JAERI-M
84-192

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PROGRAM RESENDD (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

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編集兼発行　日本原子力研究所
印　　刷　㈱高野高速印刷

JAERI-M 84-192
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INDC(JPN) 93/GL

Program RESENDD (Version 84-07) : A Program for Reconstruction of Resonance Cross Sections from Evaluated Nuclear Data in the ENDF/B Format

(Modified Version of RESEND)

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(Received September 25, 1984)

RESENDD 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 RESENDD 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RESENDD（84－07版）

ENDF／Bフォーマットの評価ずみデータから共鳴断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）

RESENDDはENDF／Bフォーマットの評価ずみ共鳴パラメータから共鳴断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RESENDD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。

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1. Introduction

In the ENDF/B format[1,2], 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[3] 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 RESENDD was developed.

The work of RESENDD 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, RESENDD 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[4] 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 RESENDD 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$^{1)}$, 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$^{2)}$. 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. RESENDD 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 RESENDD, this function was added by referring to the ENDF/B format processing program RAMP1$^{5)}$.

Multi-level Breit-Wigner formula used in RESENDD

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.

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

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 RESENDD, 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

$$\begin{aligned}\sigma_{n,n}(E)=\frac{\pi}{k^2}\sum_{l}^{NL}\{&4(2\ell+1)\sin^2\varphi_l+\sum_{J}^{NJ}g_J\,[(F_{J1})^2+(F_{J2})^2/4+2\sin 2\varphi_l\times F_{J1}\\ &-(1-\cos 2\varphi_l)F_{J2}+P_{Jl}(1-P_{Jl})f_0\\ &-P_{Jl}(1-P_{Jl})(f_1^2+f_2^2/4-f_0)/(NRL-1)]\},\end{aligned} \tag{2.2}$$

where

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

$$F_{J2}=\sum_{r}^{NRJ}\frac{\Gamma_{nr}\Gamma_r}{(E-E_r')^2+\Gamma_r^2/4}+P_{Jl}f_2, \tag{2.4}$$

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

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

and

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

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

NL	the number of ℓ-states.
NJ	the number of J-states for a particular ℓ-state.
NRL	the number of ℓ-state resonances whose J value is unknown.
NRJ	the number of ℓ-state resonances whose J value is known.
k	the neutron wave number. $k=2.196771\times10^{-3}\frac{AWR}{AWR+1}\times\sqrt{E(\mathrm{eV})}$.
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, $E_r'=E_r+\frac{S_l(\lvert E_r\rvert)-S_l(E)}{2P_l(\lvert E_r\rvert)}\times\Gamma_{nr}(\lvert E_r\rvert)$.
Γ_{nr}	the neutron width (eV) of the r-th resonance, calculated at an incident energy of E (eV) as follows. $\Gamma_{nr}=\frac{P_l(E)}{P_l(\lvert E_r\rvert)}\times\Gamma_{nr}(\lvert E_r\rvert)$, where $\Gamma_{nr}(\lvert E_r\rvert)$ is the neutron width at the resonance energy E_r and given in an input file.
Γ_{fr}	the fission width (eV) of the r-th resonance.
$\Gamma_{\gamma r}$	the radiative width (eV) of the r-th resonance.
Γ_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).

φ_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. RESENDD considers that, if a given J value is an impossible value from the combination of ℓ 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 ℓ of incident neutrons. In RESENDD, by assuming that it is proportional to (2J+1), P_{Jl} is calculated as

$$P_{Jl} = N_{Jl} g_J \,/\, \sum_J N_{Jl} . g_J, \tag{2.8}$$

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.

$$\sigma_{n,f}(E)=\frac{\pi}{k^2}\sum_{l}^{NL}\sum_{J}^{NJ}g_J\sum_{r=1}^{NR}\frac{\Gamma_{nr}\Gamma_{fr}}{(E-E_r{}')^2+\Gamma_r^2/4}, \qquad (2.9)$$

$$\sigma_{n,\gamma}(E)=\frac{\pi}{k^2}\sum_{l}^{NL}\sum_{J}^{NJ}g_J\sum_{r=1}^{NR}\frac{\Gamma_{nr}\Gamma_{\gamma r}}{(E-E_r{}')^2+\Gamma_r^2/4}, \qquad (2.10)$$

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

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

Reich-Moore formula used in RESENDD

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.

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

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

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

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

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

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[6] 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 /
P_1, P_2, - - -
- - - -, P_{NTM}) 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 cm^{-12} at the neutron energy E(eV) is calculated as follows;

$$R(E) = P_1 + P_2E + \ldots + P_{NTM}E^{(NTM-1)}$$

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

(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 /
E_1, R_1, E_2, R_2, - -
- - , E_{NP}, R_{NP}) 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:

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

where $E_c=(E_i+E_{i+1})/2$, $\sigma^I(E_c)$ 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 ε 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 ε. 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 ==> E_{i+1},

E_{i+1} ==> E_{i+2}, 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, RESENDD has the following option.

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

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

where E_k and Γ_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:

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

where σ^N and σ^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. RESENDD 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,

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

$$-\exp[-\alpha(\sqrt{E'}+\sqrt{E})^2]\},\qquad(3.1)$$

where T is temperature in Kelvin and

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

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

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 RESENDD, Eq. (3.1) is calculated directly with almost the same numerical integration method as that applied in SIGMA1[4].

3.1 Numerical Integration

Eq. (3.1) can be rewritten as follows:

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

where

$x^2\equiv\alpha E'$, 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 ε (see Section 2.3). Therefore $\sigma(x,0)$ can be written as follows in the range from x_i and x_{i+1}:

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

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,

$$\sigma(y,T)=\sigma(y)^*-\sigma(-y)^*, \tag{3.4}$$

where

$$\sigma(y)^* \equiv \frac{1}{\pi^{1/2}y^2}\int_0^\infty x^2\sigma(x,0)\exp[-(x-y)^2]\,dx,$$

$$=\frac{1}{\pi^{1/2}y^2}\sum_i\int_{x_i}^{x_{i+1}} x^2[\sigma(x_i)+(x^2-x_i^2)S_i]\exp[-(x-y)^2]\,dx,$$

$$=\frac{1}{\pi^{1/2}y^2}\sum_i\int_{x_i-y}^{x_{i+1}-y} (z+y)^2[\sigma(x_i)-S_i x_i^2+(z+y)^2 S_i]\exp[-z^2]\,dz,$$

$$=\sum_i\{A_i[\sigma(x_i)-S_i x_i]+B_i S_i\}, \tag{3.5}$$

where

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

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

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:

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

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

$$=F_n(a)-F_n(b). \tag{3.9}$$

By using a recurrence formula of F_n:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

In RESENDD, 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:

$$y-4<x<y+4, \text{ and } 0<x, \tag{3.15}$$

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 1.13×10^{-7} which is small enough. For $\sigma(-y)^*$,

$$0<x<4-y, \tag{3.16}$$

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 $y\geqq4$, in other words $E\geqq16/\alpha$.

3.2 Data Handling in RESENDD

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 ε. 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),

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

For INT=4 (log-linear),

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

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

For INT=5 (log-log),

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

$$E_c = \exp\{\frac{1}{B-1}\ln(\frac{\sigma_i - \sigma_{i+1}}{E_i - E_{i+1}} \times \frac{1}{B})$$

$$- [\ln\sigma_{i+1}\ln E_i - \ln\sigma_i \ln E_{i+1}]/\ln(E_i/E_{i+1})\}, \quad \text{for } B \geqq 3.0, \qquad (3.19')$$

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

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

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

where $\sigma^L(E_c)$ and $\sigma^C(E_c)$ are the cross sections interpolated with linear-linear interpolation and with originally given interpolation, respectively, and ε is accuracy which is assumed to be the same as the value of ε 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 calculation 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, RESENDD 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.

RESENDD 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.0 .......
    OPTP
//*PROC=J2608.PROCLIB.CNTL
// EXEC RESENDD
// (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 RESENDD 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 RESENDD-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 inpiut file of EINF. If MATE is zero, the same MAT number as MAT is assumed.

ERR = (0.01) Accuracy of calculation (ε 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 α 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 $\geqq$ 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},20×10^{6}) An energy range of the Doppler broadening. The lower and upper boundaries are given in the form of

$E= E_1,E_2$. (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) LABFL 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 RESENDD 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 RESENDD                                       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 RESENDD, 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}Cu data of JENDL-2[7) by applying various values of accuracy. Table 4 lists number of energy points generated to reproduce cross section curves within the required accuracy ε, 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.

```
                                                 Card No.
MAT=2291,TEMP=300                                    4
GO                                                   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 RESENDD was used by Dr. Hasegawa, JAERI, to participate in the comparison. Some errors of RESENDD could be found through this comparison, and they have been corrected. The author acknowledges all of these valuable contributions.

References

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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

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

Table 2 Penetration factors

ℓ	P_l
0	ρ
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

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

Table 3 Hard-sphere scattering phase shifts

Hard-sphere scattering phase shists are calculated as shown in this table, by using the effective scattering radius given in an input file. Here, $\hat{\rho} = kR$.

ℓ	φ_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

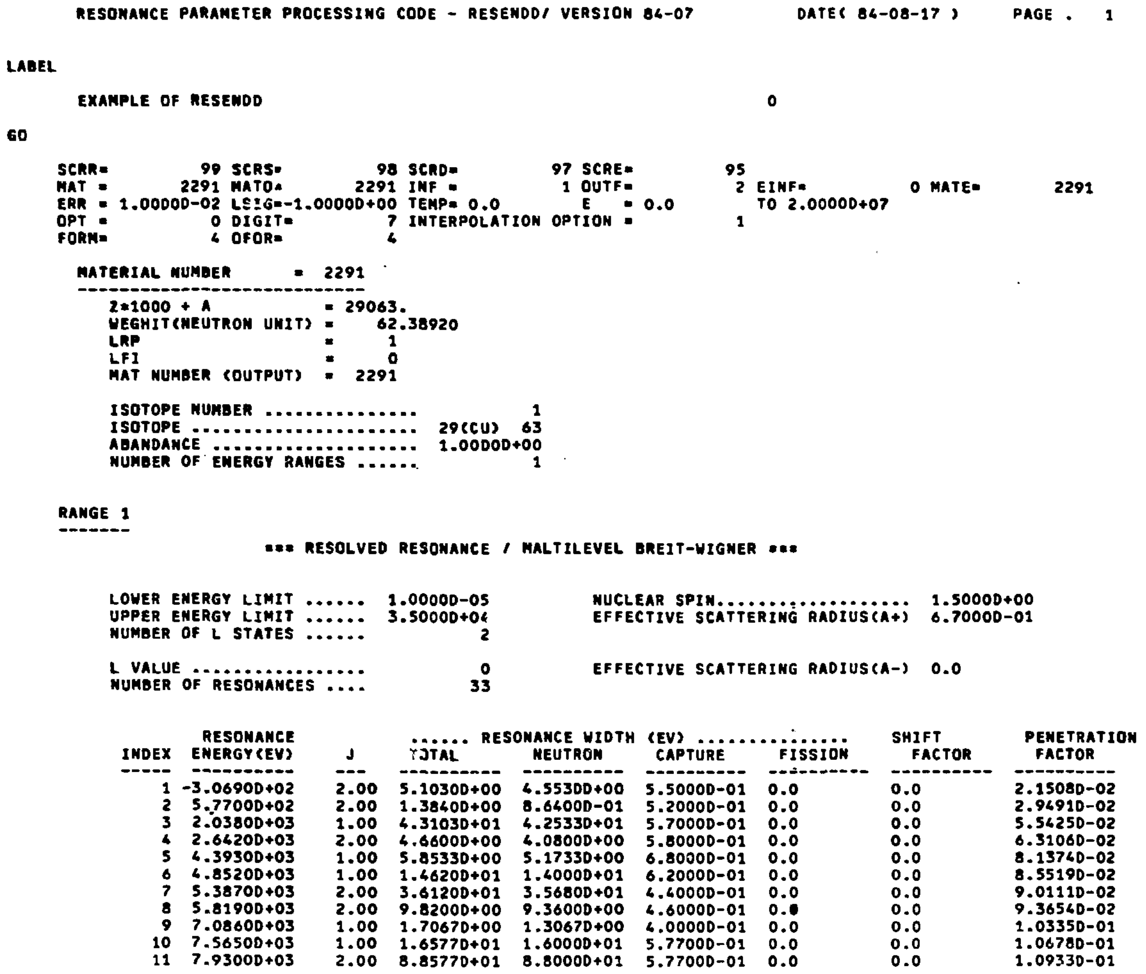
Resonance cross sections were calculated from the Cu-63 data of JENDL-2 with several kinds of accuracy. The number of energy points obtained in the resonance region and spent CPU time of FACOM-M 380 are compared.

ε	energy points	CPU time (sec)
0.5	602	1.1
0.1	1156	1.9
0.05	1641	2.5
0.01	3585	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



```
       RESONANCE PARAMETER PROCESSING CODE - RESENDD/ VERSION 84-07         DATE( 84-08-17 )     PAGE .   1

LABEL

       EXAMPLE OF RESENDD                                                  0

GO

     SCRR=          99 SCRS=          98 SCRD=          97 SCRE=          95
     MAT =        2291 MATO=        2291 INF =           1 OUTF=           2 EINF=           0 MATE=        2291
     ERR = 1.0000D-02 LS:G=-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.
          WEGHIT(NEUTRON UNIT) =     62.38920
          LRP                  =      1
          LFI                  =      0
          MAT NUMBER (OUTPUT)  =  2291

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


     RANGE 1
     -------
                         *** RESOLVED RESONANCE / MALTILEVEL 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


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

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

```
      RESONANCE PARAMETER PROCESSING CODE - RESENDD/ VERSION 84-07          DATE( 84-08-17 )     PAGE .   2

                 RESONANCE                ...... RESONANCE WIDTH (EV) ...............     SHIFT         PENETRATION
           INDEX  ENERGY(EV)       J      TOTAL        NEUTRON      CAPTURE      FISSION      FACTOR        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      1.00  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  3.6200D+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

                 RESONANCE                ...... RESONANCE WIDTH (EV) ...............     SHIFT         PENETRATION
           INDEX  ENERGY(EV)       J      TOTAL        NEUTRON      CAPTURE      FISSION      FACTOR        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 RESENDD                                                   0
 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
                     2200 M/S      RES. INTEG.                       2291 1451   24
        ELASTIC       4.979 B          -                             2291 1451   25
        CAPTURE       4.492 B        5.41 B                          2291 1451   26
        TOTAL         9.471 B          -                             2291 1451   27
                                                                     2291 1451   28
MF=3  NEUTRON CROSS SECTIONS                                         2291 1451   29
  BELOW 35 KEV, ALL BACKGROUND CROSS SECTIONS ARE ZERO.              2291 1451   30
  ABOVE 35 KEV, DATA WERE EVALUATED AS FOLLOWS,                      2291 1451   31
  MT=1    TOTAL                                                      2291 1451   32
     OPTICAL AND STATISTICAL MODEL CALCULATION WAS MADE WITH         2291 1451   33
     CODE CASTHY /3/.  THE OPTICAL POTENTIAL PARAMETERS USED ARE     2291 1451   34
     AS FOLLOWS (IN THE UNITS OF MEV AND FERMI),                     2291 1451   35
      V   = 46.0 - 0.250*E    , RO = 1.16*A**1/3+0.6, AO = 0.62      2291 1451   36
      WI =0.125*E-0.0004*E**2, RI = 1.16*A**1/3+0.6, AI = 0.62       2291 1451   37
      WS = 7.0                , RS = 1.16*A**1/3+1.1, AS = 0.35      2291 1451   38
      WSO= 7.0                , RSO= 1.16*A**1/3+0.6, ASO= 0.60      2291 1451   39
  MT=2    ELASTIC SCATTERING                                         2291 1451   40
     (TOTAL)-(ALL OTHER PARTIAL CROSS SECTIONS)                      2291 1451   41
  MT=4,51-57,91  INELASTIC SCATTERING                                2291 1451   42
     OPTICAL AND STATISTICAL MODEL CALCULATION WAS MADE BY TAKING 2291 1451   43
     INTO ACCOUNT OF (N,2N), (N,N'A) AND (N,A) REACTIONS AS COM-     2291 1451   44
     PETING PROCESSES.  THE LEVEL SCHEME WAS TAKEN FROM REF. /4/. 2291 1451   45
         NO.     ENERGY(MEV)    SPIN-PARITY                          2291 1451   46
         G.S.     0.0            3/2 -                               2291 1451   47
          1       0.66962        1/2 -                               2291 1451   48
          2       0.96206        5/2 -                               2291 1451   49
          3       1.32703        7/2 -                               2291 1451   50
          4       1.41203        5/2 -                               2291 1451   51
          5       1.54702        3/2 -                               2291 1451   52
          6       1.8613         5/2 -                               2291 1451   53
          7       2.0111         3/2 -                               2291 1451   54
      LEVELS ABOVE 2.05 MEV WERE ASSUMED TO BE OVERLAPPING.          2291 1451   55
  MT=16,22,107  (N,2N),(N,N'A) AND (N,A)                             2291 1451   56
     RECOMMENDED BY KOBAYASHI /5/.                                   2291 1451   57
  MT=102  CAPTURE                                                    2291 1451   58
     CALCULATED WITH CASTHY /3/ AND NORMALIZED TO THE VALUE OF       2291 1451   59
     23.7 MILLI-BARNS AT 230 KEV WHICH WAS MEASURED BY ZAIKIN /6/.2291 1451   60
  MT=251  MU-BAR                                                     2291 1451   61
     CALCULATED WITH CASTHY /3/.                                     2291 1451   62
                                                                     2291 1451   63
MF=4  ANGULAR DISTRIBUTIONS OF SECONDARY NEUTRONS                    2291 1451   64
  MT=2,51-57  : CALCULATED WITH CASTHY /3/.                          2291 1451   65
  MT=16,22    : ASSUMED TO BE ISOTROPIC IN THE LAB SYSTEM.           2291 1451   66
  MT=91       : ASSUMED THE SAME DISTRIBUTIONS IN THE LAB SYSTEM     2291 1451   67
                AS THOSE CALCULATED WITH CASTHY IN THE CENTER-       2291 1451   68
                OF-MASS SYSTEM.                                      2291 1451   69
                                                                     2291 1451   70
MF=5  ENERGY DISTRIBUTIONS OF SECONDARY NEUTRONS                     2291 1451   71
```

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

```
  MT=16,22,91 : EVAPORATION SPECTRA.                              2291 1451   72
                                                                  2291 1451   73
REFERENCES                                                        2291 1451   74
 1) MUGHABGHAB S.F. AND GARBER D.I.: BNL 325, 3RD ED., VOL. 1     2291 1451   75
    (1973).                                                       2291 1451   76
 2) MUGHABGHAB S.F. ET AL.: "NEUTRON CROSS SECTIONS, VOL. 1,      2291 1451   77
    PART A", ACADEMIC PRESS (1981).                               2291 1451   78
 3) IGARASI S.: J. NUCL. SCI. TECHNOL., 12, 67 (1975).            2291 1451   79
 4) AUBLE R.L.: NUCLEAR DATA SHEETS, 14, 119 (1975).              2291 1451   80
 5) KOBAYASHI K.: PRIVATE COMMUNICATION.                          2291 1451   81
 6) ZAIKIN G.G. ET AL.: ATOMNAYA ENERGIYA, 25, 526 (1968).        2291 1451   82
                                                                  2291 1451   83
                                                                  2291 1451   84
 ***** RESENDD CALCULATION UNDER THE FOLLOWING PARAMETERS *****   2291 1451   85
                                                                  2291 1451   86
  ACCURACY ............. 0.0100    MINIMUM X-SECTION ...-1.000D+00 2291 1451   87
  INTERPOLATION OPT. .. X-SECT.    OUTPUT OPTION .......     0    2291 1451   88
  TEMPERATURE ......... 0.0                                       2291 1451   89
                                                                  2291 1451   90
                                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
                                                                  2291 1  0  123
                                                                  2291 0  0  124
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+ 22291 3  1  134
2.234862-5 1.56149+ 2 2.852293-5 1.38790+ 2 3.469725-5 1.26302+ 22291 3  1  135
4.704587-5 1.09170+ 2 5.939450-5 9.77083+ 1 7.174312-5 8.93513+ 12291 3  1  136
8.409175-5 8.29106+ 1 1.087890-4 7.34959+ 1 1.334862-4 6.68336+ 12291 3  1  137
1.581835-4 6.18001+ 1 2.075781-4 5.45811+ 1 2.569726-4 4.95598+ 12291 3  1  138
3.063671-4 4.58081+ 1 4.051562-4 4.04832+ 1 5.039452-4 3.68136+ 12291 3  1  139
6.027343-4 3.40881+ 1 8.003125-4 3.02406+ 1 9.978907-4 2.76020+ 12291 3  1  140
1.195469-3 2.56481+ 1 1.590625-3 2.28977+ 1 1.985781-3 2.10161+ 12291 3  1  141
2.380937-3 1.96249+ 1 3.171250-3 1.76694+ 1 3.961562-3 1.63332+ 12291 3  1  142
4.751875-3 1.53460+ 1 6.332500-3 1.39594+ 1 7.913125-3 1.30125+ 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+ 12291 3  1  216
6.495402+2 1.41450+ 1 6.495756+2 1.55363+ 1 6.496110+2 1.72325+ 12291 3  1  217
6.496464+2 1.93193+ 1 6.496818+2 2.19085+ 1 6.497172+2 2.51447+ 12291 3  1  218
6.497526+2 2.92065+ 1 6.497880+2 3.42973+ 1 6.498234+2 4.06012+ 12291 3  1  219
6.498588+2 4.81679+ 1 6.498942+2 5.66781+ 1 6.499471+2 6.87042+ 12291 3  1  220
6.499735+2 7.26275+ 1 6.500000+2 7.40522+ 1 6.500264+2 7.26397+ 12291 3  1  221
6.500529+2 6.87074+ 1 6.501058+2 5.66829+ 1 6.501438+2 4.75776+ 12291 3  1  222
6.501818+2 3.95985+ 1 6.502198+2 3.30792+ 1 6.502578+2 2.79163+ 12291 3  1  223
6.502958+2 2.38691+ 1 6.503338+2 2.06937+ 1 6.503718+2 1.81859+ 12291 3  1  224
6.504099+2 1.61823+ 1 6.504479+2 1.45734+ 1 6.504859+2 1.32641+ 12291 3  1  225
6.505239+2 1.21875+ 1 6.505620+2 1.12916+ 1 6.506380+2 9.91053+ 02291 3  1  226
6.507141+2 8.90838+ 0 6.507901+2 8.16223+ 0 6.508661+2 7.59210+ 02291 3  1  227
6.509421+2 7.14723+ 0 6.510182+2 6.79331+ 0 6.510942+2 6.50798+ 02291 3  1  228
6.511703+2 6.27408+ 0 6.512463+2 6.08046+ 0 6.513224+2 5.91798+ 02291 3  1  229
6.514744+2 5.66332+ 0 6.516265+2 5.47459+ 0 6.517786+2 5.33078+ 02291 3  1  230
6.519307+2 5.21854+ 0 6.520827+2 5.12918+ 0 6.522348+2 5.05667+ 02291 3  1  231
6.523869+2 4.99693+ 0 6.525390+2 4.94705+ 0 6.528431+2 4.86883+ 02291 3  1  232
6.531473+2 4.81052+ 0 6.534514+2 4.76552+ 0 6.537556+2 4.72969+ 02291 3  1  233
6.540597+2 4.70045+ 0 6.543639+2 4.67601+ 0 6.549722+2 4.63717+ 02291 3  1  234
6.555805+2 4.60714+ 0 6.561888+2 4.58271+ 0 6.567971+2 4.56202+ 02291 3  1  235
6.574054+2 4.54394+ 0 6.586220+2 4.51299+ 0 6.598386+2 4.48651+ 02291 3  1  236
6.610552+2 4.46287+ 0 6.622718+2 4.44118+ 0 6.647050+2 4.40182+ 02291 3  1  237
6.671382+2 4.36620+ 0 6.695715+2 4.33330+ 0 6.744379+2 4.27364+ 02291 3  1  238
6.793044+2 4.22032+ 0 6.890373+2 4.12795+ 0 6.987702+2 4.04994+ 02291 3  1  239
7.085031+2 3.98265+ 0 7.182360+2 3.92368+ 0 7.279689+2 3.87130+ 02291 3  1  240
7.474346+2 3.78156+ 0 7.669004+2 3.70668+ 0 7.766333+2 3.67370+ 02291 3  1  241
7.814997+2 3.65835+ 0 7.863662+2 3.64402+ 0 7.887994+2 3.63743+ 02291 3  1  242
7.912326+2 3.63145+ 0 7.936658+2 3.62653+ 0 7.948824+2 3.62474+ 02291 3  1  243
7.960991+2 3.62369+ 0 7.973157+2 3.62382+ 0 7.979240+2 3.62455+ 02291 3  1  244
7.985323+2 3.62592+ 0 7.991406+2 3.62817+ 0 7.997489+2 3.63164+ 02291 3  1  245
8.003572+2 3.63691+ 0 8.009655+2 3.64486+ 0 8.012696+2 3.65030+ 02291 3  1  246
8.015738+2 3.65708+ 0 8.018779+2 3.66559+ 0 8.021821+2 3.67643+ 02291 3  1  247
8.024862+2 3.69041+ 0 8.027904+2 3.70878+ 0 8.030945+2 3.73340+ 02291 3  1  248
8.033987+2 3.76735+ 0 8.035507+2 3.78928+ 0 8.037028+2 3.81572+ 02291 3  1  249
8.038549+2 3.84795+ 0 8.040070+2 3.88772+ 0 8.041590+2 3.93751+ 02291 3  1  250
8.043111+2 4.00099+ 0 8.044632+2 4.08349+ 0 8.046153+2 4.19326+ 02291 3  1  251
8.047673+2 4.34330+ 0 8.048433+2 4.43975+ 0 8.049194+2 4.55563+ 02291 3  1  252
8.049954+2 4.69595+ 0 8.050715+2 4.86830+ 0 8.051475+2 5.08215+ 02291 3  1  253
8.052236+2 5.35193+ 0 8.052996+2 5.69656+ 0 8.053757+2 6.14521+ 02291 3  1  254
8.054517+2 6.73741+ 0 8.055278+2 7.53334+ 0 8.056038+2 8.61203+ 02291 3  1  255
8.056799+2 1.00768+ 1 8.057559+2 1.20072+ 1 8.058320+2 1.43477+ 12291 3  1  256
8.059160+2 1.68326+ 1 8.059580+2 1.76442+ 1 8.060000+2 1.79376+ 12291 3  1  257
8.060420+2 1.76450+ 1 8.060840+2 1.68340+ 1 8.061680+2 1.43498+ 12291 3  1  258
8.062606+2 1.15494+ 1 8.063069+2 1.03791+ 1 8.063532+2 9.38725+ 02291 3  1  259
8.063995+2 8.55908+ 0 8.064458+2 7.87179+ 0 8.064921+2 7.30181+ 02291 3  1  260
8.065384+2 6.82791+ 0 8.065847+2 6.43213+ 0 8.066310+2 6.09977+ 02291 3  1  261
8.067236+2 5.58032+ 0 8.068162+2 5.20053+ 0 8.069088+2 4.91624+ 02291 3  1  262
8.070014+2 4.69881+ 0 8.070940+2 4.52927+ 0 8.071866+2 4.39478+ 02291 3  1  263
8.072792+2 4.28645+ 0 8.073718+2 4.19799+ 0 8.074644+2 4.12488+ 02291 3  1  264
8.076497+2 4.01218+ 0 8.078349+2 3.93064+ 0 8.080201+2 3.86973+ 02291 3  1  265
8.082053+2 3.82303+ 0 8.083905+2 3.78644+ 0 8.085757+2 3.75721+ 02291 3  1  266
8.087609+2 3.73348+ 0 8.089461+2 3.71393+ 0 8.091314+2 3.69762+ 02291 3  1  267
8.095018+2 3.67212+ 0 8.098722+2 3.65325+ 0 8.102426+2 3.63882+ 02291 3  1  268
8.106131+2 3.62747+ 0 8.109835+2 3.61833+ 0 8.113539+2 3.61082+ 02291 3  1  269
8.120948+2 3.59916+ 0 8.128356+2 3.59047+ 0 8.135765+2 3.58365+ 02291 3  1  270
8.143173+2 3.57806+ 0 8.150582+2 3.57333+ 0 8.165399+2 3.56552+ 02291 3  1  271
8.180217+2 3.55909+ 0 8.195034+2 3.55347+ 0 8.209851+2 3.54837+ 02291 3  1  272
8.239486+2 3.53912+ 0 8.269120+2 3.53062+ 0 8.298755+2 3.52257+ 02291 3  1  273
8.358024+2 3.50729+ 0 8.417293+2 3.49272+ 0 8.535831+2 3.46497+ 02291 3  1  274
8.772907+2 3.41338+ 0 9.009983+2 3.36560+ 0 9.247058+2 3.32081+ 02291 3  1  275
9.365596+2 3.29941+ 0 9.484134+2 3.27873+ 0 9.543403+2 3.26874+ 02291 3  1  276
9.602672+2 3.25909+ 0 9.661941+2 3.24998+ 0 9.691575+2 3.24576+ 02291 3  1  277
9.721210+2 3.24191+ 0 9.750844+2 3.23863+ 0 9.780479+2 3.23632+ 02291 3  1  278
9.795296+2 3.23575+ 0 9.810113+2 3.23579+ 0 9.824930+2 3.23672+ 02291 3  1  279
9.839748+2 3.23900+ 0 9.847156+2 3.24087+ 0 9.854565+2 3.24343+ 02291 3  1  280
9.861973+2 3.24687+ 0 9.869382+2 3.25152+ 0 9.876790+2 3.25781+ 02291 3  1  281
9.884199+2 3.26642+ 0 9.891608+2 3.27839+ 0 9.899017+2 3.29545+ 02291 3  1  282
9.902721+2 3.30675+ 0 9.906425+2 3.32059+ 0 9.910129+2 3.33777+ 02291 3  1  283
9.913834+2 3.35938+ 0 9.917538+2 3.38702+ 0 9.921242+2 3.42309+ 02291 3  1  284
9.924946+2 3.47129+ 0 9.928651+2 3.53762+ 0 9.930503+2 3.58050+ 02291 3  1  285
9.932355+2 3.63221+ 0 9.934207+2 3.69534+ 0 9.936059+2 3.77347+ 02291 3  1  286
9.937911+2 3.87168+ 0 9.939763+2 3.99741+ 0 9.941615+2 4.16183+ 02291 3  1  287
```

Fig. 2 (Continued)

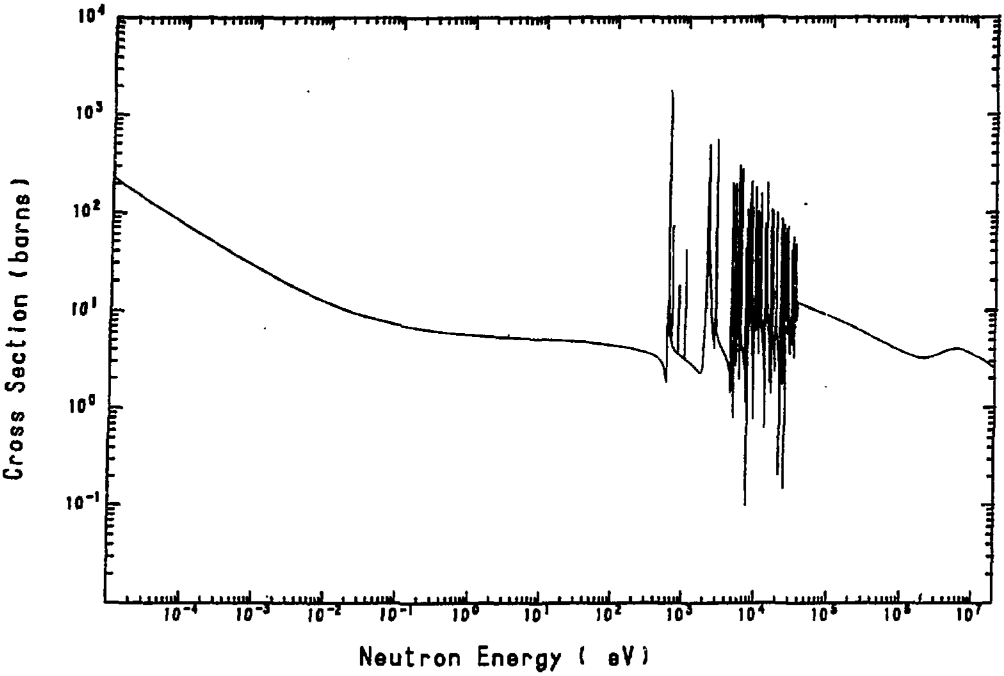


Fig. 3 Total cross section obtained by Example 1.

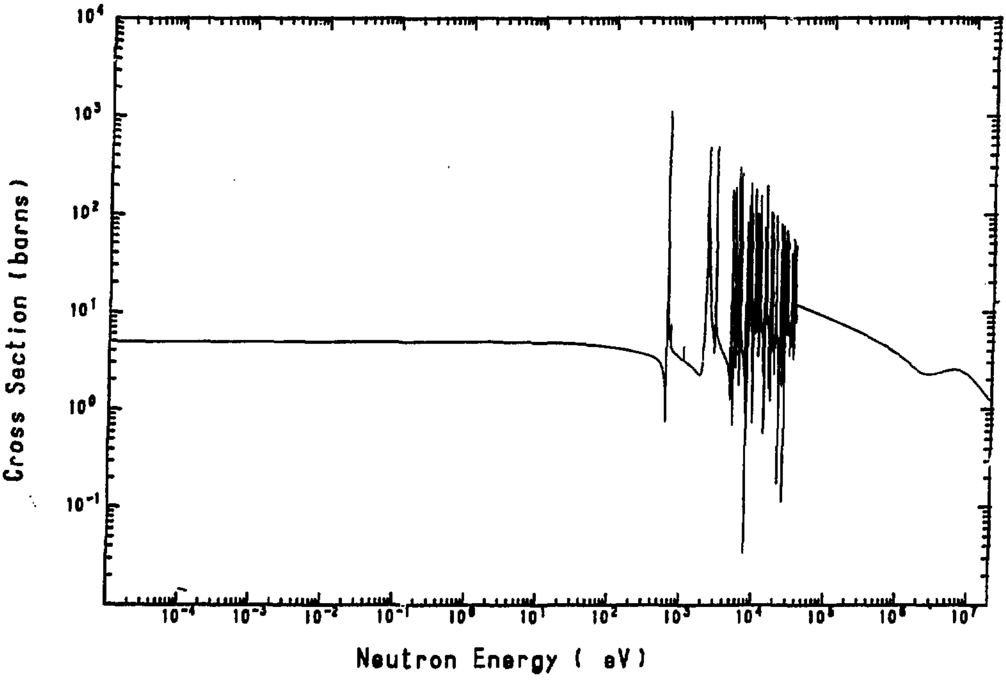


Fig. 4 Elastic scattering cross section obtained by Example 1.

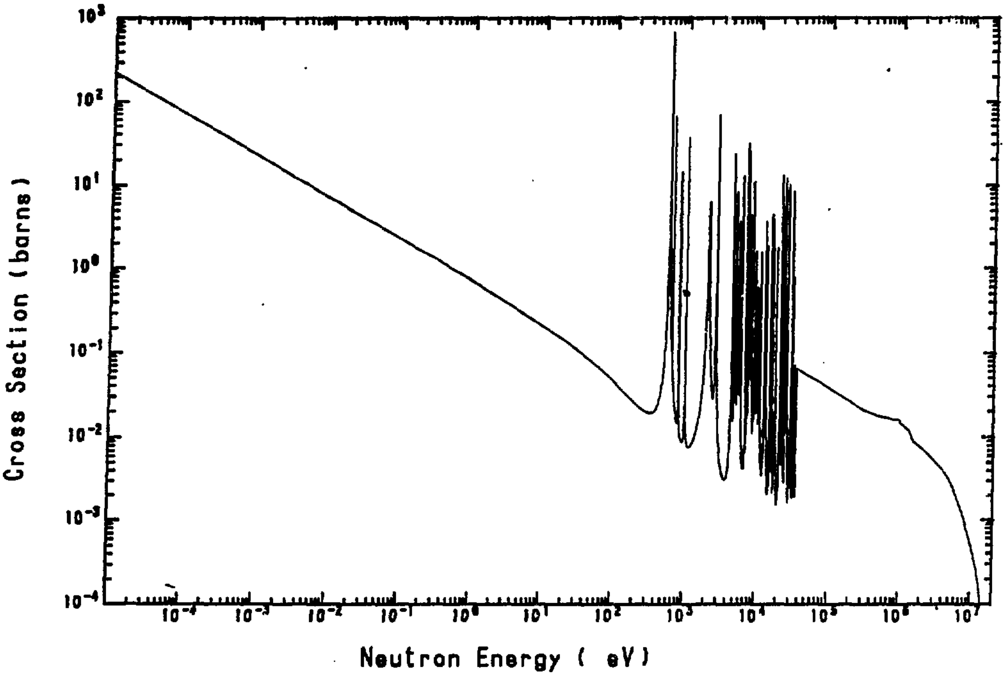


Fig. 5 Capture cross section obtained by Example 1.

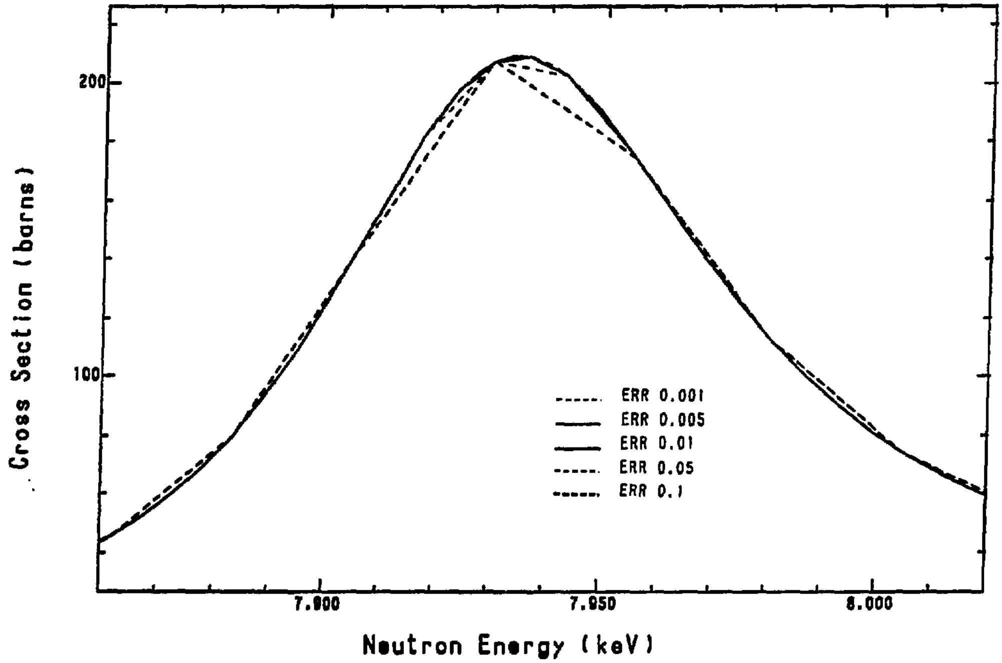


Fig. 6 Total cross section of Cu-63, around the 7.93-keV resonance. The cross section was calculated with various values of ε.

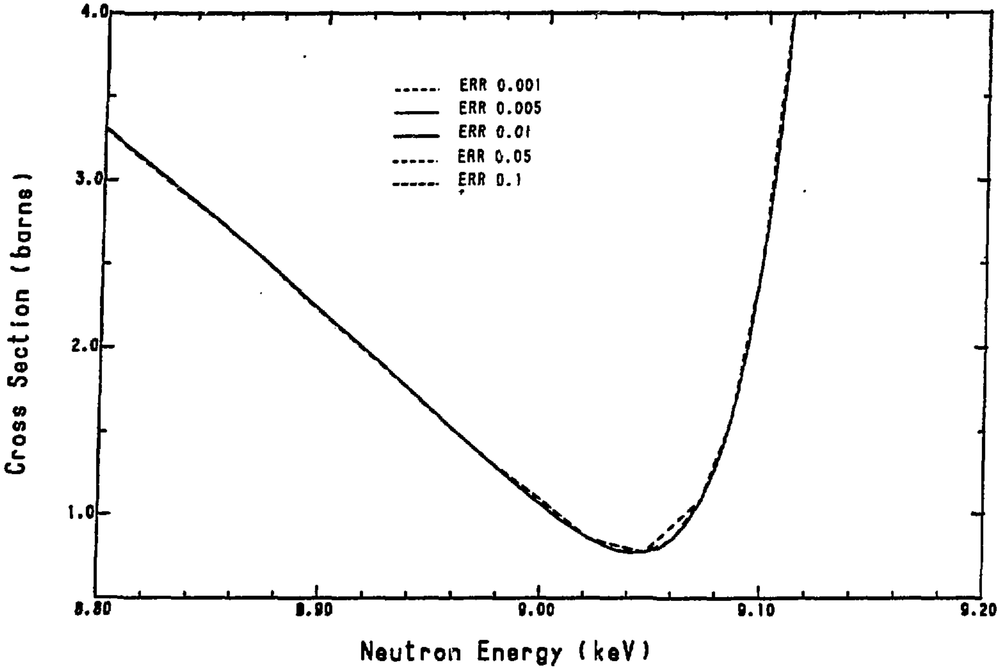
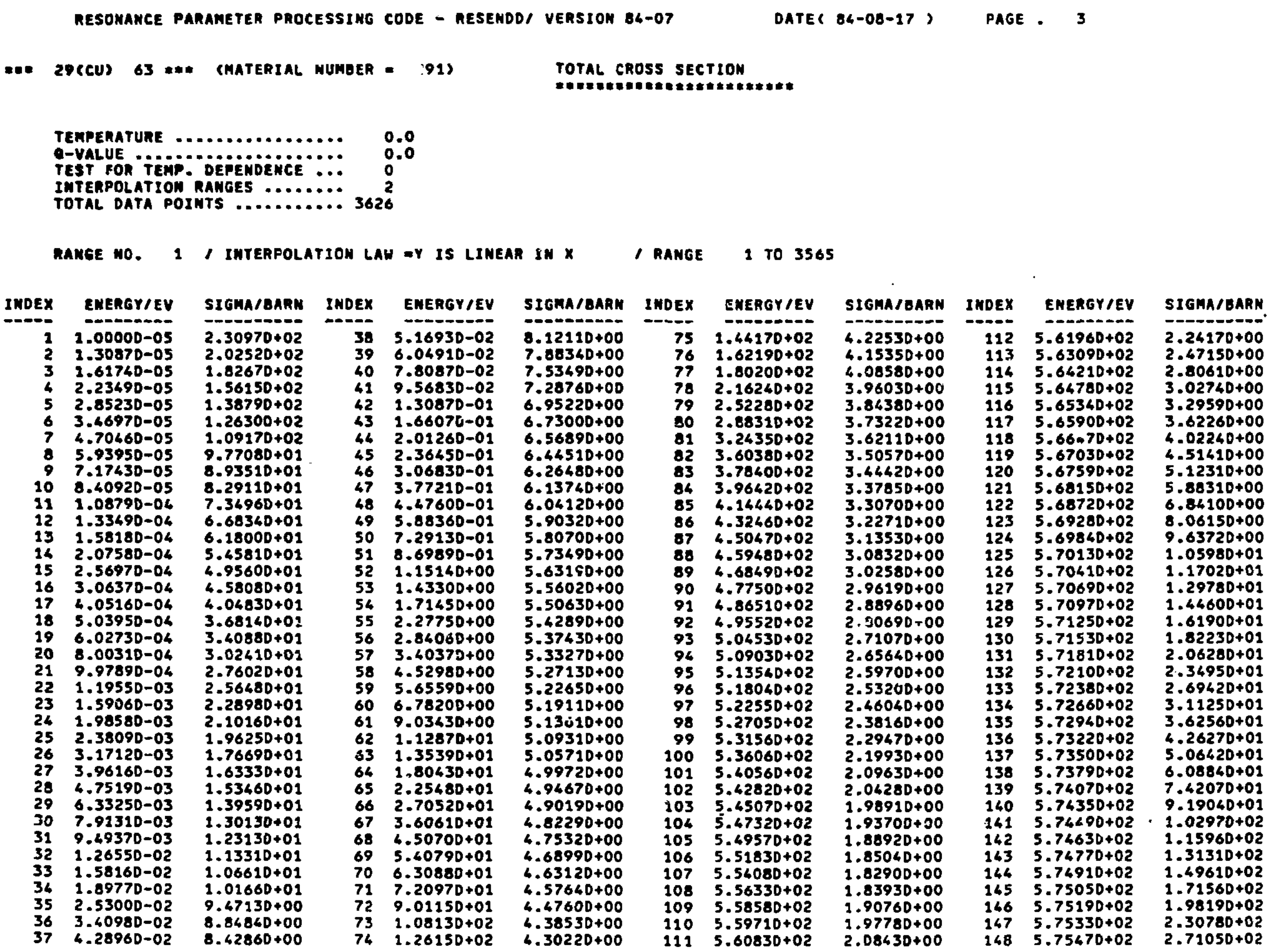


Fig. 7 Total cross section of Cu-63, around a cross-section minimum. The cross section was calculated with various values of ε.



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     RESONANCE PARAMETER PROCESSING CODE - RESENDD/ VERSION 84-07          DATE( 84-08-17 )     PAGE .   3

***  29(CU)  63 ***  (MATERIAL NUMBER =  :91)          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  1.0000D-05    2.3097D+02      38  5.1693D-02    8.1211D+00      75  1.4417D+02    4.2253D+00     112  5.6196D+02    2.2417D+00
    2  1.3087D-05    2.0252D+02      39  6.0491D-02    7.8834D+00      76  1.6219D+02    4.1535D+00     113  5.6309D+02    2.4715D+00
    3  1.6174D-05    1.8267D+02      40  7.8087D-02    7.5349D+00      77  1.8020D+02    4.0858D+00     114  5.6421D+02    2.8061D+00
    4  2.2349D-05    1.5615D+02      41  9.5683D-02    7.2876D+0D      78  2.1624D+02    3.9603D+00     115  5.6478D+02    3.0274D+00
    5  2.8523D-05    1.3879D+02      42  1.3087D-01    6.9522D+00      79  2.5228D+02    3.8438D+00     116  5.6534D+02    3.2959D+00
    6  3.4697D-05    1.2630D+02      43  1.6607D-01    6.7300D+00      80  2.8831D+02    3.7322D+00     117  5.6590D+02    3.6226D+00
    7  4.7046D-05    1.0917D+02      44  2.0126D-01    6.5689D+00      81  3.2435D+02    3.6211D+00     118  5.6647D+02    4.0224D+00
    8  5.9395D-05    9.7708D+01      45  2.3645D-01    6.4451D+00      82  3.6038D+02    3.5057D+00     119  5.6703D+02    4.5141D+00
    9  7.1743D-05    8.9351D+01      46  3.0683D-01    6.2648D+00      83  3.7840D+02    3.4442D+00     120  5.6759D+02    5.1231D+00
   10  8.4092D-05    8.2911D+01      47  3.7721D-01    6.1374D+00      84  3.9642D+02    3.3785D+00     121  5.6815D+02    5.8831D+00
   11  1.0879D-04    7.3496D+01      48  4.4760D-01    6.0412D+00      85  4.1444D+02    3.3070D+00     122  5.6872D+02    6.8410D+00
   12  1.3349D-04    6.6834D+01      49  5.8836D-01    5.9032D+00      86  4.3246D+02    3.2271D+00     123  5.6928D+02    8.0615D+00
   13  1.5818D-04    6.1800D+01      50  7.2913D-01    5.8070D+00      87  4.5047D+02    3.1353D+00     124  5.6984D+02    9.6372D+00
   14  2.0758D-04    5.4581D+01      51  8.6989D-01    5.7349D+00      88  4.5948D+02    3.0832D+00     125  5.7013D+02    1.0598D+01
   15  2.5697D-04    4.9560D+01      52  1.1514D+00    5.6319D+00      89  4.6849D+02    3.0258D+00     126  5.7041D+02    1.1702D+01
   16  3.0637D-04    4.5808D+01      53  1.4330D+00    5.5602D+00      90  4.7750D+02    2.9619D+00     127  5.7069D+02    1.2978D+01
   17  4.0516D-04    4.0483D+01      54  1.7145D+00    5.5063D+00      91  4.8651D+02    2.8896D+00     128  5.7097D+02    1.4460D+01
   18  5.0395D-04    3.6814D+01      55  2.2775D+00    5.4289D+00      92  4.9552D+02    2.8069D+00     129  5.7125D+02    1.6190D+01
   19  6.0273D-04    3.4088D+01      56  2.8406D+00    5.3743D+00      93  5.0453D+02    2.7107D+00     130  5.7153D+02    1.8223D+01
   20  8.0031D-04    3.0241D+01      57  3.4037D+00    5.3327D+00      94  5.0903D+02    2.6564D+00     131  5.7181D+02    2.0628D+01
   21  9.9789D-04    2.7602D+01      58  4.5298D+00    5.2713D+00      95  5.1354D+02    2.5970D+00     132  5.7210D+02    2.3495D+01
   22  1.1955D-03    2.5648D+01      59  5.6559D+00    5.2265D+00      96  5.1804D+02    2.5320D+00     133  5.7238D+02    2.6942D+01
   23  1.5906D-03    2.2898D+01      60  6.7820D+00    5.1911D+00      97  5.2255D+02    2.4604D+00     134  5.7266D+02    3.1125D+01
   24  1.9858D-03    2.1016D+01      61  9.0343D+00    5.1361D+00      98  5.2705D+02    2.3816D+00     135  5.7294D+02    3.6256D+01
   25  2.3809D-03    1.9625D+01      62  1.1287D+01    5.0931D+00      99  5.3156D+02    2.2947D+00     136  5.7322D+02    4.2627D+01
   26  3.1712D-03    1.7669D+01      63  1.3539D+01    5.0571D+00     100  5.3606D+02    2.1993D+00     137  5.7350D+02    5.0642D+01
   27  3.9616D-03    1.6333D+01      64  1.8043D+01    4.9972D+00     101  5.4056D+02    2.0963D+00     138  5.7379D+02    6.0884D+01
   28  4.7519D-03    1.5346D+01      65  2.2548D+01    4.9467D+00     102  5.4282D+02    2.0428D+00     139  5.7407D+02    7.4207D+01
   29  6.3325D-03    1.3959D+01      66  2.7052D+01    4.9019D+00     103  5.4507D+02    1.9891D+00     140  5.7435D+02    9.1904D+01
   30  7.9131D-03    1.3013D+01      67  3.6061D+01    4.8229D+00     104  5.4732D+02    1.9370D+00     141  5.7449D+02    1.0297D+02
   31  9.4937D-03    1.2313D+01      68  4.5070D+01    4.7532D+00     105  5.4957D+02    1.8892D+00     142  5.7463D+02    1.1596D+02
   32  1.2655D-02    1.1331D+01      69  5.4079D+01    4.6899D+00     106  5.5183D+02    1.8504D+00     143  5.7477D+02    1.3131D+02
   33  1.5816D-02    1.0661D+01      70  6.3088D+01    4.6312D+00     107  5.5408D+02    1.8290D+00     144  5.7491D+02    1.4961D+02
   34  1.8977D-02    1.0166D+01      71  7.2097D+01    4.5764D+00     108  5.5633D+02    1.8393D+00     145  5.7505D+02    1.7156D+02
   35  2.5300D-02    9.4713D+00      72  9.0115D+01    4.4760D+00     109  5.5858D+02    1.9076D+00     146  5.7519D+02    1.9819D+02
   36  3.4098D-02    8.8484D+00      73  1.0813D+02    4.3853D+00     110  5.5971D+02    1.9778D+00     147  5.7533D+02    2.3078D+02
   37  4.2896D-02    8.4286D+00      74  1.2615D+02    4.3022D+00     111  5.6083D+02    2.0843D+00     148  5.7547D+02    2.7105D+02
```

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

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     RESONANCE PARAMETER PROCESSING CODE - RESENDD/ VERSION 84-07          DATE( 84-08-17 )     PAGE .   4

***  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  5.7547D+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    1.3418D+01    243  6.4912D+02    7.5046D+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  6.0005D+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  6.2271D+02    5.5572D+00    259  6.4986D+02    4.8168D+01    306  6.5680D+02    4.5620D+00
  166  5.7797D+02    6.7123D+02    213  6.2724D+02    5.3291D+00    260  6.4989D+02    5.6678D+01    307  6.5741D+02    4.5439D+00
  167  5.7811D+02    5.6269D+02    214  6.3177D+02    5.1443D+00    261  6.4995D+02    6.8704D+01    308  6.5862D+02    4.5130D+00
  168  5.7825D+02    4.7655D+02    215  6.3630D+02    4.9938D+00    262  6.4997D+02    7.2627D+01    309  6.5984D+02    4.4865D+00
  169  5.7839D+02    4.0780D+02    216  6.3857D+02    4.9306D+00    263  6.5000D+02    7.4052D+01    310  6.6106D+02    4.4629D+00
  170  5.7853D+02    3.5247D+02    217  6.4083D+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  6.4196D+02    4.8556D+00    265  6.5005D+02    6.8707D+01    312  6.6470D+02    4.4018D+00
  172  5.7882D+02    2.7064D+02    219  6.4310D+02    4.8396D+00    266  6.5011D+02    5.6683D+01    313  6.6714D+02    4.3662D+00
  173  5.7896D+02    2.4006D+02    220  6.4366D+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  6.4423D+02    4.8329D+00    268  6.5018D+02    3.9598D+01    315  6.7444D+02    4.2736D+00
  175  5.7938D+02    1.7452D+02    222  6.4480D+02    4.8354D+00    269  6.5022D+02    3.3079D+01    316  6.7930D+02    4.2203D+00
  176  5.7966D+02    1.4516D+02    223  6.4536D+02    4.8443D+00    270  6.5026D+02    2.7916D+01    317  6.8904D+02    4.1280D+00
  177  5.7995D+02    1.2300D+02    224  6.4593D+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  6.4621D+02    4.8785D+00    272  6.5033D+02    2.0694D+01    319  7.0850D+02    3.9827D+00
  179  5.8051D+02    9.2315D+01    226  6.4650D+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  7.7663D+02    3.6737D+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  7.8880D+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  7.9488D+02    3.6247D+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    3.6245D+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)

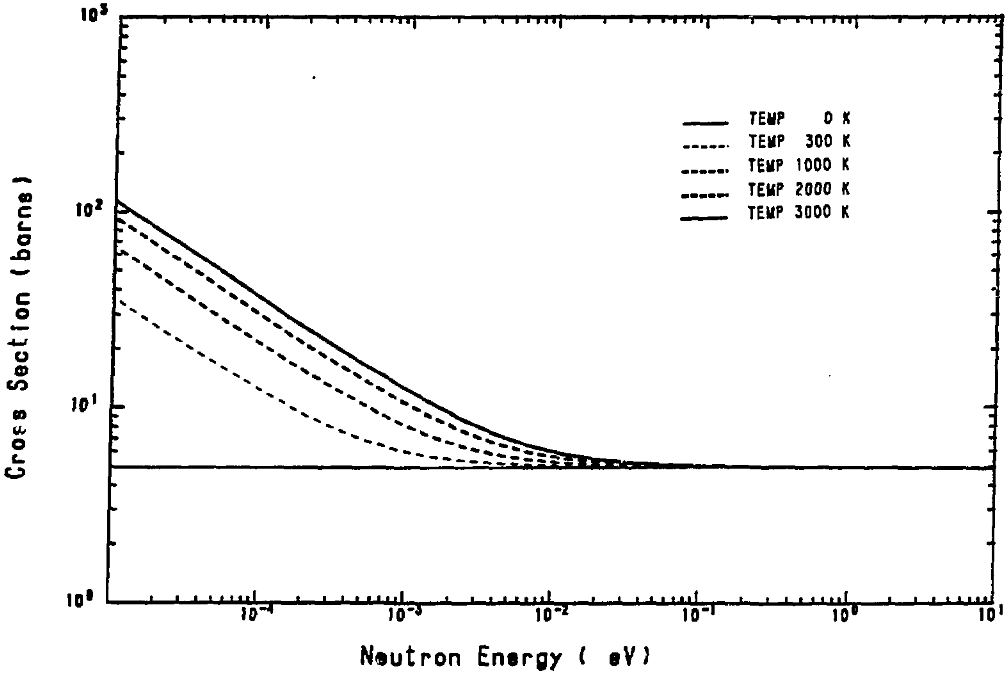

Fig. 9 Doppler broadened cross sections. The elastic scattering cross section in low energy region.

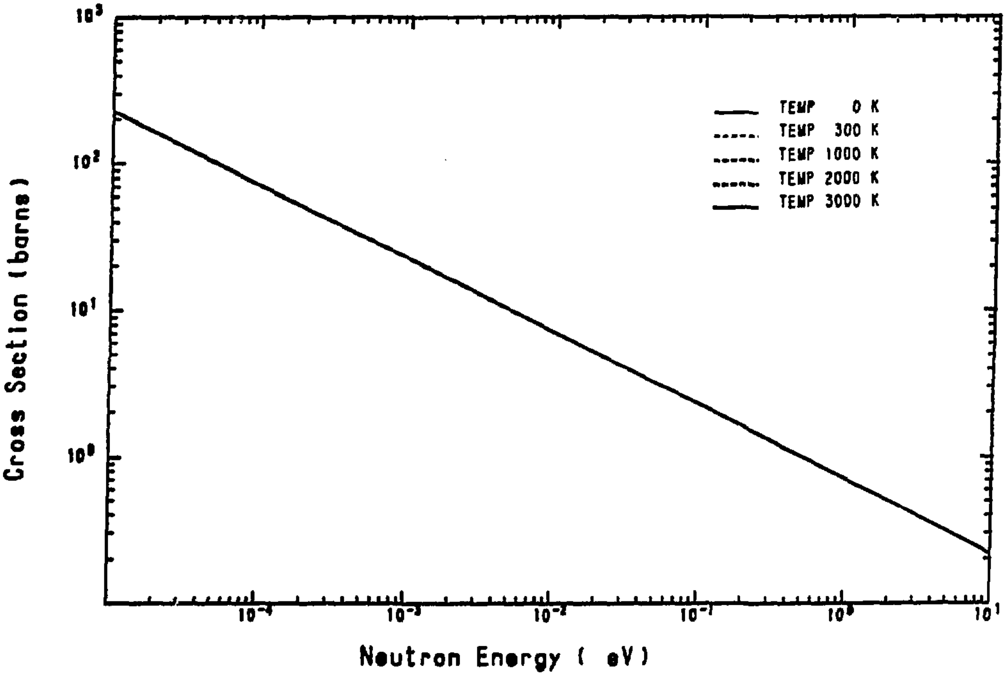

Fig. 10 Doppler broadened cross sections. The capture cross section in low energy region. The cross section in a form of 1/v is not changed by the Doppler effect.

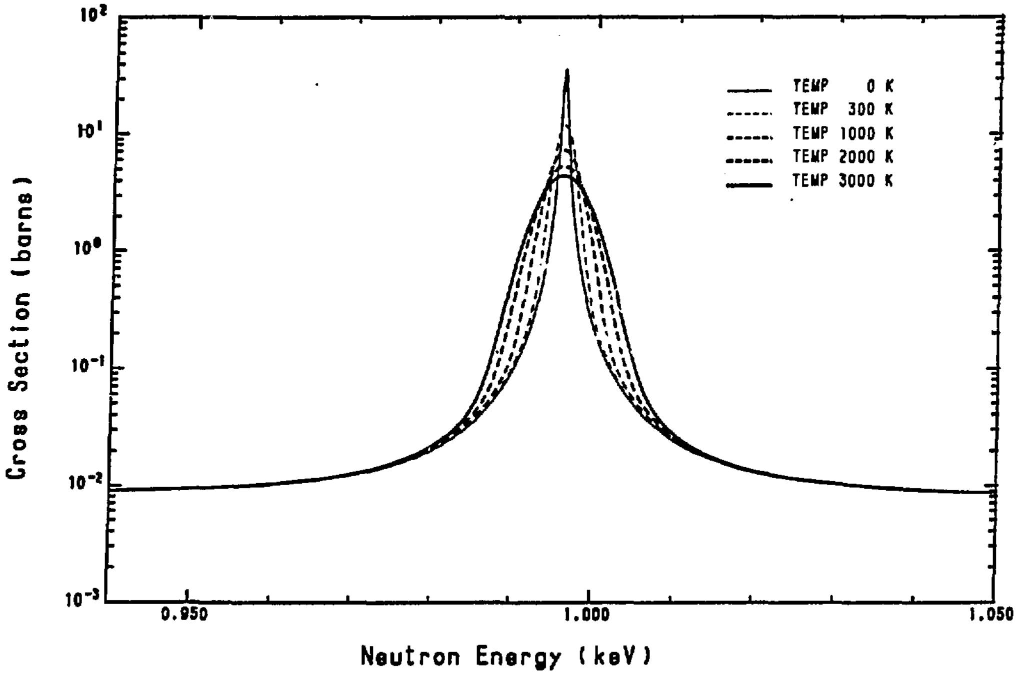

Fig. 11 Doppler broadened cross sections. The capture cross section around a narrow resonance.

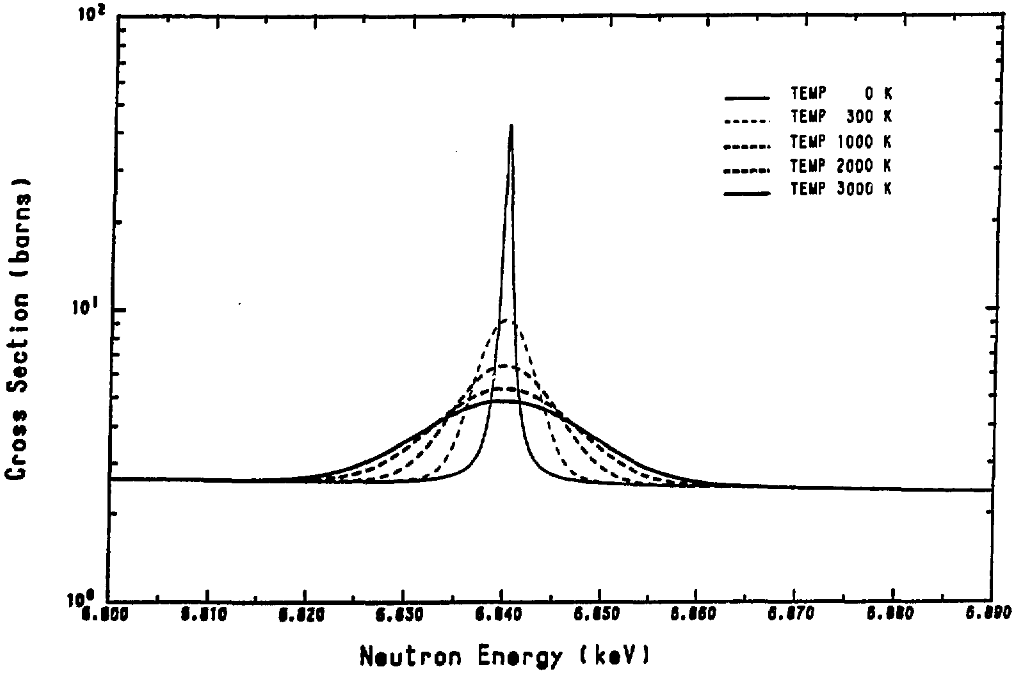

Fig. 12 Doppler broadened cross sections. The total cross section around a narrow resonance.

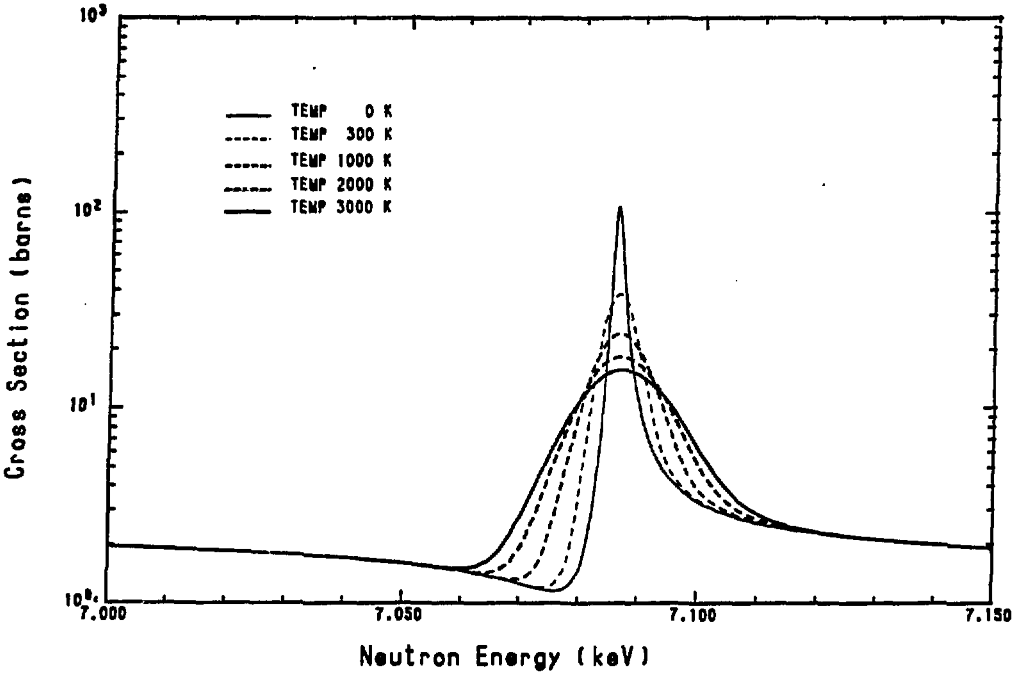

Fig. 13 Doppler broadened cross sections. The total cross section with a shape of s-wave potential interference.

Appendix

Derivation of Multi-level Breit-Wigner Formula Used in RESENDD

The multi-level Breit-Wigner formula used in RESENDD 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.

$$\sigma_{n,n}(E)=\frac{\pi}{k^2}\sum_{l}\sum_{J}g_J\left|1-U^J_{n,n}(E)\right|^2. \tag{A.1}$$

Usually the scattering matrix is approximated as

$$U^J_{n,c} = \exp(-2i\varphi_l)\left[\delta_{n,c}+i\sum_{r}^{NR}\frac{\Gamma_{nr}^{1/2}\Gamma_{cr}^{1/2}}{E_r{}'-E-i\Gamma_r/2}\right]. \tag{A.2}$$

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

$$U^J_{n,c} = \exp(-2i\varphi_l)\left[\delta_{n,c}+i\sum_{r}^{NRJ}\frac{\Gamma_{nr}^{1/2}\Gamma_{cr}^{1/2}}{E_r{}'-E-i\Gamma_r/2}+i\sum_{u}^{NRL}\frac{\delta_{Ju}\Gamma_{nu}^{1/2}\Gamma_{cu}^{1/2}}{E_u{}'-E-i\Gamma_u/2}\right], \tag{A.3}$$

where the first summation is for J-known resonances and the second summation for J-unknown resonances, and the quantity δ_{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.

$$\sigma_{n,n}(E)=\frac{\pi}{k^2}\sum_{l}\Big\{4(2\ell+1)\sin^2\varphi_l+\sum_{J}g_J\Big[(G_{J1})^2+\frac{1}{4}(G_{J2})^2$$

$$+2\sin 2\varphi_l\times G_{J1}-(1-\cos 2\varphi_l)G_{J2}\Big]\Big\}, \tag{A.4}$$

where

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

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

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

$$(G_{J1})^2 = \left[\sum_{r}^{NRJ}\frac{\Gamma_{nr}(E-E_r')}{(E-E_r')^2+\Gamma_r^2/4}\right]^2+2\sum_{r}^{NRJ}\frac{\Gamma_{nr}(E-E_r')}{(E-E_r')^2+\Gamma_r^2/4}\times\sum_{u}^{NRL}\frac{\delta_{Ju}\Gamma_{nu}(E-E_u')}{(E-E_u')^2+\Gamma_u^2/4}$$

$$+\left[\sum_{u}^{NRL}\frac{\delta_{Ju}\Gamma_{nu}(E-E_u')}{(E-E_u')^2+\Gamma_u^2/4}\right]^2 \tag{A.7}$$

The second term can be written as follows;

$$2P_{Jl}\sum_{r}^{NRJ}\frac{\Gamma_{nr}(E-E_r')}{(E-E_r')^2+\Gamma_r^2/4}\times\sum_{u}^{NRL}\frac{\Gamma_{nu}(E-E_u')}{(E-E_u')^2+\Gamma_u^2/4}, \tag{A.8}$$

by assuming that

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

where the quantity P_{Jl} 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_{Jl}. The third term of Eq. (A.7) is

$$\left[\sum_{u}^{NRL}\frac{\delta_{Ju}\Gamma_{nu}(E-E_u')}{(E-E_u')^2+\Gamma_u^2/4}\right]^2$$

$$=\sum_{u}^{NRL}\frac{\delta_{Ju}\Gamma_{nu}^2(E-E_u')^2}{[(E-E_u')^2+\Gamma_u^2/4]^2}+\sum_{u}^{NRL}\sum_{\substack{u'\\u'\neq u}}^{NRL}\frac{\delta_{Ju}\delta_{Ju'}\Gamma_{nu}\Gamma_{nu'}(E-E_u')(E-E_{u'}')}{[(E-E_u')^2+\Gamma_u^2/4]\,[(E-E_{u'}')^2+\Gamma_{u'}^2/4]}$$

$$=P_{Jl}\sum_{u}^{NRL}\frac{\Gamma_{nu}^2(E-E_u')^2}{[(E-E_u')^2+\Gamma_u^2/4]^2}+P_{Jl}'\sum_{u}^{NRL}\sum_{\substack{u'\\u'\neq u}}^{NRL}\frac{\Gamma_{nu}\Gamma_{nu'}(E-E_u')(E-E_{u'}')}{[(E-E_u')^2+\Gamma_u^2/4]\,[(E-E_{u'}')^2+\Gamma_{u'}^2/4]}$$

$$=P_{Jl}\sum_{u}^{NRL}\frac{\Gamma_{nu}^{2}(E-E_u')^2}{[(E-E_u')^2+\Gamma_u^2/4]^2}$$

$$+P_{Jl}'\left\{\{\sum_{u}^{NRL}\frac{\Gamma_{nu}(E-E_u')}{[(E-E_u')^2+\Gamma_u^2/4]}\}^2-\sum_{u}^{NRL}\frac{\Gamma_{nu}^{2}(E-E_u')^2}{[(E-E_u')^2+\Gamma_u^2/4]^2}\right\} \qquad (A.10)$$

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

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

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

$$(G_{J1})^2+\frac{1}{4}(G_{J2})^2$$

$$=\{\sum_{r}^{NRJ}\frac{\Gamma_{nr}(E-E_r')}{(E-E_r')^2+\Gamma_r^2/4}\}^2+\frac{1}{4}\{\sum_{r}^{NRJ}\frac{\Gamma_{nr}\Gamma_r}{(E-E_r')^2+\Gamma_r^2/4}\}^2$$

$$+2P_{Jl}\left[\sum_{r}^{NRJ}\frac{\Gamma_{nr}(E-E_r')}{(E-E_r')^2+\Gamma_r^2/4}\times\sum_{u}^{NRL}\frac{\Gamma_{nu}(E-E_u')}{(E-E_u')^2+\Gamma_u^2/4}\right.$$

$$\left.+\frac{1}{4}\sum_{r}^{NRJ}\frac{\Gamma_{nr}\Gamma_r}{(E-E_r')^2+\Gamma_r^2/4}\times\sum_{u}^{NRL}\frac{\Gamma_{nu}\Gamma_u}{(E-E_u')^2+\Gamma_u^2/4}\right]$$

$$+P_{Jl}\sum_{u}^{NRL}\frac{\Gamma_{nu}^2}{(E-E_u')^2+\Gamma_u^2/4}+\frac{P_{Jl}(P_{Jl}NRL-1)}{(NRL-1)}\left[\{\sum_{u}^{NRL}\frac{\Gamma_{nu}(E-E_u')}{(E-E_u')^2+\Gamma_u^2/4}\}^2\right.$$

$$\left.+\frac{1}{4}\{\sum_{u}^{NRL}\frac{\Gamma_{nu}\Gamma_u}{(E-E_u')^2+\Gamma_u^2/4}\}^2-\sum_{u}^{NRL}\frac{\Gamma_{nu}\Gamma_u}{(E-E_u')^2+\Gamma_u^2/4}\right]. \qquad (A.11)$$

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

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

$$F_{J2}\equiv\sum_{r}^{NRJ}\frac{\Gamma_{nr}\Gamma_r}{(E-E_r')^2+\Gamma_r^2/4}+P_{Jl}\sum_{u}^{NRL}\frac{\Gamma_{nu}\Gamma_u}{(E-E_u')^2+\Gamma_u^2/4}, \qquad (A.13)$$

Then,

$$G_{J1} \doteqdot F_{J1},$$

$$G_{J2} \doteqdot F_{J2},$$

$$(G_{J1})^2+\frac{1}{4}(G_{J2})^2 = (F_{J1})^2+\frac{1}{4}(F_{J2})^2+P_{Jl}(1-P_{Jl})f_0$$

$$-\frac{P_{Jl}(1-P_{Jl})}{NRL-1}(f_1^2+\frac{1}{4}f_2^2-f_0). \qquad (A.14)$$

Therefore

$$\sigma_{n,n}(E)=\frac{\pi}{k^2}\sum_{l}^{NL}\Big\{(2\ell+1)\sin^2\varphi_l+\sum_{J}^{NJ}g_J\Big[(F_{J1})^2+\frac{1}{4}(F_{J2})^2+2\sin2\varphi_l\times F_{J1}$$

$$-(1-\cos2\varphi_l)F_{J2}+P_{Jl}(1-P_{Jl})f_0-\frac{P_{Jl}(1-P_{Jl})}{NRL-1}(f_1^2+\frac{1}{4}f_2^2-f_0)\Big]\Big\} . \qquad (A.15)$$

where

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

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

and

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

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.