581D-01	6.4334D-03
10	2.5779D+04	1.50	2.1770D+00	1.6000D+00	5.7700D-01	0.0	-9.6260D-01	7.3731D-03
11	3.0285D+04	1.50	2.1770D+00	1.6000D+00	5.7700D-01	0.0	-9.5634D-01	9.3275D-03

FILE-2 PROCESS COMPLETED. 3565 POINTS GENERATED

..... THIS MATERIAL COMPLETED .....

EOF WRITTEN (OUTF= 2)

STOP

Fig. 1 (Continued)

```

EXAMPLE OF RESEND
2.90630+ 4 6.23892+ 1          0          0          .0          322291 1451 1
0.0      + 0 0.0      + 0          0          0          88          02291 1451 2
29-CU- 63 JAERI,MAPI EVAL-MAR82 S.IGARASI,M.SASAKI          2291 1451 3
          DIST-MAR83 REV1-JAN84          2291 1451 4
HISTORY          2291 1451 5
75-03 EVALUATION WAS MADE FOR JENDL-1 BY M.SAKAKI(MAPI).          2291 1451 6
83-03 DATA IN THE ENERGY REGION ABOVE 35 KEV WERE RE-EVALUATED          2291 1451 7
      FOR JENDL-2 BY S.IGARASI (JAERI), AND THE BACKGROUND DATA          2291 1451 8
      IN THE RESONANCE REGION WERE MODIFIED.          2291 1451 9
84-01 COMMENT WAS ADDED.          2291 1451 10
          2291 1451 11
MF=1 GENERAL INFORMATION          2291 1451 12
MT=451 DESCRIPTIVE DATA AND DICTIONARY          2291 1451 13
          2291 1451 14
MF=2 RESONANCE PARAMETERS          2291 1451 15
MT=151 RESOLVED RESONANCE PARAMETERS FOR MLBW FORMULA          2291 1451 16
      RESONANCE REGION = 1.0E-5 EV TO 35 KEV.          2291 1451 17
      PARAMETERS WERE MAINLY TAKEN FROM BNL-325 3RD EDITION /1/.          2291 1451 18
      A BOUND LEVEL WAS ADDED TO REPRODUCE THE 2200-M/SEC CAPTURE          2291 1451 19
      CROSS SECTION OF 4.5 +- 0.1 BARNS /1/. THE EFFECTIVE SCAT-          2291 1451 20
      TERING RADIUS OF 6.70 FM WAS TAKEN FROM REF. /2/.          2291 1451 21
          2291 1451 22
      CALCULATED 2200-M/S CROSS SECTIONS AND RES. INTEGRALS.          2291 1451 23
          2291 1451 24
          2200 M/S          RES. INTEG.          2291 1451 25
      ELASTIC          4.979 B          -          2291 1451 26
      CAPTURE          4.492 B          5.41 B          2291 1451 27
      TOTAL          9.471 B          -          2291 1451 28
          2291 1451 29
MF=3 NEUTRON CROSS SECTIONS          2291 1451 30
      BELOW 35 KEV, ALL BACKGROUND CROSS SECTIONS ARE ZERO.          2291 1451 31
      ABOVE 35 KEV, DATA WERE EVALUATED AS FOLLOWS,          2291 1451 32
      MT=1 TOTAL          2291 1451 33
          OPTICAL AND STATISTICAL MODEL CALCULATION WAS MADE WITH          2291 1451 34
          CODE CASTHY /3/. THE OPTICAL POTENTIAL PARAMETERS USED ARE          2291 1451 35
          AS FOLLOWS (IN THE UNITS OF MEV AND FERMI),          2291 1451 36
          V = 46.0 - 0.250*E , RO = 1.16*A**1/3+0.6, AO = 0.62          2291 1451 37
          WI = 0.125*E-0.0004*E**2, RI = 1.16*A**1/3+0.6, AI = 0.62          2291 1451 38
          WS = 7.0 , RS = 1.16*A**1/3+1.1, AS = 0.35          2291 1451 39
          WSO= 7.0 , RSO= 1.16*A**1/3+0.6, ASO= 0.60          2291 1451 40
      MT=2 ELASTIC SCATTERING          2291 1451 41
      (TOTAL)-(ALL OTHER PARTIAL CROSS SECTIONS)          2291 1451 42
      MT=4,51-57,91 INELASTIC SCATTERING          2291 1451 43
          OPTICAL AND STATISTICAL MODEL CALCULATION WAS MADE BY TAKING          2291 1451 44
          INTO ACCOUNT OF (N,2N), (N,N'A) AND (N,A) REACTIONS AS COM-          2291 1451 45
          PETING PROCESSES. THE LEVEL SCHEME WAS TAKEN FROM REF. /4/.          2291 1451 46
          NO.          ENERGY(MEV)          SPIN-PARITY          2291 1451 47
          G.S.          0.0          3/2 -          2291 1451 48
          1          0.66962          1/2 -          2291 1451 49
          2          0.96206          5/2 -          2291 1451 50
          3          1.32703          7/2 -          2291 1451 51
          4          1.41203          5/2 -          2291 1451 52
          5          1.54702          3/2 -          2291 1451 53
          6          1.8613          5/2 -          2291 1451 54
          7          2.0111          3/2 -          2291 1451 55
          LEVELS ABOVE 2.05 MEV WERE ASSUMED TO BE OVERLAPPING.          2291 1451 56
      MT=16,22,107 (N,2N),(N,N'A) AND (N,A)          2291 1451 57
      RECOMMENDED BY KOBAYASHI /5/.          2291 1451 58
      MT=102 CAPTURE          2291 1451 59
          CALCULATED WITH CASTHY /3/ AND NORMALIZED TO THE VALUE OF          2291 1451 60
          23.7 MILLI-BARNS AT 230 KEV WHICH WAS MEASURED BY ZAIKIN /6/.          2291 1451 61
      MT=251 MU-BAR          2291 1451 62
          CALCULATED WITH CASTHY /3/.          2291 1451 63
          2291 1451 64
MF=4 ANGULAR DISTRIBUTIONS OF SECONDARY NEUTRONS          2291 1451 65
      MT=2,51-57 : CALCULATED WITH CASTHY /3/.          2291 1451 66
      MT=16,22 : ASSUMED TO BE ISOTROPIC IN THE LAB SYSTEM.          2291 1451 67
      MT=91 : ASSUMED THE SAME DISTRIBUTIONS IN THE LAB SYSTEM          2291 1451 68
          AS THOSE CALCULATED WITH CASTHY IN THE CENTER-          2291 1451 69
          OF-MASS SYSTEM.          2291 1451 70
          2291 1451 71
MF=5 ENERGY DISTRIBUTIONS OF SECONDARY NEUTRONS

```

Fig. 2 Output on a magnetic disk by Example 1. Only a first few hundred records are shown.

MT=16,22,91 : EVAPORATION SPECTRA.

REFERENCES

- 1) MUGHABGHAB S.F. AND GARBER D.I.: BNL 325, 3RD ED., VOL. 1 (1973).
- 2) MUGHABGHAB S.F. ET AL.: "NEUTRON CROSS SECTIONS, VOL. 1, PART A", ACADEMIC PRESS (1981).
- 3) IGARASI S.: J. NUCL. SCI. TECHNOL., 12, 67 (1975).
- 4) AUBLE R.L.: NUCLEAR DATA SHEETS, 14, 119 (1975).
- 5) KOBAYASHI K.: PRIVATE COMMUNICATION.
- 6) ZAIKIN G.G. ET AL.: ATOMNAYA ENERGIYA, 25, 526 (1968).

2291 1451 72  
 2291 1451 73  
 2291 1451 74  
 2291 1451 75  
 2291 1451 76  
 2291 1451 77  
 2291 1451 78  
 2291 1451 79  
 2291 1451 80  
 2291 1451 81  
 2291 1451 82  
 2291 1451 83  
 2291 1451 84

\*\*\*\*\* RESEND CALCULATION UNDER THE FOLLOWING PARAMETERS \*\*\*\*\*

ACCURACY ..... 0.0100      MINIMUM X-SECTION ...-1.00D+00  
 INTERPOLATION OPT. .. X-SECT.      OUTPUT OPTION ..... 0  
 TEMPERATURE ..... 0.0

2291 1451 85  
 2291 1451 86  
 2291 1451 87  
 2291 1451 88  
 2291 1451 89  
 2291 1451 90  
 2291 1451 91  
 2291 1451 92  
 2291 1451 93  
 2291 1451 94  
 2291 1451 95  
 2291 1451 96  
 2291 1451 97  
 2291 1451 98  
 2291 1451 99  
 2291 1451 100  
 2291 1451 101  
 2291 1451 102  
 2291 1451 103  
 2291 1451 104  
 2291 1451 105  
 2291 1451 106  
 2291 1451 107  
 2291 1451 108  
 2291 1451 109  
 2291 1451 110  
 2291 1451 111  
 2291 1451 112  
 2291 1451 113  
 2291 1451 114  
 2291 1451 115  
 2291 1451 116  
 2291 1451 117  
 2291 1451 118  
 2291 1451 119  
 2291 1451 120  
 2291 1451 121  
 2291 1451 122  
 2291 1 0 123  
 2291 0 0 124

1	451	115	2291 1451 91
2	151	50	2291 1451 92
3	1	24	2291 1451 93
3	2	17	2291 1451 94
3	4	13	2291 1451 95
3	16	10	2291 1451 96
3	22	11	2291 1451 97
3	51	13	2291 1451 98
3	52	13	2291 1451 99
3	53	12	2291 1451 100
3	54	12	2291 1451 101
3	55	11	2291 1451 102
3	56	11	2291 1451 103
3	57	10	2291 1451 104
3	91	10	2291 1451 105
3	102	17	2291 1451 106
3	107	15	2291 1451 107
3	251	18	2291 1451 108
4	2	213	2291 1451 109
4	16	10	2291 1451 110
4	22	10	2291 1451 111
4	51	106	2291 1451 112
4	52	100	2291 1451 113
4	53	91	2291 1451 114
4	54	89	2291 1451 115
4	55	82	2291 1451 116
4	56	80	2291 1451 117
4	57	73	2291 1451 118
4	91	71	2291 1451 119
5	16	15	2291 1451 120
5	22	9	2291 1451 121
5	91	10	2291 1451 122
2.90630+ 4 6.23892+ 1	0	0	1 02291 2151 125
2.90630+ 4 1.00000+ 0	0	0	1 02291 2151 126
1.00000- 5 3.50000+ 4	0	0	0 02291 2151 127
1.50000+ 0 6.70000- 1	0	0	0 02291 2151 128
			2291 2 0 129
			2291 0 0 130
2.90630+ 4 6.23892+ 1	0	0	0 02291 3 1 131
0.0 + 0 0.0 + 0	0	0	2 36262291 3 1 132
3565	2	3626	5 2291 3 1 133
1.000000-5 2.30969+ 2	1.308715-5 2.02524+ 2	1.617431-5 1.82675+ 2	22291 3 1 134
2.234862-5 1.56149+ 2	2.852293-5 1.38790+ 2	3.469725-5 1.26302+ 2	22291 3 1 135
4.704587-5 1.09170+ 2	5.939450-5 9.77083+ 1	7.174312-5 8.93513+ 1	12291 3 1 136
8.409175-5 8.29106+ 1	1.087890-4 7.34959+ 1	1.334862-4 6.68336+ 1	12291 3 1 137
1.581835-4 6.18001+ 1	2.075781-4 5.45811+ 1	2.569726-4 4.95598+ 1	12291 3 1 138
3.063671-4 4.58081+ 1	4.051562-4 4.04832+ 1	5.039452-4 3.68136+ 1	12291 3 1 139
6.027343-4 3.40881+ 1	8.003125-4 3.02406+ 1	9.978907-4 2.76020+ 1	12291 3 1 140
1.195469-3 2.56481+ 1	1.590625-3 2.28977+ 1	1.985781-3 2.10161+ 1	12291 3 1 141
2.380937-3 1.96249+ 1	3.171250-3 1.76694+ 1	3.961562-3 1.63332+ 1	12291 3 1 142
4.751875-3 1.53460+ 1	6.332500-3 1.39594+ 1	7.913125-3 1.30125+ 1	12291 3 1 143

Fig. 2 (Continued)

9.493750-3	1.23133+	1	1.265500-2	1.13314+	1	1.581625-2	1.06611+	12291	3	1	144
1.897750-2	1.01662+	1	2.530000-2	9.47134+	0	3.409783-2	8.84838+	02291	3	1	145
4.289566-2	8.42859+	0	5.169349-2	8.12113+	0	6.049132-2	7.88344+	02291	3	1	146
7.808698-2	7.53492+	0	9.568265-2	7.28758+	0	1.308740-1	6.95220+	02291	3	1	147
1.660653-1	6.72998+	0	2.012566-1	6.56885+	0	2.364480-1	6.44511+	02291	3	1	148
3.068307-1	6.26475+	0	3.772134-1	6.13738+	0	4.475961-1	6.04122+	02291	3	1	149
5.883615-1	5.90321+	0	7.291268-1	5.80700+	0	8.698922-1	5.73488+	02291	3	1	150
1.151423+0	5.63188+	0	1.432953+0	5.56018+	0	1.714484+0	5.50632+	02291	3	1	151
2.277546+0	5.42890+	0	2.840607+0	5.37431+	0	3.403669+0	5.33268+	02291	3	1	152
4.529792+0	5.27134+	0	5.655915+0	5.22652+	0	6.782038+0	5.19106+	02291	3	1	153
9.034285+0	5.13606+	0	1.128653+1	5.09312+	0	1.353878+1	5.05712+	02291	3	1	154
1.804327+1	4.99717+	0	2.254776+1	4.94665+	0	2.705226+1	4.90185+	02291	3	1	155
3.606125+1	4.82293+	0	4.507023+1	4.75324+	0	5.407922+1	4.68986+	02291	3	1	156
6.308821+1	4.63123+	0	7.209720+1	4.57644+	0	9.011515+1	4.47601+	02291	3	1	157
1.081331+2	4.38528+	0	1.261511+2	4.30219+	0	1.441691+2	4.22529+	02291	3	1	158
1.621870+2	4.15347+	0	1.802050+2	4.08584+	0	2.162410+2	3.96032+	02291	3	1	159
2.522769+2	3.84383+	0	2.883129+2	3.73217+	0	3.243488+2	3.62114+	02291	3	1	160
3.603848+2	3.50569+	0	3.784027+2	3.44418+	0	3.964207+2	3.37852+	02291	3	1	161
4.144387+2	3.30699+	0	4.324567+2	3.22711+	0	4.504746+2	3.13527+	02291	3	1	162
4.594836+2	3.08322+	0	4.684926+2	3.02585+	0	4.775016+2	2.96187+	02291	3	1	163
4.865106+2	2.88964+	0	4.955196+2	2.80692+	0	5.045286+2	2.71072+	02291	3	1	164
5.090330+2	2.65636+	0	5.135375+2	2.59701+	0	5.180420+2	2.53197+	02291	3	1	165
5.225465+2	2.46043+	0	5.270510+2	2.38158+	0	5.315555+2	2.29467+	02291	3	1	166
5.360600+2	2.19933+	0	5.405645+2	2.09627+	0	5.428167+2	2.04277+	02291	3	1	167
5.450690+2	1.98912+	0	5.473212+2	1.93698+	0	5.495735+2	1.88915+	02291	3	1	168
5.518257+2	1.85042+	0	5.540780+2	1.82898+	0	5.563302+2	1.83928+	02291	3	1	169
5.585825+2	1.90763+	0	5.597086+2	1.97777+	0	5.608347+2	2.08430+	02291	3	1	170
5.619608+2	2.24174+	0	5.630870+2	2.47154+	0	5.642131+2	2.80607+	02291	3	1	171
5.647761+2	3.02738+	0	5.653392+2	3.29585+	0	5.659022+2	3.62264+	02291	3	1	172
5.664653+2	4.02240+	0	5.670284+2	4.51411+	0	5.675915+2	5.12306+	02291	3	1	173
5.681545+2	5.88309+	0	5.687176+2	6.84105+	0	5.692806+2	8.06147+	02291	3	1	174
5.698437+2	9.63721+	0	5.701252+2	1.05980+	1	5.704067+2	1.17025+	12291	3	1	175
5.706882+2	1.29783+	1	5.709698+2	1.44601+	1	5.712513+2	1.61899+	12291	3	1	176
5.715329+2	1.82231+	1	5.718144+2	2.06277+	1	5.720960+2	2.34954+	12291	3	1	177
5.723775+2	2.69420+	1	5.726590+2	3.11249+	1	5.729405+2	3.62557+	12291	3	1	178
5.732221+2	4.26272+	1	5.735036+2	5.06418+	1	5.737851+2	6.08837+	12291	3	1	179
5.740666+2	7.42066+	1	5.743482+2	9.19041+	1	5.744889+2	1.02969+	22291	3	1	180
5.746297+2	1.15963+	2	5.747704+2	1.31311+	2	5.749112+2	1.49605+	22291	3	1	181
5.750519+2	1.71563+	2	5.751927+2	1.98193+	2	5.753335+2	2.30777+	22291	3	1	182
5.754743+2	2.71048+	2	5.756150+2	3.21292+	2	5.757558+2	3.84700+	22291	3	1	183
5.758966+2	4.65391+	2	5.760374+2	5.68730+	2	5.761781+2	7.01083+	22291	3	1	184
5.763189+2	8.69201+	2	5.764597+2	1.07644+	3	5.766005+2	1.31577+	32291	3	1	185
5.768002+2	1.64801+	3	5.769001+2	1.76434+	3	5.770000+2	1.81694+	32291	3	1	186
5.770998+2	1.79556+	3	5.771997+2	1.70690+	3	5.773995+2	1.41146+	32291	3	1	187
5.775410+2	1.18271+	3	5.776826+2	9.78011+	2	5.778242+2	8.07919+	22291	3	1	188
5.779658+2	6.71231+	2	5.781074+2	5.62692+	2	5.782490+2	4.76546+	22291	3	1	189
5.783906+2	4.07797+	2	5.785322+2	3.52470+	2	5.786737+2	3.07542+	22291	3	1	190
5.788153+2	2.70642+	2	5.789569+2	2.40061+	2	5.790985+2	2.14480+	22291	3	1	191
5.793817+2	1.74519+	2	5.796649+2	1.45162+	2	5.799480+2	1.22998+	22291	3	1	192
5.802312+2	1.05850+	2	5.805144+2	9.23149+	1	5.807976+2	8.14397+	12291	3	1	193
5.810808+2	7.25655+	1	5.813640+2	6.52251+	1	5.816472+2	5.90798+	12291	3	1	194
5.819304+2	5.38799+	1	5.824967+2	4.56115+	1	5.830631+2	3.93812+	12291	3	1	195
5.836294+2	3.45595+	1	5.841958+2	3.07414+	1	5.847621+2	2.76607+	12291	3	1	196
5.853285+2	2.51331+	1	5.858949+2	2.30302+	1	5.864613+2	2.12587+	12291	3	1	197
5.875940+2	1.84532+	1	5.887267+2	1.63449+	1	5.898594+2	1.47127+	12291	3	1	198
5.909922+2	1.34179+	1	5.921249+2	1.23697+	1	5.932576+2	1.15064+	12291	3	1	199
5.943903+2	1.07848+	1	5.955231+2	1.01737+	1	5.966558+2	9.65065+	02291	3	1	200
5.977885+2	9.19838+	0	6.000540+2	8.45712+	0	6.023194+2	7.87673+	02291	3	1	201
6.045849+2	7.41108+	0	6.068503+2	7.02992+	0	6.091158+2	6.71256+	02291	3	1	202
6.113813+2	6.44450+	0	6.136468+2	6.21526+	0	6.159122+2	6.01710+	02291	3	1	203
6.181777+2	5.84417+	0	6.227086+2	5.55716+	0	6.272395+2	5.32905+	02291	3	1	204
6.317705+2	5.14427+	0	6.363014+2	4.99379+	0	6.385668+2	4.93062+	02291	3	1	205
6.408323+2	4.87718+	0	6.419650+2	4.85564+	0	6.430977+2	4.83963+	02291	3	1	206
6.436640+2	4.83472+	0	6.442304+2	4.83288+	0	6.447968+2	4.83536+	02291	3	1	207
6.453632+2	4.84428+	0	6.459295+2	4.86331+	0	6.462127+2	4.87854+	02291	3	1	208
6.464959+2	4.89928+	0	6.467791+2	4.92751+	0	6.470623+2	4.96621+	02291	3	1	209
6.473455+2	5.02002+	0	6.476287+2	5.09650+	0	6.477702+2	5.14691+	02291	3	1	210
6.479118+2	5.20851+	0	6.480534+2	5.28458+	0	6.481950+2	5.37975+	02291	3	1	211
6.483366+2	5.50066+	0	6.484782+2	5.65713+	0	6.486198+2	5.86404+	02291	3	1	212
6.487614+2	6.14495+	0	6.488322+2	6.32443+	0	6.489030+2	6.53880+	02291	3	1	213
6.489738+2	6.79755+	0	6.490446+2	7.11354+	0	6.491154+2	7.50460+	02291	3	1	214
6.491862+2	7.99592+	0	6.492570+2	8.62396+	0	6.493278+2	9.44285+	02291	3	1	215

Fig. 2 (Continued)

6.493986+2	1.05353+1	6.494694+2	1.20318+1	6.495048+2	1.29933+1	12291	3	1	216
6.495402+2	1.41450+1	6.495756+2	1.55363+1	6.496110+2	1.72325+1	12291	3	1	217
6.496464+2	1.93193+1	6.496818+2	2.19085+1	6.497172+2	2.51447+1	12291	3	1	218
6.497526+2	2.92065+1	6.497880+2	3.42973+1	6.498234+2	4.06012+1	12291	3	1	219
6.498588+2	4.81679+1	6.498942+2	5.66781+1	6.499471+2	6.87042+1	12291	3	1	220
6.499735+2	7.26275+1	6.500000+2	7.40522+1	6.500264+2	7.26397+1	12291	3	1	221
6.500529+2	6.87074+1	6.501058+2	5.66829+1	6.501438+2	4.75776+1	12291	3	1	222
6.501818+2	3.95985+1	6.502198+2	3.30792+1	6.502578+2	2.79163+1	12291	3	1	223
6.502958+2	2.38691+1	6.503338+2	2.06937+1	6.503718+2	1.81859+1	12291	3	1	224
6.504099+2	1.61823+1	6.504479+2	1.45734+1	6.504859+2	1.32641+1	12291	3	1	225
6.505239+2	1.21875+1	6.505620+2	1.12916+1	6.506380+2	9.91053+0	02291	3	1	226
6.507141+2	8.90838+0	6.507901+2	8.16223+0	6.508661+2	7.59210+0	02291	3	1	227
6.509421+2	7.14723+0	6.510182+2	6.79331+0	6.510942+2	6.50798+0	02291	3	1	228
6.511703+2	6.27408+0	6.512463+2	6.08046+0	6.513224+2	5.91798+0	02291	3	1	229
6.514744+2	5.66332+0	6.516265+2	5.47459+0	6.517786+2	5.33078+0	02291	3	1	230
6.519307+2	5.21854+0	6.520827+2	5.12918+0	6.522348+2	5.05667+0	02291	3	1	231
6.523869+2	4.99693+0	6.525390+2	4.94705+0	6.528431+2	4.86883+0	02291	3	1	232
6.531473+2	4.81052+0	6.534514+2	4.76552+0	6.537556+2	4.72969+0	02291	3	1	233
6.540597+2	4.70045+0	6.543639+2	4.67601+0	6.549722+2	4.63717+0	02291	3	1	234
6.555805+2	4.60714+0	6.561888+2	4.58271+0	6.567971+2	4.56202+0	02291	3	1	235
6.574054+2	4.54394+0	6.586220+2	4.51299+0	6.598386+2	4.48651+0	02291	3	1	236
6.610552+2	4.46287+0	6.622718+2	4.44118+0	6.647050+2	4.40182+0	02291	3	1	237
6.671382+2	4.36620+0	6.695715+2	4.33330+0	6.744379+2	4.27364+0	02291	3	1	238
6.793044+2	4.22032+0	6.890373+2	4.12795+0	6.987702+2	4.04994+0	02291	3	1	239
7.085031+2	3.98265+0	7.182360+2	3.92368+0	7.279689+2	3.87130+0	02291	3	1	240
7.474346+2	3.78156+0	7.669004+2	3.70668+0	7.766333+2	3.67370+0	02291	3	1	241
7.814997+2	3.65835+0	7.863662+2	3.64402+0	7.887994+2	3.63743+0	02291	3	1	242
7.912326+2	3.63145+0	7.936658+2	3.62653+0	7.948824+2	3.62474+0	02291	3	1	243
7.960991+2	3.62369+0	7.973157+2	3.62382+0	7.979240+2	3.62455+0	02291	3	1	244
7.985323+2	3.62592+0	7.991406+2	3.62817+0	7.997489+2	3.63164+0	02291	3	1	245
8.003572+2	3.63691+0	8.009655+2	3.64486+0	8.012696+2	3.65030+0	02291	3	1	246
8.015738+2	3.65708+0	8.018779+2	3.66559+0	8.021821+2	3.67643+0	02291	3	1	247
8.024862+2	3.69041+0	8.027904+2	3.70878+0	8.030945+2	3.73340+0	02291	3	1	248
8.033987+2	3.76735+0	8.035507+2	3.78928+0	8.037028+2	3.81572+0	02291	3	1	249
8.038549+2	3.84795+0	8.040070+2	3.88772+0	8.041590+2	3.93751+0	02291	3	1	250
8.043111+2	4.00099+0	8.044632+2	4.08349+0	8.046153+2	4.19326+0	02291	3	1	251
8.047673+2	4.34033+0	8.048433+2	4.43975+0	8.049194+2	4.55563+0	02291	3	1	252
8.049954+2	4.69595+0	8.050715+2	4.86830+0	8.051475+2	5.08215+0	02291	3	1	253
8.052236+2	5.35193+0	8.052996+2	5.69656+0	8.053757+2	6.14521+0	02291	3	1	254
8.054517+2	6.73741+0	8.055278+2	7.53334+0	8.056038+2	8.61203+0	02291	3	1	255
8.056799+2	1.00768+1	8.057559+2	1.20072+1	8.058320+2	1.43477+1	12291	3	1	256
8.059160+2	1.68326+1	8.059580+2	1.76442+1	8.060000+2	1.79376+1	12291	3	1	257
8.060420+2	1.76450+1	8.060840+2	1.68340+1	8.061680+2	1.43498+1	12291	3	1	258
8.062606+2	1.15494+1	8.063069+2	1.03791+1	8.063532+2	9.38725+0	02291	3	1	259
8.063995+2	8.55908+0	8.064458+2	7.87179+0	8.064921+2	7.30181+0	02291	3	1	260
8.065384+2	6.82791+0	8.065847+2	6.43213+0	8.066310+2	6.09977+0	02291	3	1	261
8.067236+2	5.58032+0	8.068162+2	5.20053+0	8.069088+2	4.91624+0	02291	3	1	262
8.070014+2	4.69881+0	8.070940+2	4.52927+0	8.071866+2	4.39478+0	02291	3	1	263
8.072792+2	4.28645+0	8.073718+2	4.19799+0	8.074644+2	4.12488+0	02291	3	1	264
8.076497+2	4.01218+0	8.078349+2	3.93064+0	8.080201+2	3.86973+0	02291	3	1	265
8.082053+2	3.82303+0	8.083905+2	3.78644+0	8.085757+2	3.75721+0	02291	3	1	266
8.087609+2	3.73348+0	8.089461+2	3.71393+0	8.091314+2	3.69762+0	02291	3	1	267
8.095018+2	3.67212+0	8.098722+2	3.65325+0	8.102426+2	3.63882+0	02291	3	1	268
8.106131+2	3.62747+0	8.109835+2	3.61833+0	8.113539+2	3.61082+0	02291	3	1	269
8.120948+2	3.59916+0	8.128356+2	3.59047+0	8.135765+2	3.58365+0	02291	3	1	270
8.143173+2	3.57806+0	8.150582+2	3.57333+0	8.165399+2	3.56552+0	02291	3	1	271
8.180217+2	3.55909+0	8.195034+2	3.55347+0	8.209851+2	3.54837+0	02291	3	1	272
8.239486+2	3.53912+0	8.269120+2	3.53062+0	8.298755+2	3.52257+0	02291	3	1	273
8.358024+2	3.50729+0	8.417293+2	3.49272+0	8.535831+2	3.46497+0	02291	3	1	274
8.772907+2	3.41338+0	9.009983+2	3.36560+0	9.247058+2	3.32081+0	02291	3	1	275
9.365596+2	3.29941+0	9.484134+2	3.27873+0	9.543403+2	3.26874+0	02291	3	1	276
9.602672+2	3.25909+0	9.661941+2	3.24998+0	9.691575+2	3.24576+0	02291	3	1	277
9.721210+2	3.24191+0	9.750844+2	3.23863+0	9.780479+2	3.23632+0	02291	3	1	278
9.795296+2	3.23575+0	9.810113+2	3.23579+0	9.824930+2	3.23672+0	02291	3	1	279
9.839748+2	3.23900+0	9.847156+2	3.24087+0	9.854565+2	3.24343+0	02291	3	1	280
9.861973+2	3.24687+0	9.869382+2	3.25152+0	9.876790+2	3.25781+0	02291	3	1	281
9.884199+2	3.26642+0	9.891608+2	3.27839+0	9.899017+2	3.29545+0	02291	3	1	282
9.902721+2	3.30675+0	9.906425+2	3.32059+0	9.910129+2	3.33777+0	02291	3	1	283
9.913834+2	3.35938+0	9.917538+2	3.38702+0	9.921242+2	3.42309+0	02291	3	1	284
9.924946+2	3.47129+0	9.928651+2	3.53762+0	9.930503+2	3.58050+0	02291	3	1	285
9.932355+2	3.63221+0	9.934207+2	3.69534+0	9.936059+2	3.77347+0	02291	3	1	286
9.937911+2	3.87168+0	9.939763+2	3.99741+0	9.941615+2	4.16183+0	02291	3	1	287

Fig. 2 (Continued)

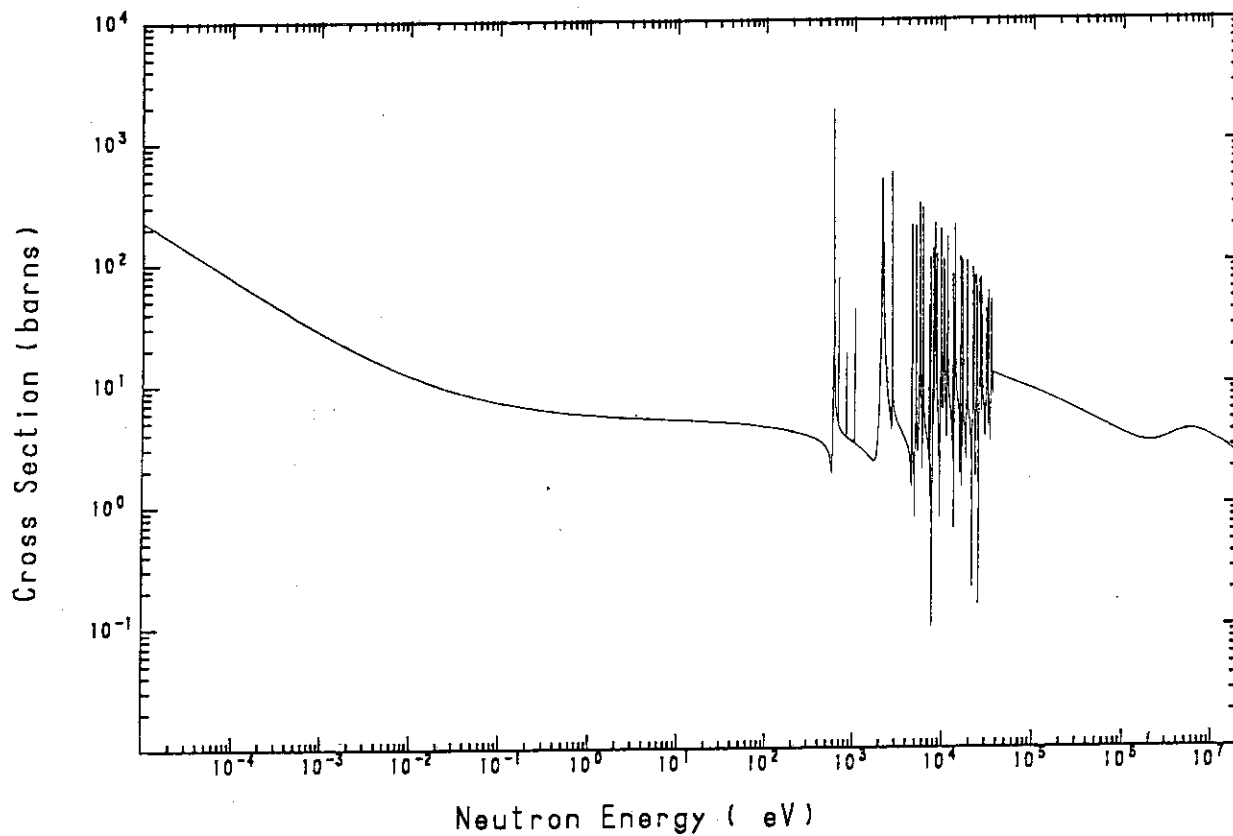


Fig. 3 Total cross section obtained by Example 1.

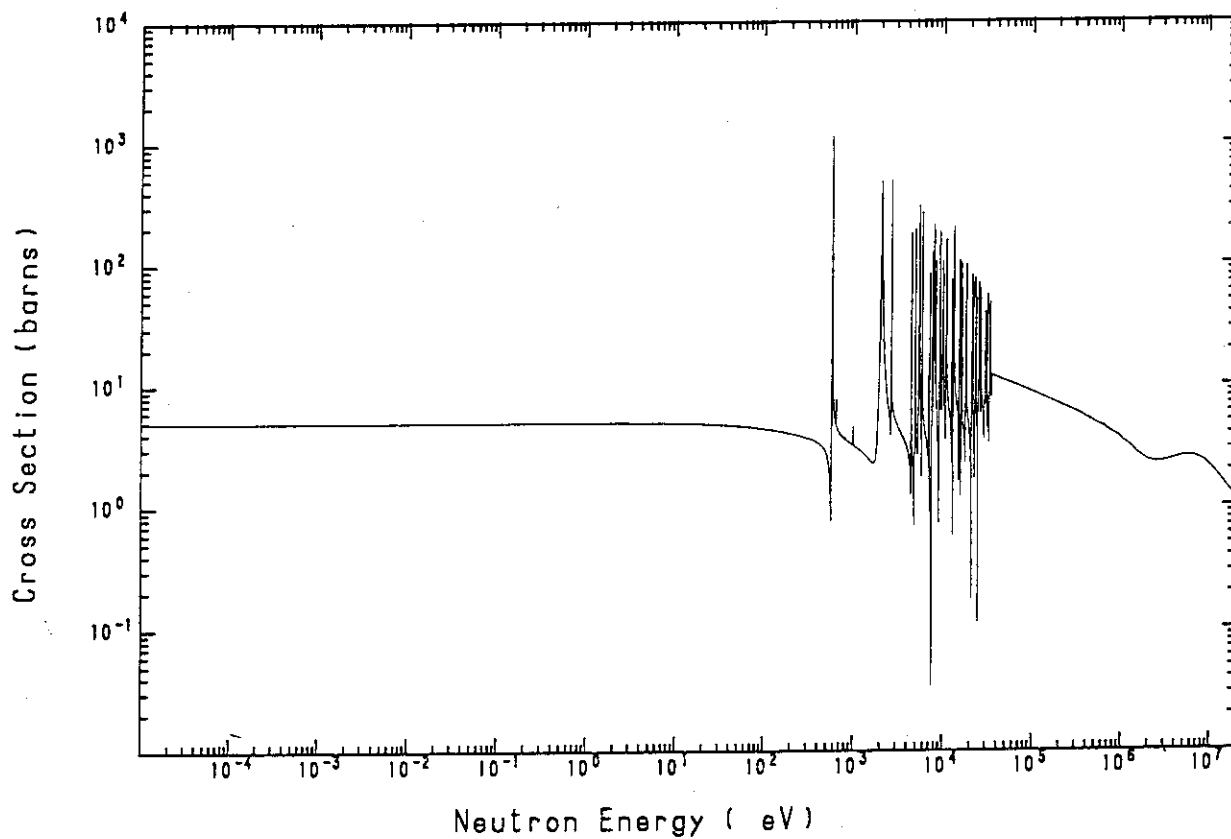


Fig. 4 Elastic scattering cross section obtained by Example 1.

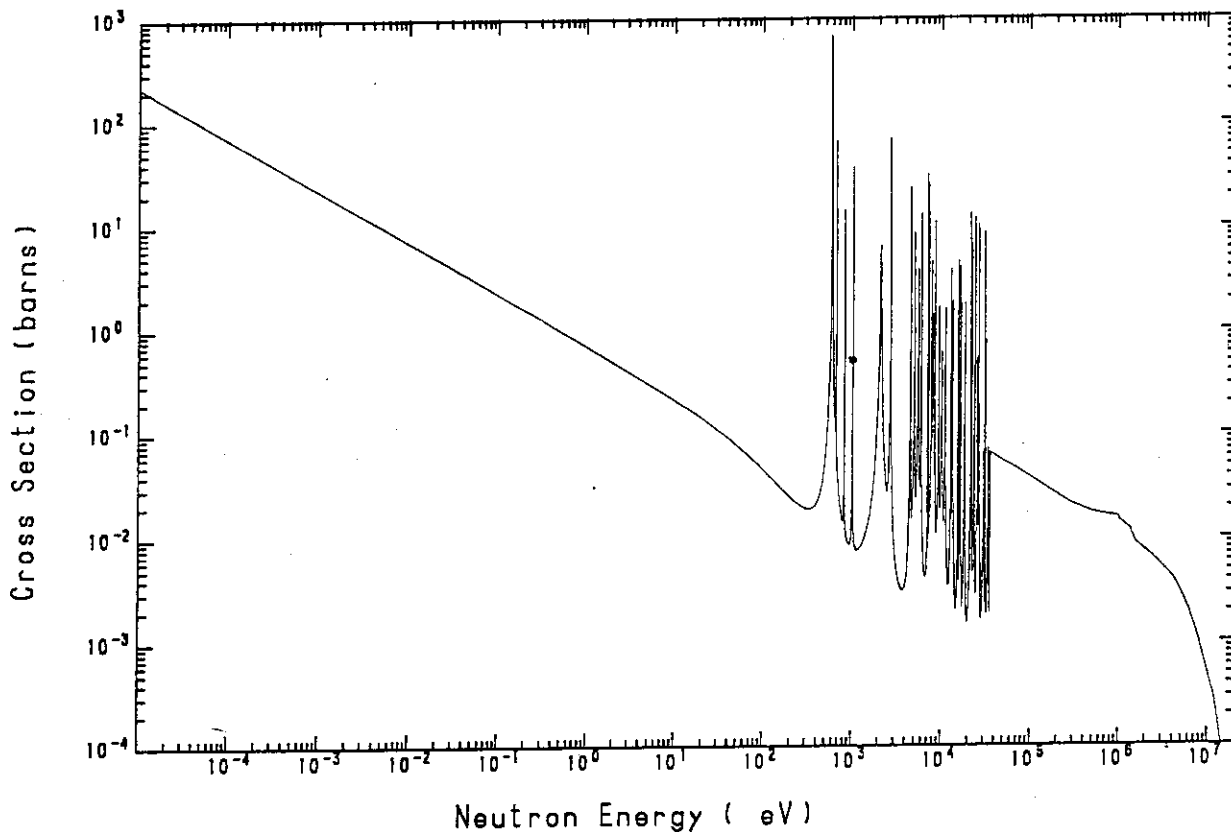


Fig. 5 Capture cross section obtained by Example 1.

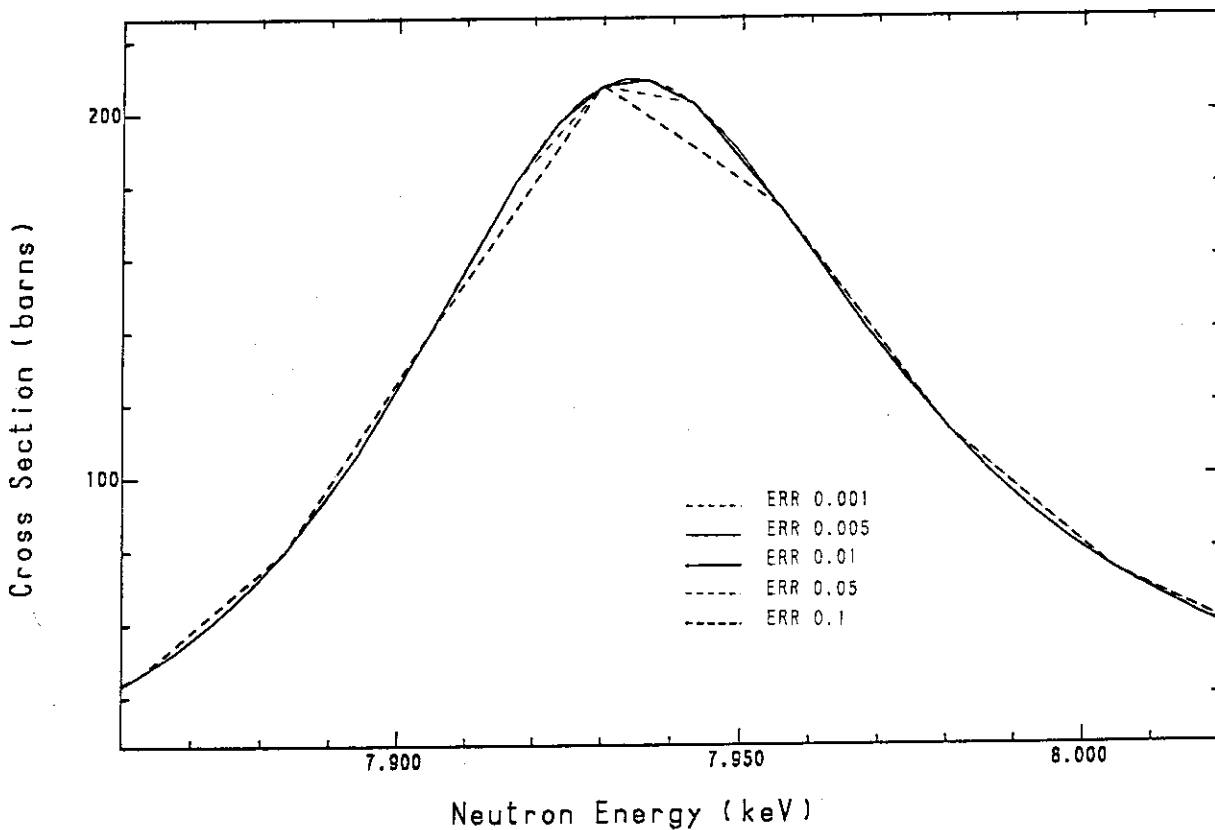


Fig. 6 Total cross section of Cu-63, around the 7.93-keV resonance. The cross section was calculated with various values of  $\epsilon$ .



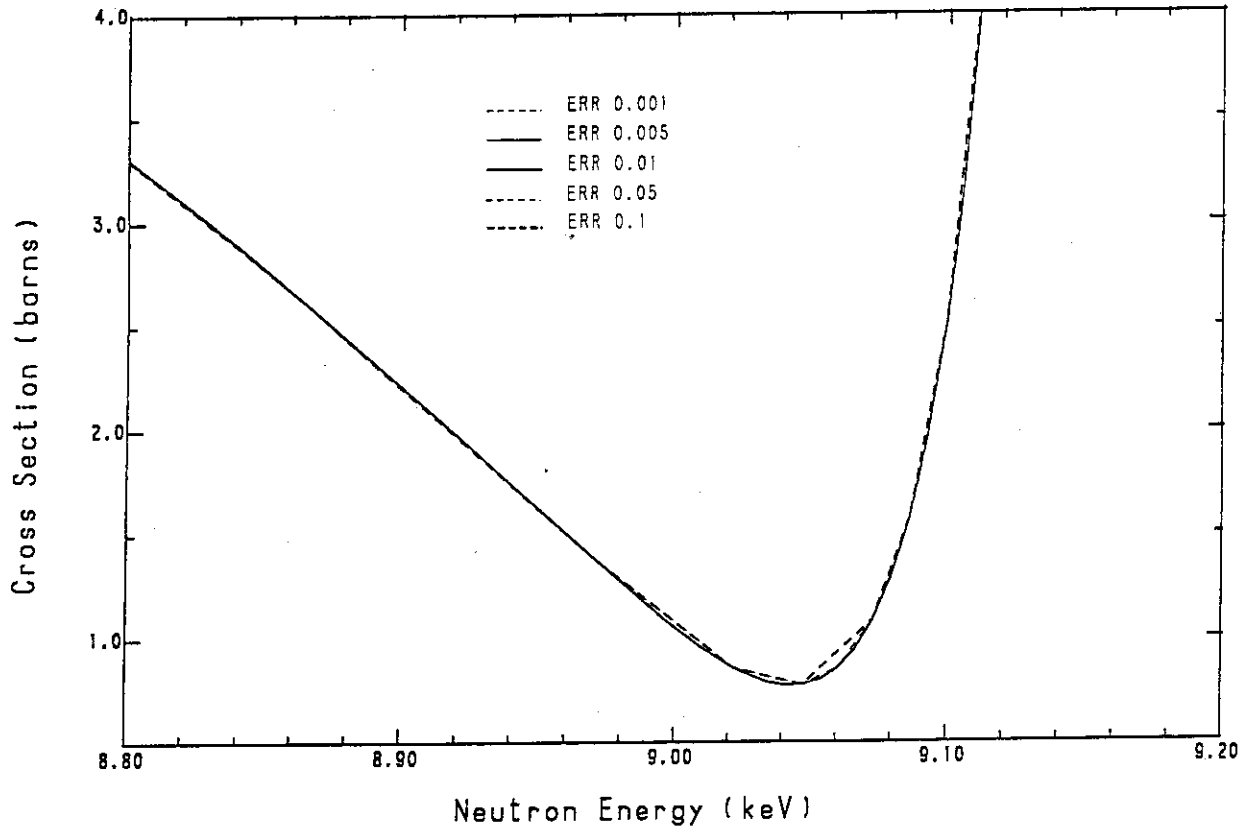


Fig. 7 Total cross section of Cu-63, around a cross-section minimum. The cross section was calculated with various values of  $\epsilon$ .

\*\*\* 29(CU) 63 \*\*\* (MATERIAL NUMBER = 2291) TOTAL CROSS SECTION  
 \*\*\*\*\*

TEMPERATURE ..... 0.0  
 Q-VALUE ..... 0.0  
 TEST FOR TEMP. DEPENDENCE ... 0  
 INTERPOLATION RANGES ..... 2  
 TOTAL DATA POINTS ..... 3626

RANGE NO. 1 / INTERPOLATION LAW =Y IS LINEAR IN X / RANGE 1 TO 3565

INDEX	ENERGY/EV	SIGMA/BARN	INDEX	ENERGY/EV	SIGMA/BARN	INDEX	ENERGY/EV	SIGMA/BARN	INDEX	ENERGY/EV	SIGMA/BARN
1	1.00000-05	2.30970+02	38	5.16930-02	8.12110+00	75	1.44170+02	4.22530+00	112	5.61960+02	2.24170+00
2	1.50870-05	2.02520+02	39	6.04910-02	7.88340+00	76	1.62190+02	4.15350+00	113	5.63090+02	2.47150+00
3	1.61740-05	1.82260+02	40	7.80870-02	7.53490+00	77	1.80200+02	4.08580+00	114	5.64210+02	2.80410+00
4	2.23490-05	1.56150+02	41	9.56830-02	7.28760+00	78	2.16240+02	3.96030+00	115	5.64780+02	3.02740+00
5	2.85230-05	1.38790+02	42	1.30870-01	6.95220+00	79	2.52280+02	3.84380+00	116	5.65340+02	3.29590+00
6	3.46970-05	1.26300+02	43	1.66070-01	6.73000+00	80	2.88310+02	3.73220+00	117	5.65900+02	3.62260+00
7	4.70460-05	1.09170+02	44	2.01260-01	6.56890+00	81	3.24350+02	3.62110+00	118	5.66470+02	4.02240+00
8	5.93950-05	9.77080+01	45	2.36450-01	6.44510+00	82	3.60380+02	3.50570+00	119	5.67030+02	4.51410+00
9	7.17430-05	8.93510+01	46	3.06830-01	6.26480+00	83	3.94200+02	3.44420+00	120	5.67590+02	5.12310+00
10	8.40920-05	8.29110+01	47	3.77210-01	6.13740+00	84	3.94200+02	3.37850+00	121	5.68150+02	5.88310+00
11	1.08790-04	7.34960+01	48	4.47600-01	6.04120+00	85	4.14440+02	3.30700+00	122	5.68720+02	6.84100+00
12	1.33490-04	6.68340+01	49	5.88360-01	5.90320+00	86	4.39460+02	3.22710+00	123	5.69280+02	8.06150+00
13	1.58180-04	6.18000+01	50	7.29130-01	5.80700+00	87	4.50470+02	3.15530+00	124	5.69840+02	9.63720+00
14	2.07580-04	5.45810+01	51	8.69890-01	5.73490+00	88	4.59480+02	3.08320+00	125	5.70130+02	1.05980+01
15	2.56970-04	4.95600+01	52	1.15140+00	5.63190+00	89	4.68490+02	3.02580+00	126	5.70410+02	1.17020+01
16	3.06370-04	4.58080+01	53	1.43300+00	5.56020+00	90	4.77500+02	2.96190+00	127	5.70690+02	1.29780+01
17	4.05160-04	4.04830+01	54	1.71450+00	5.50630+00	91	4.86510+02	2.88940+00	128	5.70970+02	1.44600+01
18	5.03950-04	3.68140+01	55	2.27750+00	5.42890+00	92	4.95520+02	2.80690+00	129	5.71250+02	1.61900+01
19	6.02730-04	3.40880+01	56	2.84060+00	5.37430+00	93	5.04530+02	2.71070+00	130	5.71530+02	1.82230+01
20	8.00310-04	3.02410+01	57	3.40370+00	5.33270+00	94	5.09030+02	2.65640+00	131	5.71810+02	2.06280+01
21	9.97890-04	2.76020+01	58	4.52980+00	5.27130+00	95	5.13540+02	2.59700+00	132	5.72100+02	2.34950+01
22	1.19550-03	2.56480+01	59	5.65590+00	5.22650+00	96	5.18040+02	2.53200+00	133	5.72380+02	2.69420+01
23	1.59060-03	2.28980+01	60	6.78200+00	5.19110+00	97	5.22550+02	2.46040+00	134	5.72660+02	3.11250+01
24	1.98580-03	2.10160+01	61	9.03430+00	5.13610+00	98	5.27050+02	2.38160+00	135	5.72940+02	3.62560+01
25	3.38090-03	1.96250+01	62	1.12870+01	5.09310+00	99	5.31560+02	2.29470+00	136	5.73220+02	4.26270+01
26	3.17120-03	1.76690+01	63	1.35390+01	5.05710+00	100	5.36060+02	2.19930+00	137	5.73500+02	5.06420+01
27	3.96160-03	1.63330+01	64	1.80430+01	4.99720+00	101	5.40560+02	2.09630+00	138	5.73790+02	6.08840+01
28	4.75190-03	1.53460+01	65	2.25480+01	4.94670+00	102	5.42820+02	2.04280+00	139	5.74070+02	7.42070+01
29	6.33250-03	1.39590+01	66	2.70320+01	4.90190+00	103	5.45070+02	1.98910+00	140	5.74350+02	9.19040+01
30	7.91310-03	1.30130+01	67	3.60610+01	4.82290+00	104	5.47320+02	1.93700+00	141	5.74630+02	1.02970+02
31	9.49370-03	1.23130+01	68	4.50700+01	4.75320+00	105	5.49570+02	1.88920+00	142	5.74910+02	1.15960+02
32	1.26550-02	1.13310+01	69	5.40790+01	4.68990+00	106	5.51830+00	1.82900+00	143	5.74770+02	1.31310+02
33	1.58160-02	1.06610+01	70	6.30880+01	4.63120+00	107	5.54080+02	1.82900+00	144	5.74910+02	1.49610+02
34	1.89770-02	1.01660+01	71	7.20370+01	4.57640+00	108	5.56330+02	1.83930+00	145	5.75050+02	1.71560+02
35	2.59000-02	9.47130+00	72	9.01150+01	4.47600+00	109	5.58580+02	1.90760+00	146	5.75190+02	1.98190+02
36	3.40980-02	8.48440+00	73	1.08130+02	4.38530+00	110	5.59710+02	1.97780+00	147	5.75330+02	2.30780+02
37	4.28960-02	8.42860+00	74	1.26150+02	4.30220+00	111	5.60830+02	2.08430+00	148	5.75470+02	2.71050+02

Fig. 8 Example of cross sections written on a line-printer.  
 Only first two pages are shown.

\*\*\* 29(CU) 63 \*\*\* (MATERIAL NUMBER = 2291)

TOTAL CROSS SECTION  
\*\*\*\*\*

INDEX	ENERGY/EV	SIGMA/BARN	INDEX	ENERGY/EV	SIGMA/BARN	INDEX	ENERGY/EV	SIGMA/BARN	INDEX	ENERGY/EV	SIGMA/BARN
148	5.75470+02	2.7105D+02	195	5.8986D+02	1.4713D+01	242	6.4904D+02	7.1135D+00	289	6.5147D+02	5.6633D+00
149	5.7561D+02	3.2129D+02	196	5.9099D+02	1.3448D+01	243	6.4912D+02	7.5066D+00	290	6.5163D+02	5.4746D+00
150	5.7576D+02	3.8470D+02	197	5.9212D+02	1.2370D+01	244	6.4919D+02	7.9959D+00	291	6.5178D+02	5.3308D+00
151	5.7590D+02	4.6539D+02	198	5.9326D+02	1.1506D+01	245	6.4926D+02	8.6240D+00	292	6.5193D+02	5.2185D+00
152	5.7604D+02	5.6873D+02	199	5.9439D+02	1.0785D+01	246	6.4933D+02	9.4429D+00	293	6.5208D+02	5.1292D+00
153	5.7618D+02	7.0108D+02	200	5.9552D+02	1.0174D+01	247	6.4940D+02	1.0535D+01	294	6.5223D+02	5.0567D+00
154	5.7632D+02	8.6920D+02	201	5.9666D+02	9.6507D+00	248	6.4947D+02	1.2032D+01	295	6.5239D+02	4.9969D+00
155	5.7646D+02	1.0764D+03	202	5.9779D+02	9.1984D+00	249	6.4950D+02	1.2993D+01	296	6.5254D+02	4.9470D+00
156	5.7660D+02	1.3158D+03	203	6.0095D+02	8.4571D+00	250	6.4954D+02	1.4145D+01	297	6.5284D+02	4.8688D+00
157	5.7680D+02	1.6480D+03	204	6.0232D+02	7.8767D+00	251	6.4958D+02	1.5536D+01	298	6.5315D+02	4.8105D+00
158	5.7690D+02	1.7643D+03	205	6.0458D+02	7.4111D+00	252	6.4961D+02	1.7233D+01	299	6.5345D+02	4.7655D+00
159	5.7700D+02	1.8169D+03	206	6.0685D+02	7.0299D+00	253	6.4965D+02	1.9319D+01	300	6.5376D+02	4.7297D+00
160	5.7710D+02	1.7956D+03	207	6.0912D+02	6.7126D+00	254	6.4968D+02	2.1909D+01	301	6.5406D+02	4.7004D+00
161	5.7720D+02	1.7069D+03	208	6.1138D+02	6.4445D+00	255	6.4972D+02	2.5145D+01	302	6.5436D+02	4.6760D+00
162	5.7740D+02	1.4115D+03	209	6.1365D+02	6.2153D+00	256	6.4975D+02	2.9207D+01	303	6.5497D+02	4.6372D+00
163	5.7754D+02	1.1827D+03	210	6.1591D+02	6.0171D+00	257	6.4979D+02	3.4297D+01	304	6.5558D+02	4.6071D+00
164	5.7768D+02	9.7801D+02	211	6.1818D+02	5.8442D+00	258	6.4982D+02	4.0601D+01	305	6.5619D+02	4.5827D+00
165	5.7782D+02	8.0792D+02	212	6.2044D+02	5.6720D+00	259	6.4986D+02	4.8168D+01	306	6.5680D+02	4.5620D+00
166	5.7797D+02	6.7123D+02	213	6.2274D+02	5.5291D+00	260	6.4989D+02	5.6678D+01	307	6.5741D+02	4.5439D+00
167	5.7811D+02	5.6269D+02	214	6.2507D+02	5.4144D+00	261	6.4995D+02	6.8704D+01	308	6.5862D+02	4.5130D+00
168	5.7825D+02	4.7655D+02	215	6.2740D+02	5.3291D+00	262	6.4997D+02	7.2627D+01	309	6.5984D+02	4.4865D+00
169	5.7839D+02	4.0780D+02	216	6.2974D+02	5.2592D+00	263	6.5000D+02	7.4052D+01	310	6.6106D+02	4.4629D+00
170	5.7853D+02	3.5247D+02	217	6.3207D+02	4.8772D+00	264	6.5003D+02	7.2640D+01	311	6.6227D+02	4.4412D+00
171	5.7867D+02	3.0754D+02	218	6.3431D+02	4.8556D+00	265	6.5010D+02	5.6683D+01	312	6.6470D+02	4.4203D+00
172	5.7882D+02	2.7064D+02	219	6.3657D+02	4.8396D+00	266	6.5018D+02	6.8704D+01	313	6.6714D+02	4.3662D+00
173	5.7896D+02	2.4006D+02	220	6.3883D+02	4.8347D+00	267	6.5014D+02	4.7578D+01	314	6.6957D+02	4.3333D+00
174	5.7910D+02	2.1448D+02	221	6.4107D+02	4.8329D+00	268	6.5018D+02	3.9598D+01	315	6.7444D+02	4.2736D+00
175	5.7925D+02	1.7452D+02	222	6.4331D+02	4.8354D+00	269	6.5022D+02	3.3079D+01	316	6.7930D+02	4.2203D+00
176	5.7939D+02	1.4516D+02	223	6.4556D+02	4.8443D+00	270	6.5026D+02	2.7916D+01	317	6.8904D+02	4.1280D+00
177	5.7953D+02	1.2300D+02	224	6.4780D+02	4.8633D+00	271	6.5030D+02	2.3869D+01	318	6.9877D+02	4.0499D+00
178	5.8023D+02	1.0585D+02	225	6.4910D+02	4.8785D+00	272	6.5033D+02	2.0894D+01	319	7.0850D+02	3.9827D+00
179	5.8051D+02	9.2315D+01	226	6.4950D+02	4.8993D+00	273	6.5037D+02	1.8186D+01	320	7.1824D+02	3.9237D+00
180	5.8080D+02	8.1440D+01	227	6.4678D+02	4.9275D+00	274	6.5041D+02	1.6182D+01	321	7.2797D+02	3.8713D+00
181	5.8108D+02	7.2566D+01	228	6.4706D+02	4.9662D+00	275	6.5045D+02	1.4573D+01	322	7.4743D+02	3.7816D+00
182	5.8136D+02	6.5225D+01	229	6.4735D+02	5.0200D+00	276	6.5049D+02	1.3264D+01	323	7.6690D+02	3.7067D+00
183	5.8165D+02	5.9080D+01	230	6.4763D+02	5.0965D+00	277	6.5052D+02	1.2188D+01	324	7.8637D+02	3.6440D+00
184	5.8193D+02	5.3880D+01	231	6.4777D+02	5.1469D+00	278	6.5056D+02	1.1292D+01	325	7.8150D+02	3.6584D+00
185	5.8250D+02	4.5612D+01	232	6.4791D+02	5.2085D+00	279	6.5064D+02	9.9105D+00	326	7.8637D+02	3.6440D+00
186	5.8306D+02	3.9381D+01	233	6.4805D+02	5.2846D+00	280	6.5071D+02	8.9084D+00	327	7.8800D+02	3.6374D+00
187	5.8363D+02	3.4560D+01	234	6.4819D+02	5.3797D+00	281	6.5079D+02	8.1622D+00	328	7.9123D+02	3.6314D+00
188	5.8420D+02	3.0741D+01	235	6.4834D+02	5.5007D+00	282	6.5087D+02	7.5921D+00	329	7.9367D+02	3.6265D+00
189	5.8476D+02	2.7661D+01	236	6.4848D+02	5.6571D+00	283	6.5094D+02	7.1472D+00	330	7.9489D+02	3.6237D+00
190	5.8533D+02	2.5133D+01	237	6.4862D+02	5.8640D+00	284	6.5102D+02	6.7933D+00	331	7.9610D+02	3.6237D+00
191	5.8589D+02	2.3030D+01	238	6.4876D+02	6.1450D+00	285	6.5109D+02	6.5080D+00	332	7.9732D+02	3.6238D+00
192	5.8646D+02	2.1259D+01	239	6.4883D+02	6.3244D+00	286	6.5117D+02	6.2741D+00	333	7.9792D+02	3.6254D+00
193	5.8759D+02	1.8453D+01	240	6.4890D+02	6.5388D+00	287	6.5125D+02	6.0805D+00	334	7.9853D+02	3.6259D+00
194	5.8873D+02	1.6345D+01	241	6.4897D+02	6.7975D+00	288	6.5132D+02	5.9180D+00	335	7.9914D+02	3.6282D+00

Fig. 8 (Continued)

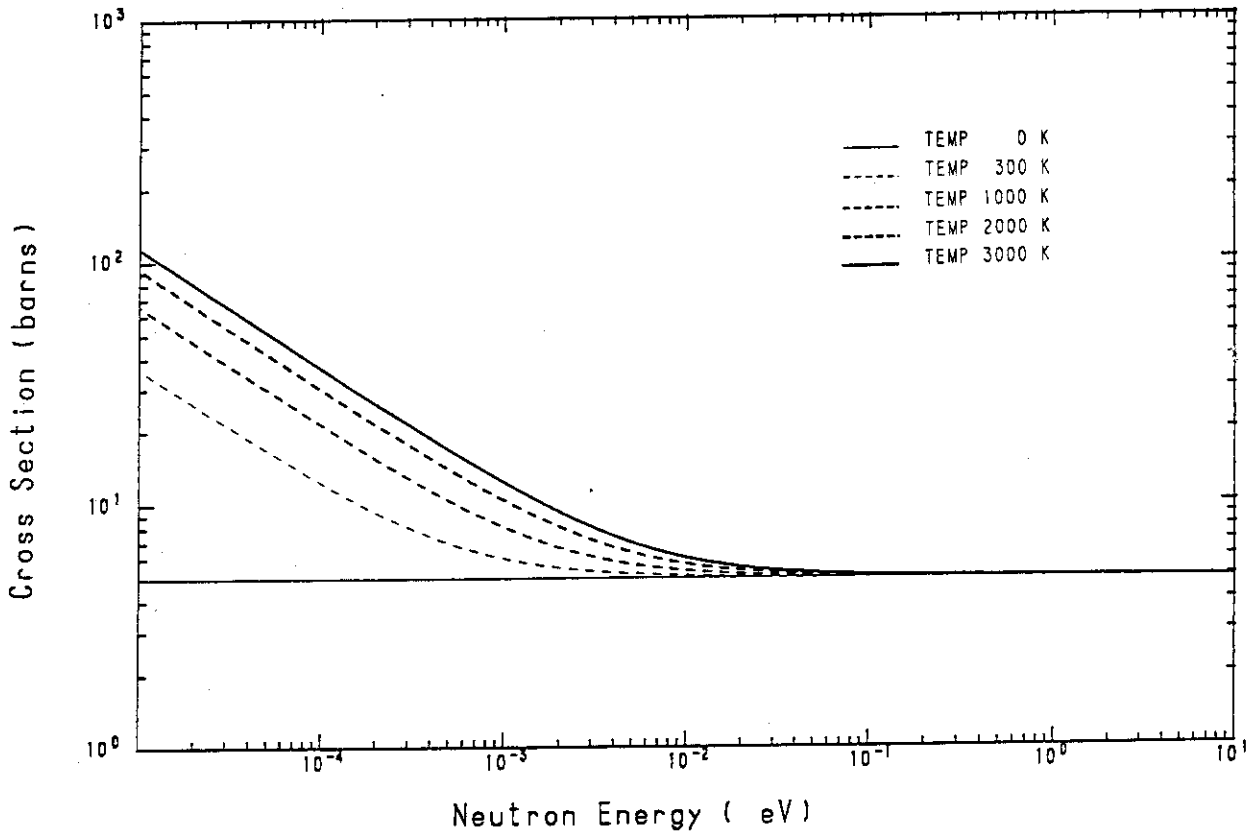


Fig. 9 Doppler broadened cross sections. The elastic scattering cross section in low energy region.

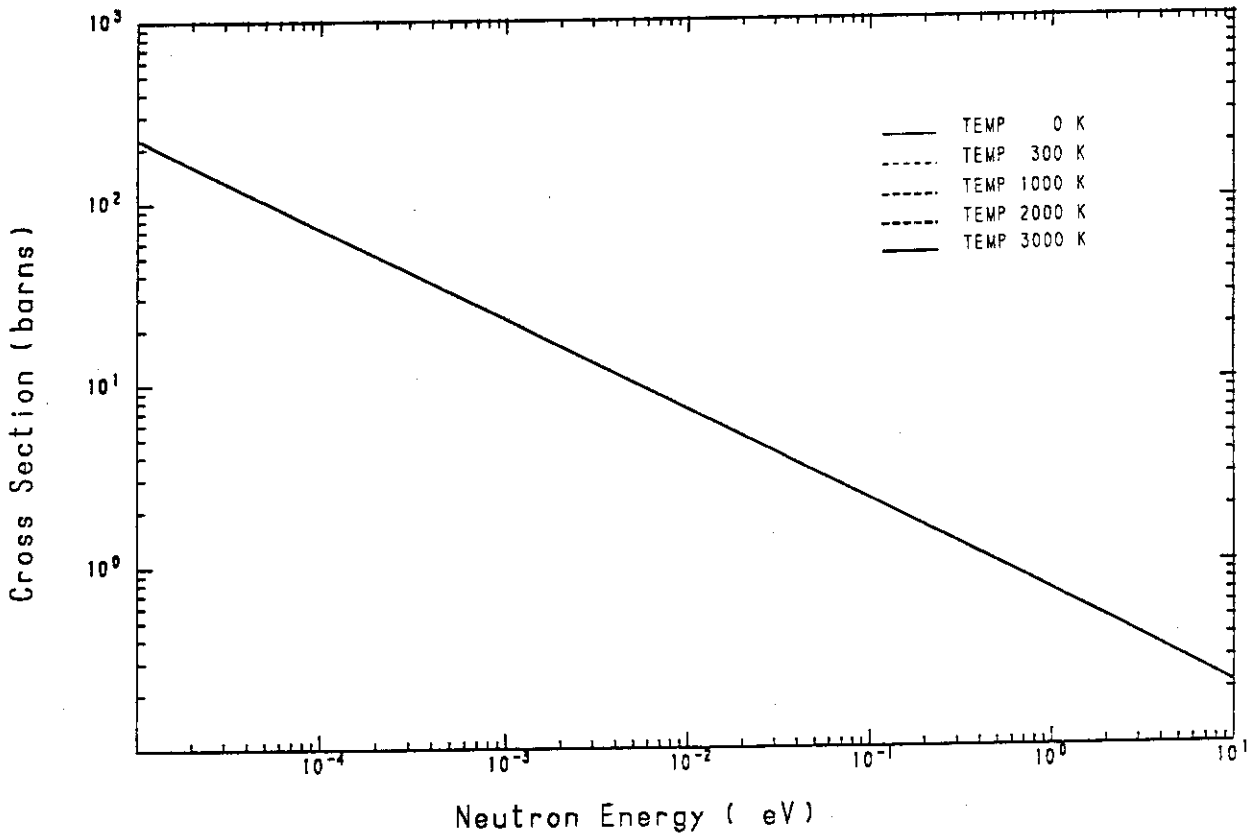


Fig. 10 Doppler broadened cross sections. The capture cross section in low energy region. The cross section in a form of  $1/v$  is not changed by the Doppler effect.

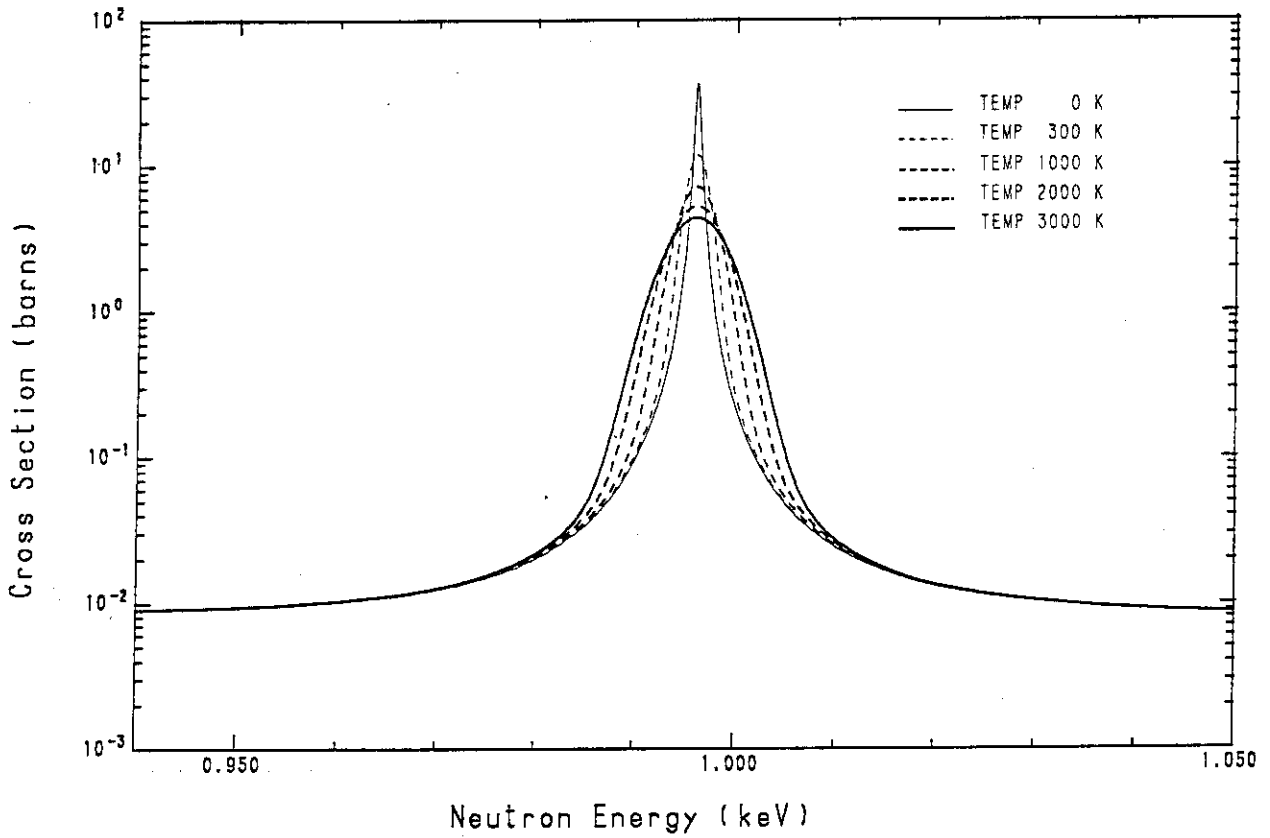


Fig. 11 Doppler broadened cross sections. The capture cross section around a narrow resonance.

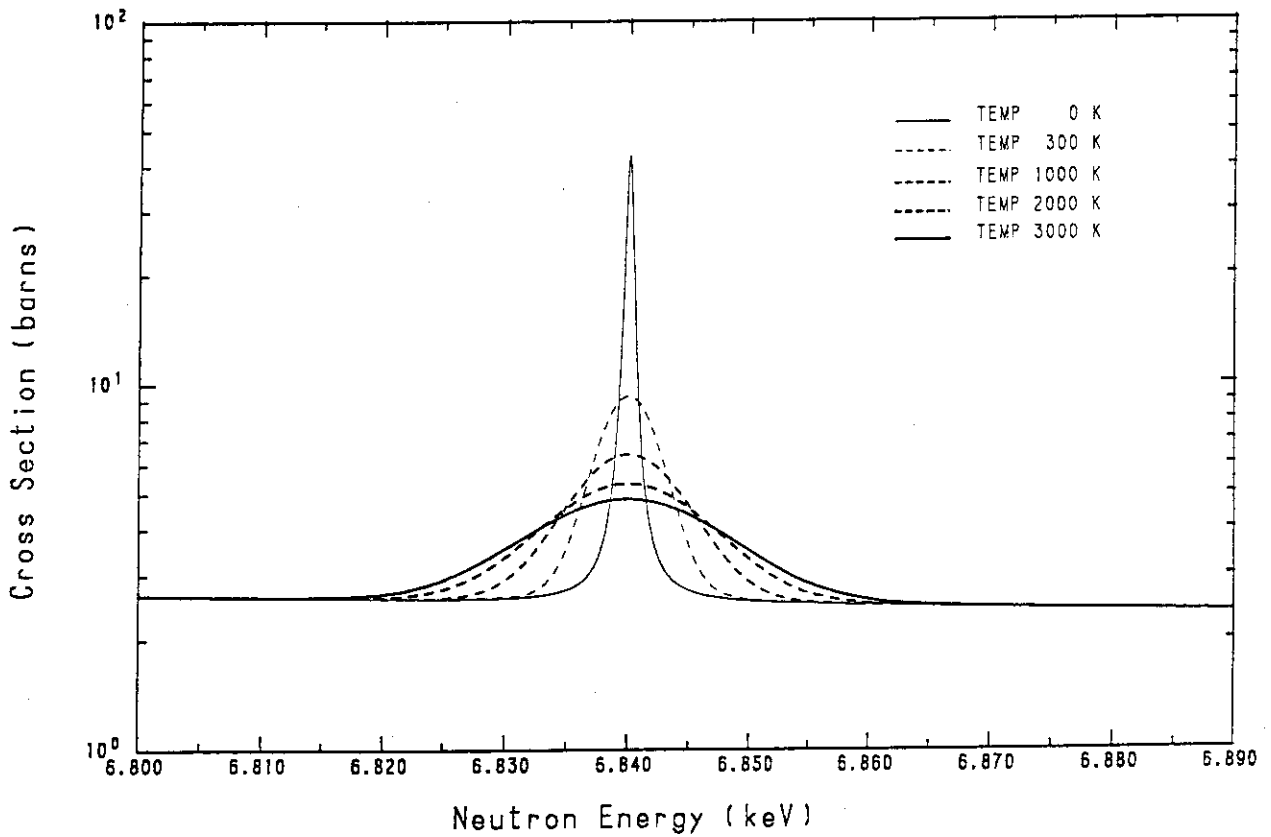


Fig. 12 Doppler broadened cross sections. The total cross section around a narrow resonance.

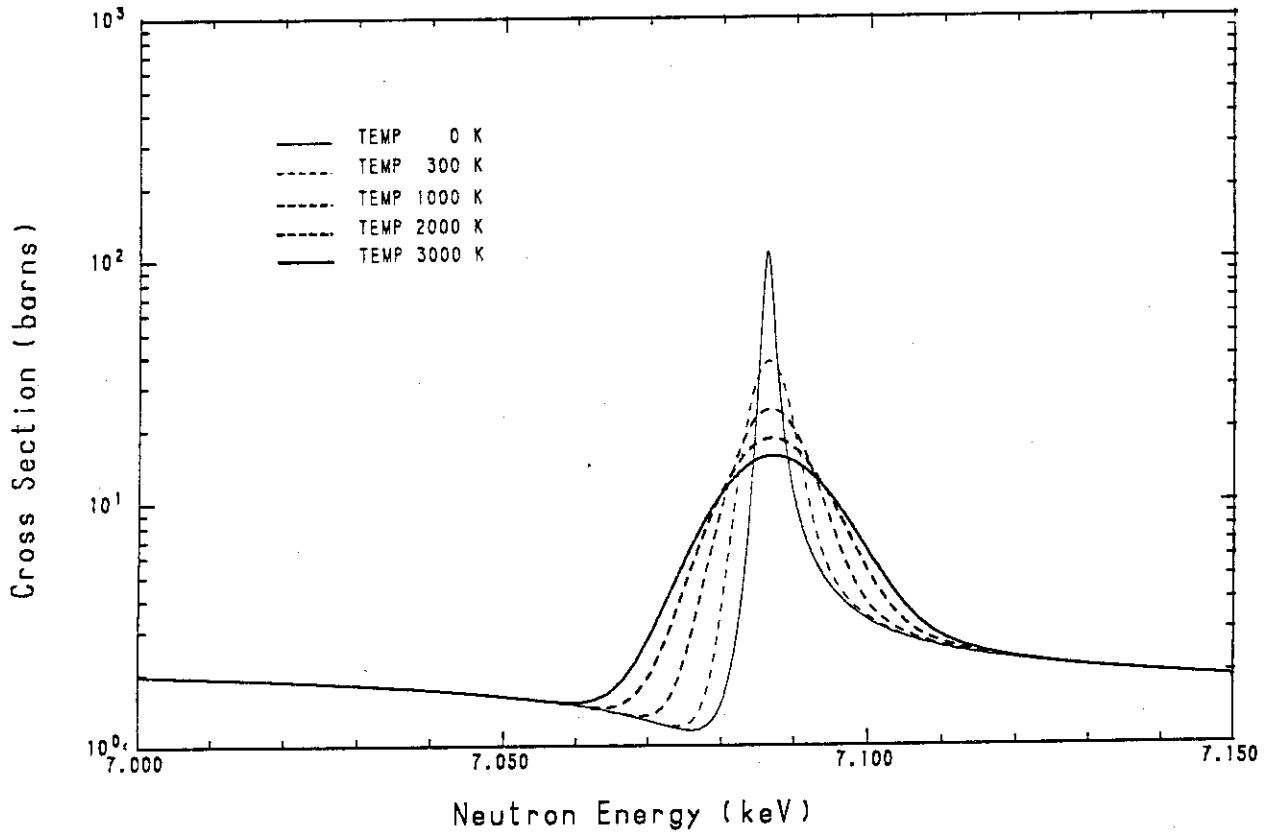


Fig. 13 Doppler broadened cross sections. The total cross section with a shape of s-wave potential interference.

## Appendix

## Derivation of Multi-level Breit-Wigner Formula Used in RESEND

The multi-level Breit-Wigner formula used in RESEND was modified to accept also J-unknown resonances and to shorten CPU time for calculation. In this appendix, derivation of Eq. (2.2) in the text is shown. The meaning of symbols used is the same as that in the text.

The elastic scattering cross section is written as follows by using the scattering matrix U.

$$\sigma_{n,n}(E) = \frac{\pi}{k^2} \sum_l \sum_J g_J |1 - U_{n,n}^J(E)|^2. \quad (\text{A.1})$$

Usually the scattering matrix is approximated as

$$U_{n,c}^J = \exp(-2i\phi_l) \left[ \delta_{n,c} + i \sum_r^{NR} \frac{\Gamma_{nr}^{1/2} \Gamma_{cr}^{1/2}}{E_r - E - i\Gamma_r/2} \right]. \quad (\text{A.2})$$

In order to take account of J-unknown resonances, we use the following scattering matrix in place of (A.2).

$$U_{n,c}^J = \exp(-2i\phi_l) \left[ \delta_{n,c} + i \sum_r^{NRJ} \frac{\Gamma_{nr}^{1/2} \Gamma_{cr}^{1/2}}{E_r - E - i\Gamma_r/2} + i \sum_u^{NRL} \frac{\delta_{Ju} \Gamma_{nu}^{1/2} \Gamma_{cu}^{1/2}}{E_u - E - i\Gamma_u/2} \right], \quad (\text{A.3})$$

where the first summation is for J-known resonances and the second summation for J-unknown resonances, and the quantity  $\delta_{Ju}$  in the second summation represents whether the J-value of the u-th resonance is J or not. It has a value of zero or one.

By using Eq. (A.3), the elastic scattering cross section is calculated as follows.

$$\sigma_{n,n}(E) = \frac{\pi}{k^2} \sum_l \left\{ 4(2\ell+1) \sin^2 \phi_l + \sum_J g_J \left[ (G_{J1})^2 + \frac{1}{4} (G_{J2})^2 + 2 \sin 2\phi_l \times G_{J1} - (1 - \cos 2\phi_l) G_{J2} \right] \right\}, \quad (\text{A.4})$$

where

$$G_{J1} \equiv \sum_r^{NRJ} \frac{\Gamma_{nr}(E-E_r')}{(E-E_r')^2 + \Gamma_r^2/4} + \sum_u^{NRL} \frac{\delta_{Ju}\Gamma_{nu}(E-E_u')}{(E-E_u')^2 + \Gamma_u^2/4}, \quad (A.5)$$

$$G_{J2} \equiv \sum_r^{NRJ} \frac{\Gamma_{nr}\Gamma_r}{(E-E_r')^2 + \Gamma_r^2/4} + \sum_u^{NRL} \frac{\delta_{Ju}\Gamma_{nu}\Gamma_u}{(E-E_u')^2 + \Gamma_u^2/4}, \quad (A.6)$$

Now, we calculate square of Eq. (A.5).

$$\begin{aligned} (G_{J1})^2 = & \left[ \sum_r^{NRJ} \frac{\Gamma_{nr}(E-E_r')}{(E-E_r')^2 + \Gamma_r^2/4} \right]^2 + 2 \sum_r^{NRJ} \frac{\Gamma_{nr}(E-E_r')}{(E-E_r')^2 + \Gamma_r^2/4} \times \sum_u^{NRL} \frac{\delta_{Ju}\Gamma_{nu}(E-E_u')}{(E-E_u')^2 + \Gamma_u^2/4} \\ & + \left[ \sum_u^{NRL} \frac{\delta_{Ju}\Gamma_{nu}(E-E_u')}{(E-E_u')^2 + \Gamma_u^2/4} \right]^2 \end{aligned} \quad (A.7)$$

The second term can be written as follows;

$$2P_{J1} \sum_r^{NRJ} \frac{\Gamma_{nr}(E-E_r')}{(E-E_r')^2 + \Gamma_r^2/4} \times \sum_u^{NRL} \frac{\Gamma_{nu}(E-E_u')}{(E-E_u')^2 + \Gamma_u^2/4}, \quad (A.8)$$

by assuming that

$$2P_{J1} \sum_u^{NRL} \frac{\Gamma_{nu}(E-E_u')}{(E-E_u')^2 + \Gamma_u^2/4} \equiv \sum_u^{NRL} \frac{\delta_{Ju}\Gamma_{nu}(E-E_u')}{(E-E_u')^2 + \Gamma_u^2/4}, \quad (A.9)$$

where the quantity  $P_{J1}$  represents a probability of resonances which have the total angular momentum of  $J$ . This quantity must be proportional to  $(2J+1)$ . In RESENDD, Eq. (2.8) is used to determine  $P_{J1}$ . The third term of Eq. (A.7) is

$$\begin{aligned} & \left[ \sum_u^{NRL} \frac{\delta_{Ju}\Gamma_{nu}(E-E_u')}{(E-E_u')^2 + \Gamma_u^2/4} \right]^2 \\ &= \sum_u^{NRL} \frac{\delta_{Ju}\Gamma_{nu}^2(E-E_u')}{[(E-E_u')^2 + \Gamma_u^2/4]^2} + \sum_u^{NRL} \sum_{u' \neq u}^{NRL} \frac{\delta_{Ju}\delta_{Ju'}\Gamma_{nu}\Gamma_{nu'}(E-E_u')(E-E_{u'})}{[(E-E_u')^2 + \Gamma_u^2/4][(E-E_{u'})^2 + \Gamma_{u'}^2/4]} \\ &= P_{J1} \sum_u^{NRL} \frac{\Gamma_{nu}^2(E-E_u')}{[(E-E_u')^2 + \Gamma_u^2/4]^2} + P_{J1} \sum_u^{NRL} \sum_{u' \neq u}^{NRL} \frac{\Gamma_{nu}\Gamma_{nu'}(E-E_u')(E-E_{u'})}{[(E-E_u')^2 + \Gamma_u^2/4][(E-E_{u'})^2 + \Gamma_{u'}^2/4]} \end{aligned}$$



$$\begin{aligned}
 &= P_{J1} \sum_u^{NRL} \frac{\Gamma_{nu}^2 (E-E_u')^2}{[(E-E_u')^2 + \Gamma_u^2/4]^2} \\
 &+ P_{J1} \cdot \left\{ \left[ \sum_u^{NRL} \frac{\Gamma_{nu} (E-E_u')}{[(E-E_u')^2 + \Gamma_u^2/4]} \right]^2 - \sum_u^{NRL} \frac{\Gamma_{nu}^2 (E-E_u')^2}{[(E-E_u')^2 + \Gamma_u^2/4]} \right\} \quad (A.10)
 \end{aligned}$$

The newly introduced quantity  $P_{J1}$  is a probability of resonances with the total angular momentum  $J$  among  $(NRL - 1)$  resonances. Therefore that can be calculated as

$$P_{J1} = \frac{P_{J1}(P_{J1}NRL-1)}{NRL-1}$$

The same calculation can be done for  $G_{J2}$ . Then,

$$\begin{aligned}
 &(G_{J1})^2 + \frac{1}{4} (G_{J2})^2 \\
 &= \left( \sum_r^{NRJ} \frac{\Gamma_{nr} (E-E_r')}{(E-E_r')^2 + \Gamma_r^2/4} \right)^2 + \frac{1}{4} \left( \sum_r^{NRJ} \frac{\Gamma_{nr} \Gamma_r}{(E-E_r')^2 + \Gamma_r^2/4} \right)^2 \\
 &+ 2P_{J1} \left[ \sum_r^{NRJ} \frac{\Gamma_{nr} (E-E_r')}{(E-E_r')^2 + \Gamma_r^2/4} \times \sum_u^{NRL} \frac{\Gamma_{nu} (E-E_u')}{(E-E_u')^2 + \Gamma_u^2/4} \right. \\
 &\quad \left. + \frac{1}{4} \sum_r^{NRJ} \frac{\Gamma_{nr} \Gamma_r}{(E-E_r')^2 + \Gamma_r^2/4} \times \sum_u^{NRL} \frac{\Gamma_{nu} \Gamma_u}{(E-E_u')^2 + \Gamma_u^2/4} \right] \\
 &+ P_{J1} \sum_u^{NRL} \frac{\Gamma_{nu}^2}{(E-E_u')^2 + \Gamma_u^2/4} + \frac{P_{J1}(P_{J1}NRL-1)}{(NRL-1)} \left[ \left( \sum_u^{NRL} \frac{\Gamma_{nu} (E-E_u')}{(E-E_u')^2 + \Gamma_u^2/4} \right)^2 \right. \\
 &\quad \left. + \frac{1}{4} \left( \sum_u^{NRL} \frac{\Gamma_{nu} \Gamma_u}{(E-E_u')^2 + \Gamma_u^2/4} \right)^2 - \sum_u^{NRL} \frac{\Gamma_{nu} \Gamma_u}{(E-E_u')^2 + \Gamma_u^2/4} \right]. \quad (A.11)
 \end{aligned}$$

We introduce the following two quantities in place of  $G_{J1}$  and  $G_{J2}$ .

$$F_{J1} \equiv \sum_r^{NRJ} \frac{\Gamma_{nr} (E-E_r')}{(E-E_r')^2 + \Gamma_r^2/4} + P_{J1} \sum_u^{NRL} \frac{\Gamma_{nu} (E-E_u')}{(E-E_u')^2 + \Gamma_u^2/4}, \quad (A.12)$$

$$F_{J2} \equiv \sum_r^{NRJ} \frac{\Gamma_{nr} \Gamma_r}{(E-E_r')^2 + \Gamma_r^2/4} + P_{J1} \sum_u^{NRL} \frac{\Gamma_{nu} \Gamma_u}{(E-E_u')^2 + \Gamma_u^2/4}, \quad (A.13)$$

Then,

$$G_{J1} = F_{J1},$$

$$G_{J2} = F_{J2},$$

$$(G_{J1})^2 + \frac{1}{4}(G_{J2})^2 = (F_{J1})^2 + \frac{1}{4}(F_{J2})^2 + P_{J1}(1-P_{J1})f_0 - \frac{P_{J1}(1-P_{J1})}{NRL-1}(f_1^2 + \frac{1}{4}f_2^2 - f_0). \quad (A.14)$$

Therefore

$$\sigma_{n,n}(E) = \frac{\pi}{k^2} \sum_l^{Nl} \left\{ (2l+1) \sin^2 \phi_l + \sum_J^{Nl} g_J \left[ (F_{J1})^2 + \frac{1}{4}(F_{J2})^2 + 2 \sin 2\phi_l \times F_{J1} - (1 - \cos 2\phi_l) F_{J2} + P_{J1}(1-P_{J1})f_0 - \frac{P_{J1}(1-P_{J1})}{NRL-1}(f_1^2 + \frac{1}{4}f_2^2 - f_0) \right] \right\}, \quad (A.15)$$

where

$$f_0 = \sum_u^{NRL} \frac{\Gamma_{nu}^2}{(E-E_u')^2 + \Gamma_u^2/4}, \quad (A.16)$$

$$f_1 = \sum_u^{NRL} \frac{\Gamma_{nu}(E-E_u')}{(E-E_u')^2 + \Gamma_u^2/4}, \quad (A.17)$$

and

$$f_2 = \sum_u^{NRL} \frac{\Gamma_{nu}\Gamma_u}{(E-E_u')^2 + \Gamma_u^2/4}. \quad (A.18)$$

This equation (A.15) is the same as Eq. (2.2) in the text. In the second summation of Eq. (A.15), the last term must be zero in the case where the number of J-unknown resonances is one. If the number of J-unknown resonances is zero, Eq. (A.15) is completely the same as the usual multi-level Breit-Wigner formula.