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BETWEEN THE CROSS SECTION DATA OF NATURAL ELEMENT
AND ITS ISOTOPES**

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A Method and Program CABEL for Adjusting Consistency Between the Cross Section Data of Natural Element and Its Isotopes

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Introduction

To meet the requirement of nuclear engineering, especially nuclear fusion research, now the data in the major evaluated libraries, such as ENDF/B-6, JENDL-3.2, JEF-2.2, BROND-2.1 and CENDL-2.1, are given not only for natural elements, but also their isotopes. It is clear that these data must be consistent in physics. Unfortunately, it is not the case, the data in the libraries usually do not satisfy the consistent relationship.

Inconsistency between element and its isotopes data is one major problems in present evaluated neutron libraries^[1]. So far, the data in the libraries are given, in most cases, only for natural elements or isotopes, not for both, to avoid this problem.

As well know, the complete data must be consistent for each nuclide itself, for example, total cross section equals the sum of elastic and noelastic cross section, nonelastic cross section equals the sum of all partial cross section except elastic cross section, and total inelastic cross section equals the sum of the cross sections of inelastic scattering to discrete and continuous states etc. The consistence between natural element and its isotopes makes the data must satisfy two kinds of consistent relationships at the same time, this is the key point and mail difficulty for this kind adjustment.

1 Adjust Method and Formulas

Let σ_{ij} express the cross section of j -th reaction for i -th isotope. σ_{i0} express the

'total' cross sections for i -th isotope, σ_{oj} express the cross section of j -th reaction for natural element, and σ_{oo} is the 'total' cross section of natural element. Suppose σ' is the cross section to be adjusted, and σ is one adjusted, so that

$$\sigma_{oj} = \sum_{i=1}^I A_i \sigma_{ij} \quad (1)$$

$$\sigma_{io} = \sum_{j=1}^J \sigma_{ij} \quad (2)$$

$$\sigma_{oo} = \sum_{j=1}^J \sigma_{oj} = \sum_{i=1}^I A_i \sigma_{io} = \sum_{i=1}^I \sum_{j=1}^J A_i \sigma_{ij} \quad (3)$$

Define objective function

$$\begin{aligned} \chi^2 &= \sum_{i=0}^I \sum_{j=0}^J w_{ij} (\sigma_{ij} - \sigma'_{ij})^2 \\ &= w_{oo} (\sigma_{oo} - \sigma'_{oo})^2 + \sum_{j=1}^J w_{oj} (\sigma_{oj} - \sigma'_{oj})^2 + \sum_{i=1}^I w_{io} (\sigma_{io} - \sigma'_{io})^2 \\ &\quad + \sum_{i=1}^I \sum_{j=1}^J w_{ij} (\sigma_{ij} - \sigma'_{ij})^2 \end{aligned} \quad (4)$$

where $w_{ij} (i = 0, 1, \dots, I, j = 0, 1, 2, \dots, J)$ is the assigned weight of the corresponding cross section for adjusting.

Substitute equations (1)–(3) into equation (4), then

$$\begin{aligned} \chi^2 &= \sum_{i=1}^I \sum_{j=1}^J w_{ij} (\sigma_{ij} - \sigma'_{ij})^2 + \sum_{i=1}^I w_{io} \left[\left(\sum_{j=1}^J \sigma_{ij} \right) - \sigma'_{io} \right]^2 \\ &\quad + \sum_{j=1}^J w_{oj} \left[\left(\sum_{i=1}^I A_i \sigma_{ij} \right) - \sigma'_{oj} \right]^2 + w_{oo} \left[\left(\sum_{i=1}^I \sum_{j=1}^J A_i \sigma_{ij} \right) - \sigma'_{oo} \right]^2 \end{aligned} \quad (5)$$

Take the partial differential to variable σ_{kl} and let them equal zero

$$\frac{\partial \chi^2}{\partial \sigma_{kl}} = 0$$

in this conditions, the linear equation group is obtained

$$\begin{aligned} w_{kl} \sigma_{kl} + w_{ko} \left(\sum_{j=1}^J \sigma_{kj} \right) + w_{ol} \left(\sum_{i=1}^I A_i \sigma_{il} \right) + w_{oo} \left(\sum_{i=1}^I \sum_{j=1}^J A_i \sigma_{ij} \right) \\ = w_{kl} \sigma'_{kl} + w_{ko} \sigma'_{ko} + w_{ol} A_k \sigma'_{ol} + w_{oo} A_k \sigma'_{oo} \end{aligned} \quad (6)$$

where $k=1, 2, \dots, I$ and $l=1, 2, \dots, J$, there are $I \times J$ equations, so the optimum values of $I \times J$ variables can be solved out. And the 'total' cross sections of each isotopes and natural element can be calculated from equations (1–3).

2 Code and Test

According to the equation group (6), the program CABEL was developed, which includes codes EPOIN, INTER, DIFFE, ADJUS and RECOV.

Code EPOIN is used for selecting and arranging energy in order. The adjusting is going on at same energy point one by one for all reactions of natural element and its isotopes, but the energy meshes of them are not the same. The energy points of each reaction are taken and collect all of them together and then put them in order from small to large by the code.

Code INTER is for interpolation of the cross section data according to interpolation mode given in the data heading of corresponding section. As mentioned above, adjusting is going on at the energy points of all reactions, the cross section may not be given at some energy points for some reactions, in this case they are calculated by the code using the given interpolation mode.

Code DIFFE is used to calculate the difference between the data of natural element and sum of its isotopes taken their abundance as weight. This is a quantitative measurement of the inconsistency.

Code ADJUS is used for solving the linear equation group (6) and adjusting the data.

Code RECOV is used to select the energy points for outputting, in usual case, recover the original energy meshes, and output the data in ENDF/B-6 format.

Taken as an example, the data of Fe from CENDL-2.1 (the data are not consistent, the authors are different for $^{54,57,58}\text{Nat. Fe}$ and ^{56}Fe) were adjusted to test the program. The results are as follows.

- 1) As desired, the difference between the data of natural element and the sum of its isotopes became zero, no matter how much the difference is before adjusted. It means that the data become consistent. Some examples are given

in Figs.1, 2 for total and nonelastic cross sections.

2) If the consistence is better before adjusted, the data keep unchanged basically; if it is worse, the data are changed larger, the worse, the larger. Some examples are given in Figs.3, 4 for the former and in Figs.5, 6 for the later. Also it can be seen from Figs.5, 6 that the changed directions are reasonable, it is clear that the original cross section curve of (n, α) is 'fat' for natural element, is 'thin' for ^{56}Fe ; after adjusted it becomes 'thinner' for natural element, and becomes 'fatter' for ^{56}Fe .

3) If the original curve is smooth, it still keep smooth after adjusted. If there are some structures for original data, there remain small structures for adjusted data (Fig.7).

4) In adjusting, the change is smaller for the isotopes having small abundance for they have small contribution to the cross section of natural element, and larger for isotopes having larger abundance for they have larger contribution. An example is given in Fig.8.

It is concluded from above that the program works well as desired in physics, and in adjusting the data change, including its direction and magnitude, is reasonable.

3 The Matter in Practical Adjusting

How to use the program, how to practically adjust a complete data, following is the matter in practical adjusting, which should be paid attention.

3.1 Weight

In principle, the weight w_{ij} for adjusting can be taken arbitrarily. It can be taken as larger for some cross sections, for which there are more experimental measurements and the errors are smaller and you want them changed smaller, and otherwise, it should be taken as smaller. For example, if you want the total cross section remain unchanged basically in the adjusting, the weight w_{io} should be taken very larger. Also if you want some cross sections, whose absolute values are very

low, change smaller to avoid the relative value change too large, the corresponding w_{ij} can be taken larger, for example as

$$w_{ij} = \frac{\sigma'_{io}}{\sigma'_{ij}} w_{ij}^o \quad (7)$$

To treat conveniently, sometime the weight can be taken as

$$w_{ij} = w_i \times w_j \quad (8)$$

that is the partial weights are taken as the same for the cross sections of same isotope and same reaction. In this case, the number of input weight parameter is reduced to $(I+J)$ from $(I \times J)$.

If the error of the cross section itself should be taken into account, then the weight can be taken as

$$w_{ij} = w_i w_j * 1/\Delta\sigma'_{ij}{}^2 \quad (9)$$

3.2 Adjustment of Complete Data

For a set complete data, except the consistence between the data of natural element and its isotopes, they also must be consistent between total, nonelastic, inelastic cross section and their corresponding partial cross sections for each isotopes. In this case, the adjusting can be done following, for example, the following steps:

(1) Total CS= elastic CS + nonelastic CS

$$(MT\ 1 = 2 + 3)$$

(2) Nonelastic CS = sum of all corresponding partial CSs

$$(MT\ 3 = 4 + 16 + \dots\dots 107)$$

Taken larger weight for nonelastic CS. to keep it unchanged during the adjusting.

(3) Inelastic CS = sum of CSs of inelastic scattering to continuous state and concrete levels

$$(MT\ 4 = 51 + 52 + \dots\dots 91)$$

Taken larger weight for inelastic CS, to keep it unchanged during the adjusting. Only do the adjusting for the consistence of each nuclide itself, not for natural element and its isotopes for there is no relationship between the CSs of inelastic scattering to concrete levels. In this case, the equation group (6) becomes

$$w_l \sigma_l + w_o (\sum_{j=1} \sigma_j) = w_l \sigma_l + w_o \sigma'_o \quad (10)$$

which is also included in the program.

The values of cross sections for different reactions and nuclides could be large different, which could lead difficulty for adjusting. To avoid this difficulty, let

$$\chi_{ij} = \frac{\sigma_{ij}}{\sigma'_{ij}} \quad (11)$$

as new variables in the equation group, the ratios of adjusted to original cross sections in physics, and then the adjusted cross sections

$$\sigma_{ij} = \chi_{ij} \sigma'_{ij} \quad (12)$$

If it is necessary, program CRECTJ5 can be used for each nuclide itself to make the energy meshes satisfy the rule requirement of ENDF/B-6 format.

3.3 The Treatment of Different Energy Region

The low energy bounds of different reactions and nuclides are different for smooth cross section (file 3), but the adjusting only can be done for file 3 and must be done in the same energy region. For this, they must be treated.

(1) If the low bounds are determined by the resonance upper bounds, the highest one is taken as low limit for all reactions of all nuclides, only in this region can be adjusted.

(2) For cross sections of continuous inelastic scattering, the highest threshold is taken as low limit for all nuclides, only in this region can be adjusted.

(3) For other threshold reactions, the lowest one is taken as low limit, the cross sections are taken as zero below this threshold for other reactions.

3.4 The Treatment of Different Reaction Channel

For some reactions, the cross sections may not be given for all nuclides, that is no data for it for some nuclides. In this case, it can be treated according to the different situations.

(1) If the reaction is not open (the threshold is higher than 20 MeV) for a nuclide, or although it is open, the cross section is small enough to be neglected, this nuclide is not included in the adjusting (see the cross section of this nuclide as zero).

(2) If the cross section is not small enough to be neglected, but is not given in the file, this isotope is not included in the adjusting, but make the abundance of main isotope plus its abundance.

3.5 Energy Point for Output and Iteration

As mentioned above, the adjusting is going on at all energy points of all reactions of all nuclides, and the cross sections are interpolated for the energy points, at which they are not given in the file. If all energy points are taken for outputting, there are too many points, and make the file too large, so the energy points must be selected for outputting, usually the original energy meshes are recovered. But in this case, the inconsistency of the new adjusted data may be appeared due to the interpolation.

To solve the problem, the iteration method is used, that is the new adjusted data can be as the input data for the next adjusting until the data is completely consistent at selected output energy meshes. To show the effecting of the iteration, some examples are given in Figs.9, 10 for the total and noelastic cross sections of ^{56}Fe respectively. It can be seen that the change is quite large in the first adjusting, only small but certainly existing corrections are made in following iterations.

4 Conclusion

The method and program CABEI have been developed to make the complete

data of natural element and its isotopes satisfy at the same time the two kinds of consistent relationships, one is for each nuclides itself, and another is between the natural element and its isotopes. The method and program have been tested, and the matter in practical adjusting, including weight taking, complete data adjusting, treatment of different energy region and reaction channel, output energy point selection and iteration, have been studied.

As an example, the method and program were successfully used to adjust the data of ^{Nat}Fe and $^{54,56,57,58}\text{Fe}$ of CENDL-2.1. It works well, As a result, the adjusted data are consistent between ^{Nat}Fe and its isotopes $^{54,56,67,58}\text{Fe}$, and at the same time keep the consistence for each nuclide itself.

The method and program were also successfully used to adjust the data of ^{Nat}Ni and its isotopes $^{58,60,61,62,64}\text{Ni}$.

The method and program can be spread to used for making the data satisfy two kinds of consistent relationships in the evaluation and evaluated libraries in ENDF/B-6 format. It can become a powerful and convenient tool for making the consistence between the data of natural element and its isotopes. Of course, it is only a mathematical method and make it optimum in mathematics, could not replace the analysing and adjusting in physics, in another words, the analysing and adjusting in physics should be done at first before using the code.

Reference

- [1] J. J. Schmidt, Proc. of International Symposium on Nuclear Data Evaluation Methodology, p. 1, BNL, USA (1992).

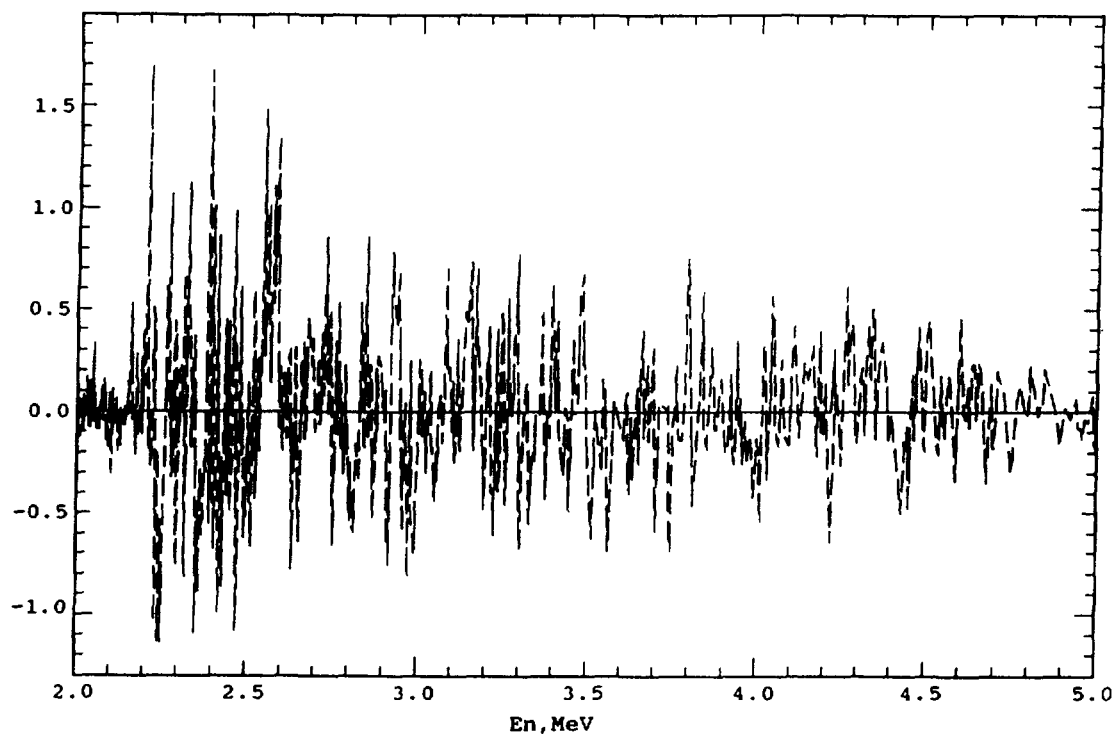


Fig.1 The difference of total CS between ^{nat}Fe and sum of its isotopes

— Adjusted - - - Original

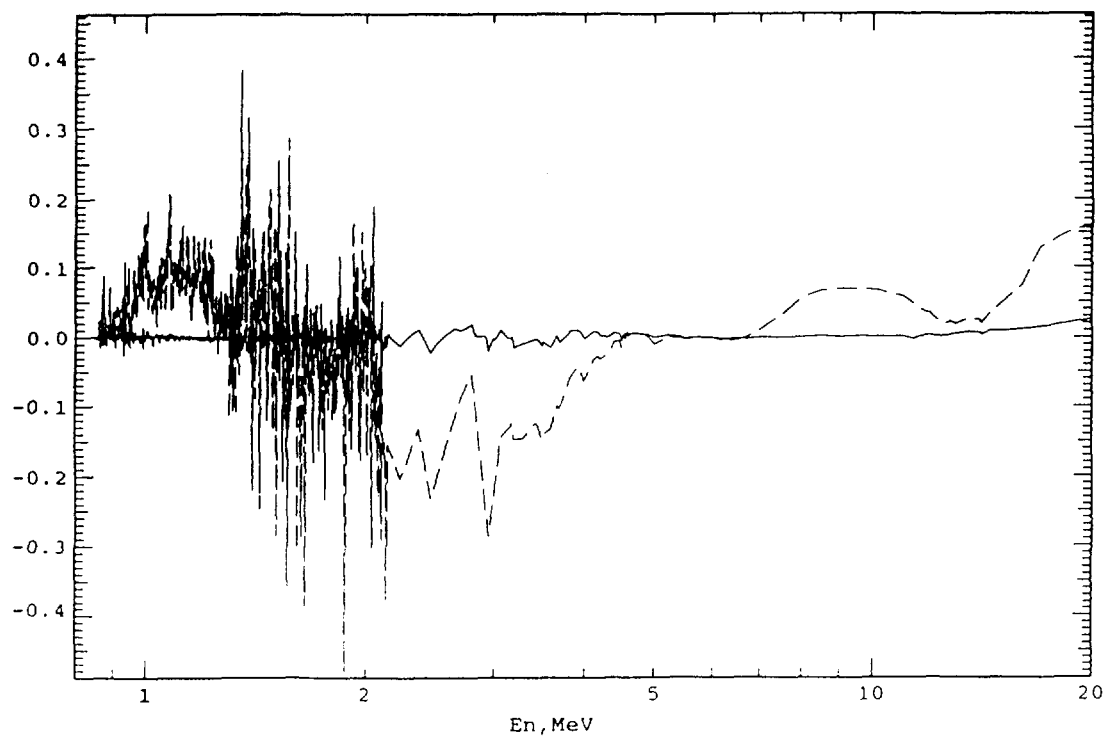


Fig.2 The difference of nonelastic CS between ^{nat}Fe and sum of its isotopes

— Adjusted - - - Original

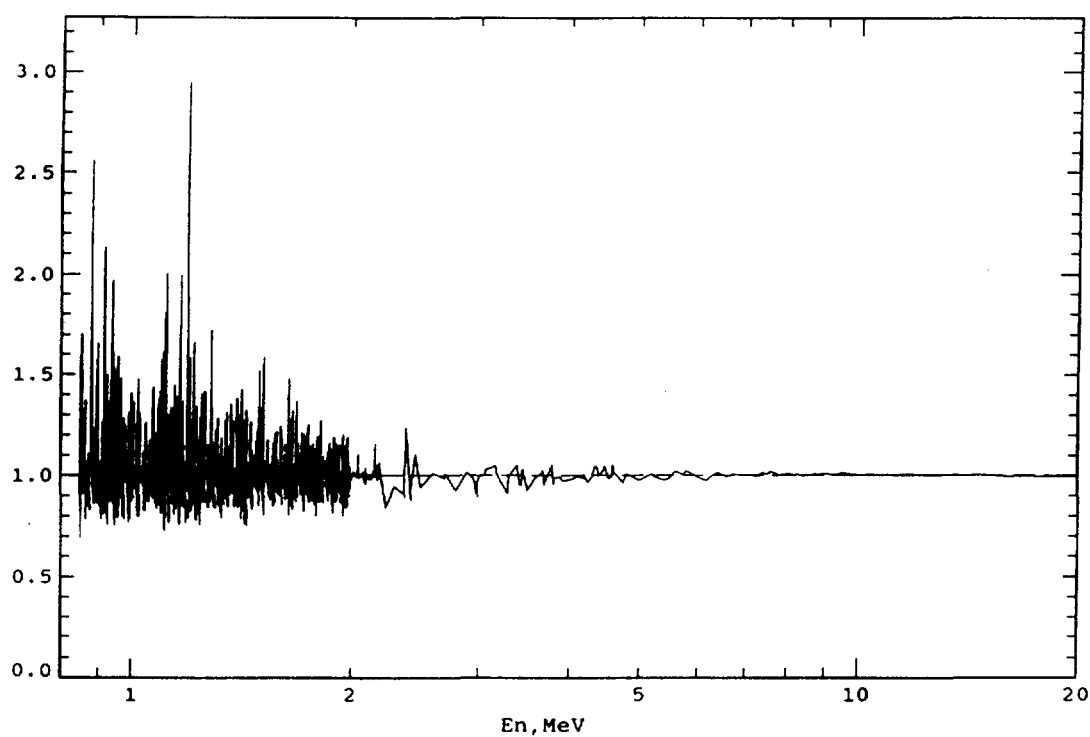


Fig 3.1 The ratios of adjusted to original ^{56}Fe total cross section

—— Adj./Orig. - - - 1.0

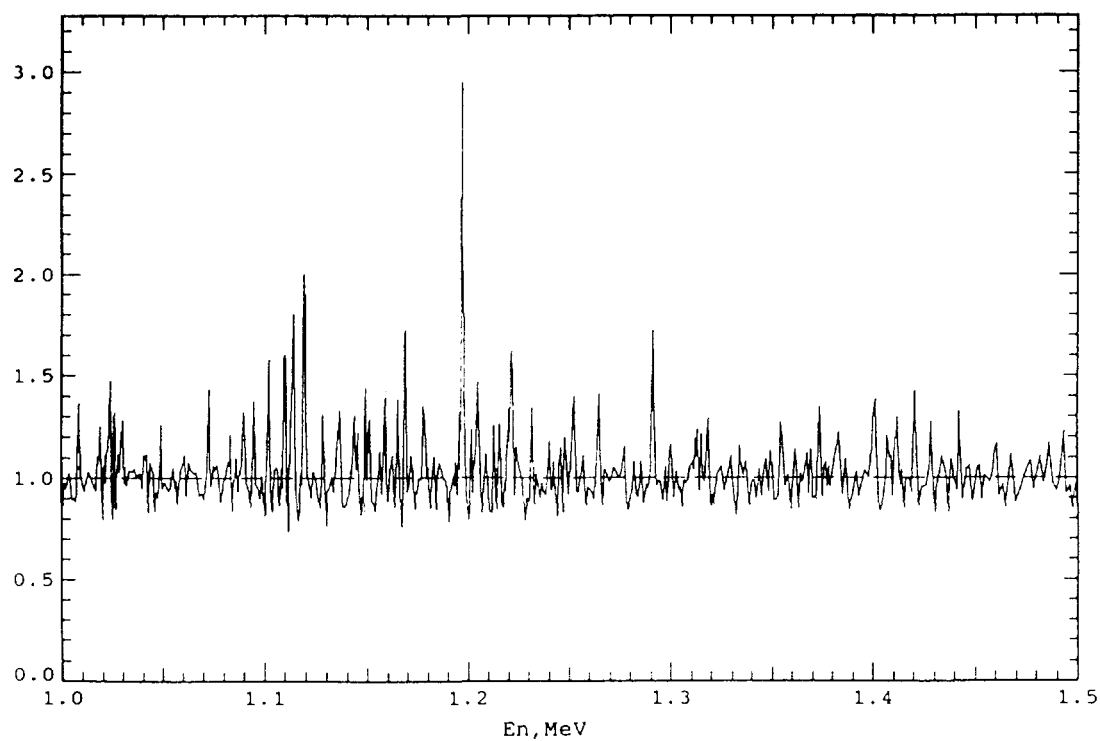


Fig.3.2 The ratios of adjusted to original ^{56}Fe total cross section

—— Adj./Orig. - - - 1.0

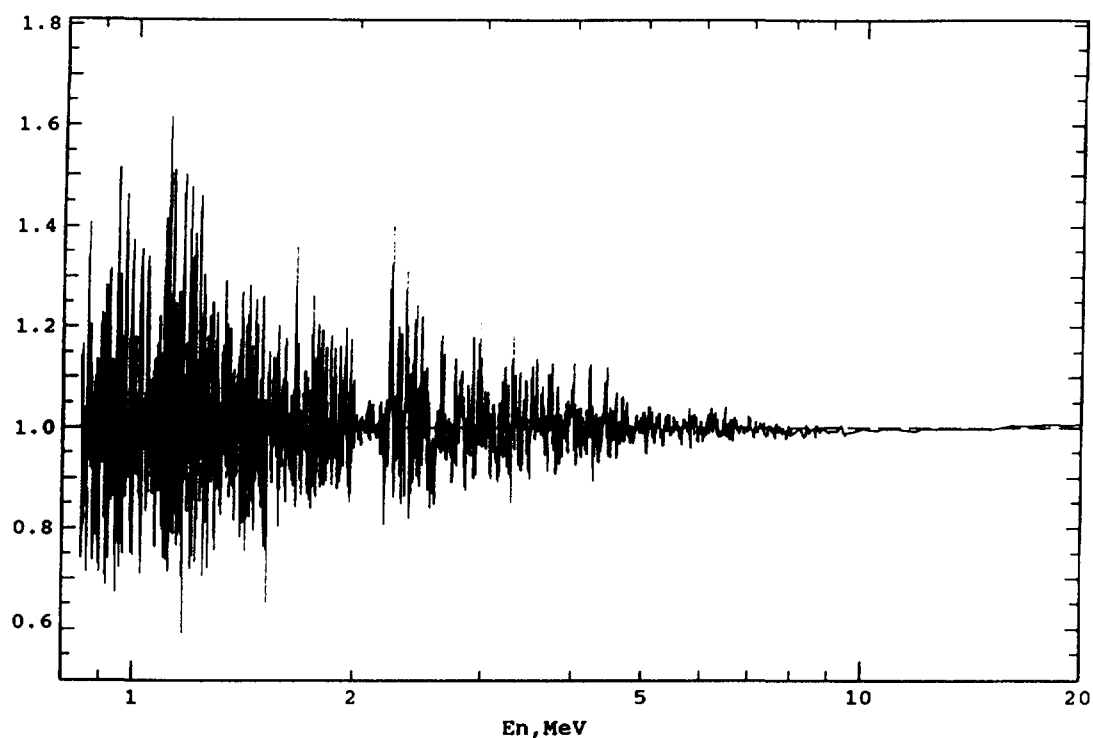


Fig.4.1 The ratios of adjusted to original ^{56}Fe total cross section

—— Adj./Orig - - - 1.0

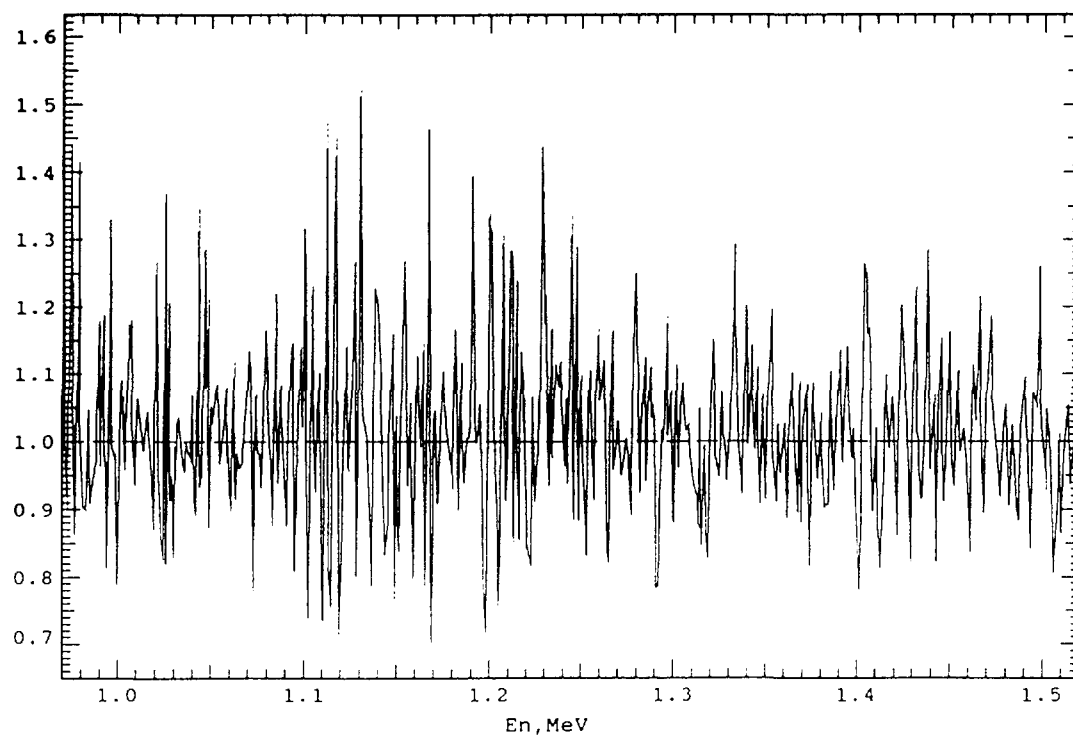


Fig.4.2 The ratios of adjusted to original ^{56}Fe total cross section

—— Adj./Orig - - - 1.0

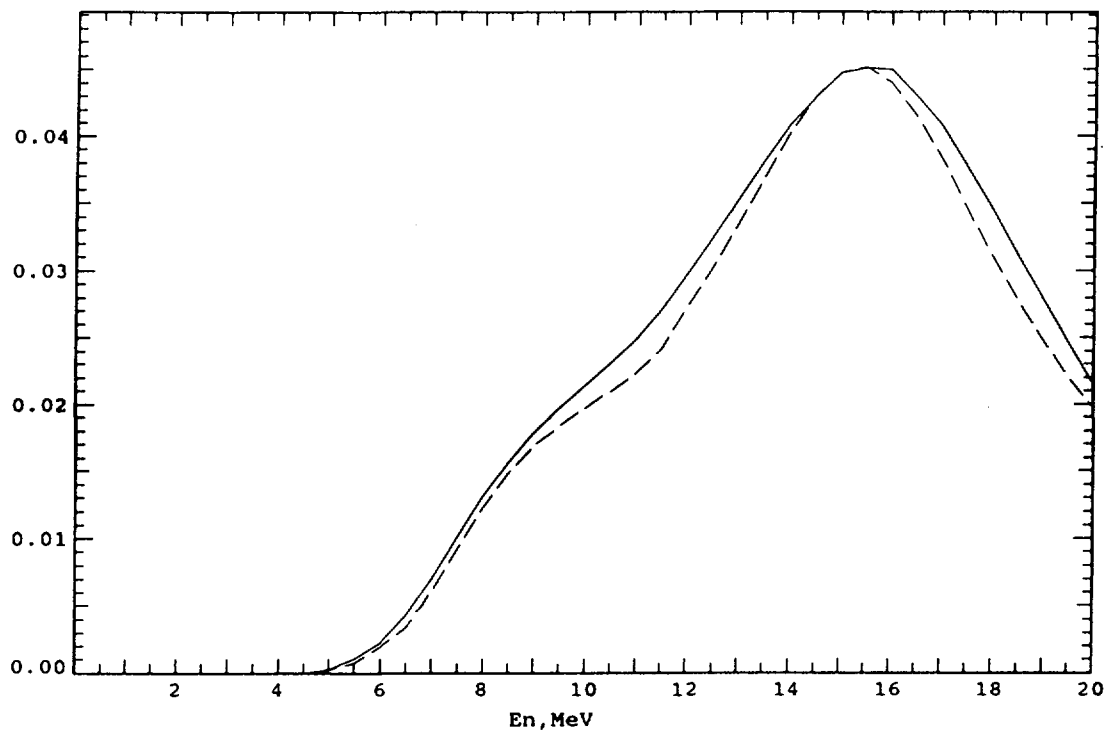


Fig.5 Adjusting of $^{56}\text{Fe}(n,\alpha)$ cross section

———— Adjusted - - - - Original

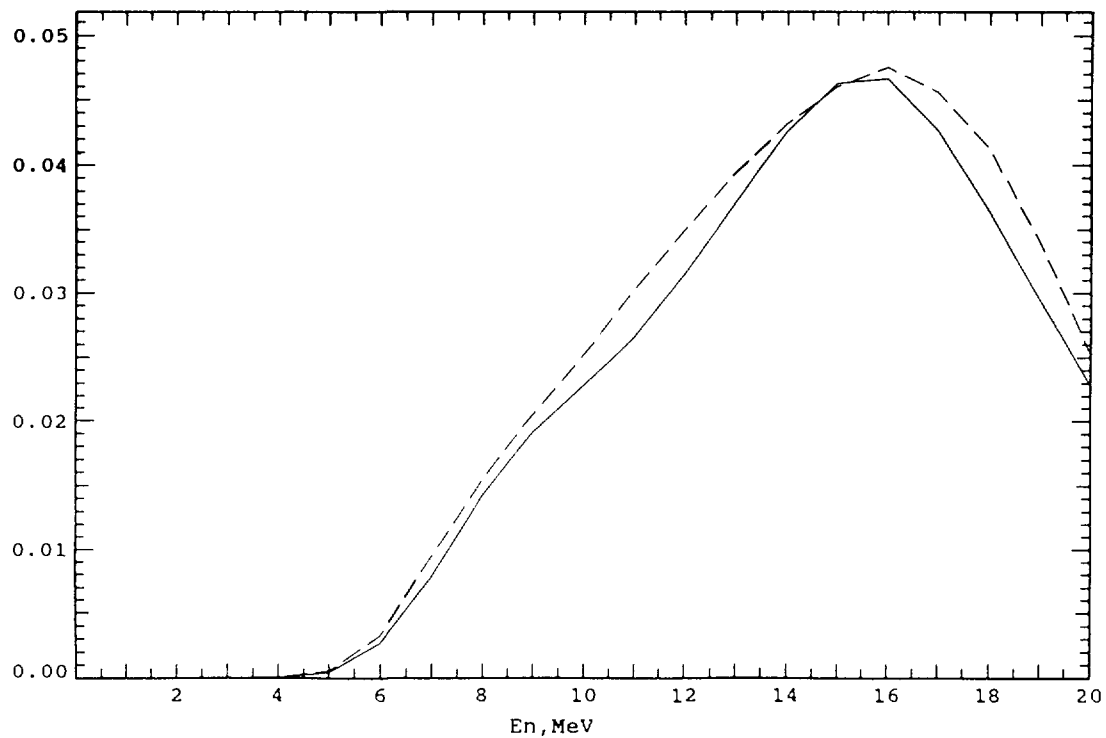


Fig.6 Adjusting of $^{\text{Nat}}\text{Fe}(n,\alpha)$ cross section

———— Adjusted - - - - Original

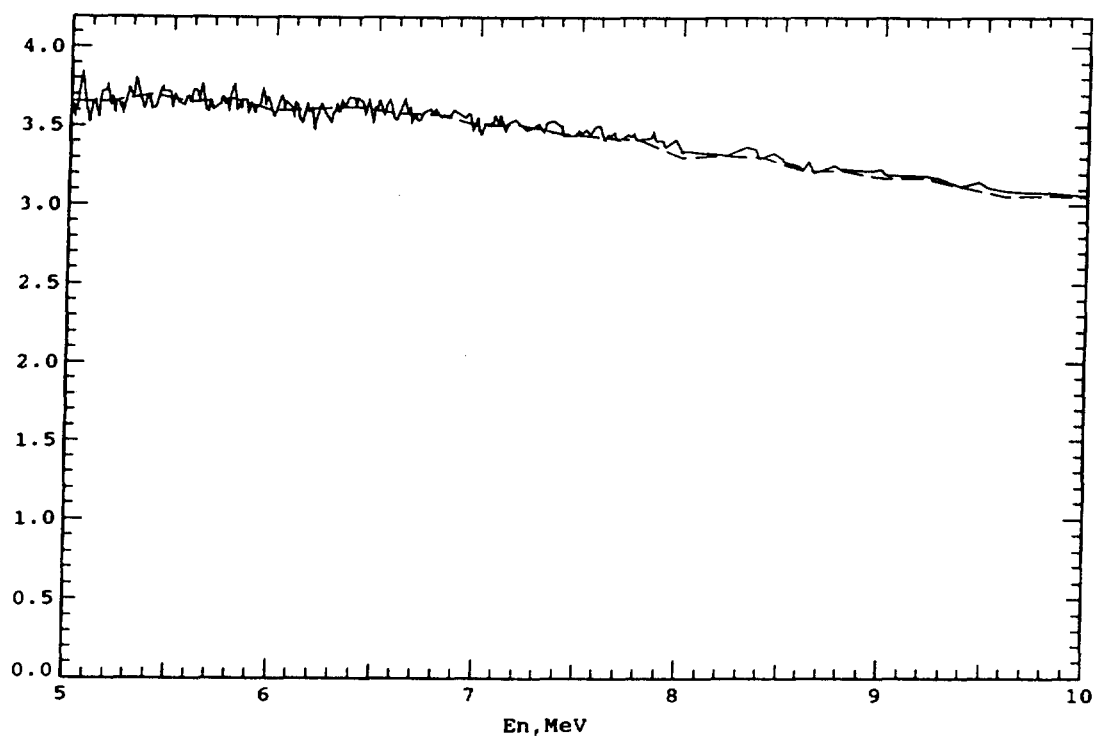


Fig.7 Adjusting of ^{56}Fe total cross section

———— Adjusted - - - - Original

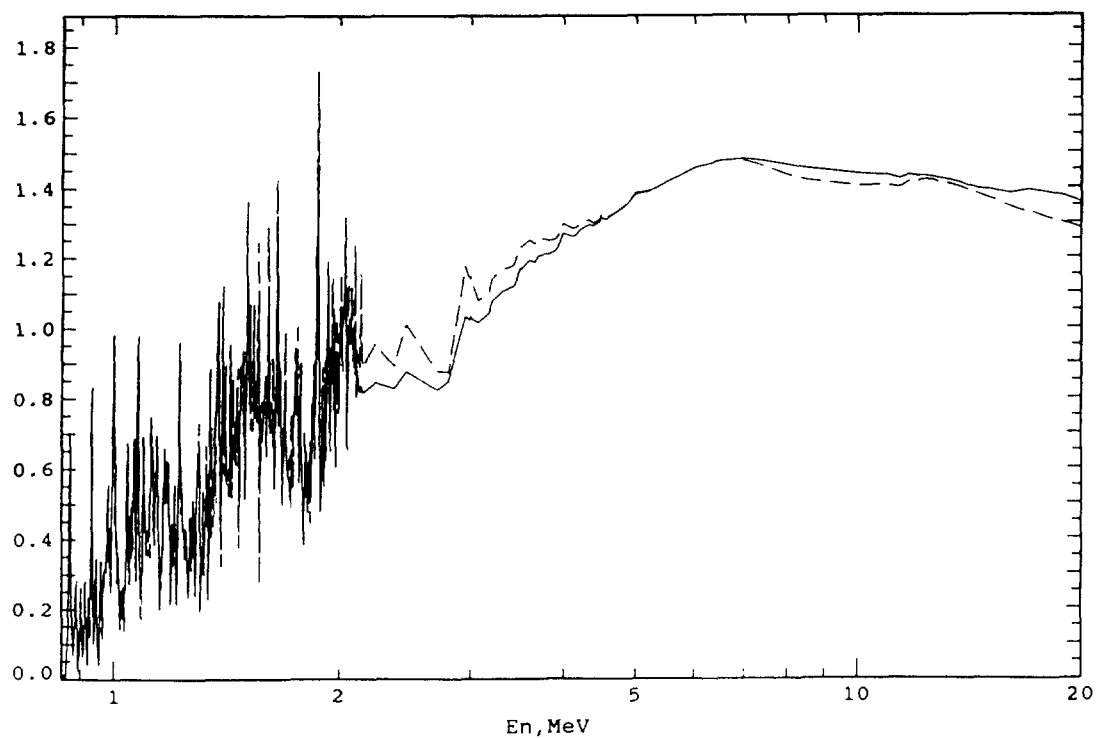


Fig.8.1 Adjusting of ^{56}Fe nonelastic cross section

———— Adjusted - - - - Original

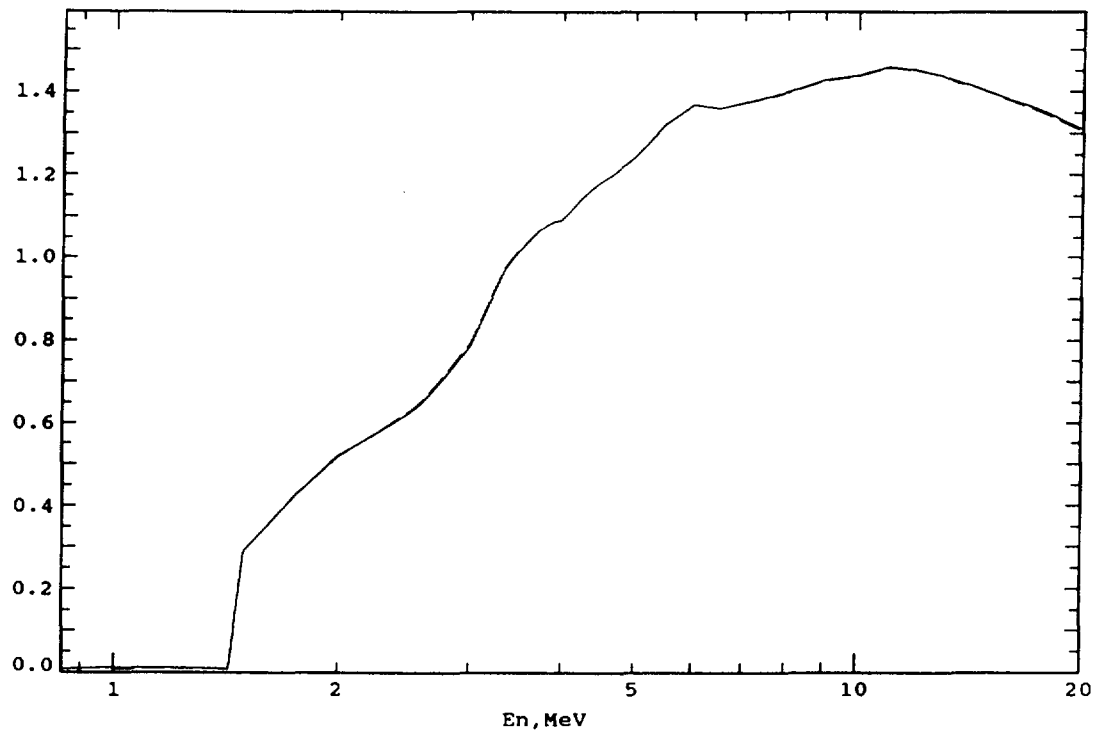


Fig.8.2 Adjusting of ^{54}Fe nonelastic cross section

— Adjusted - - - Original

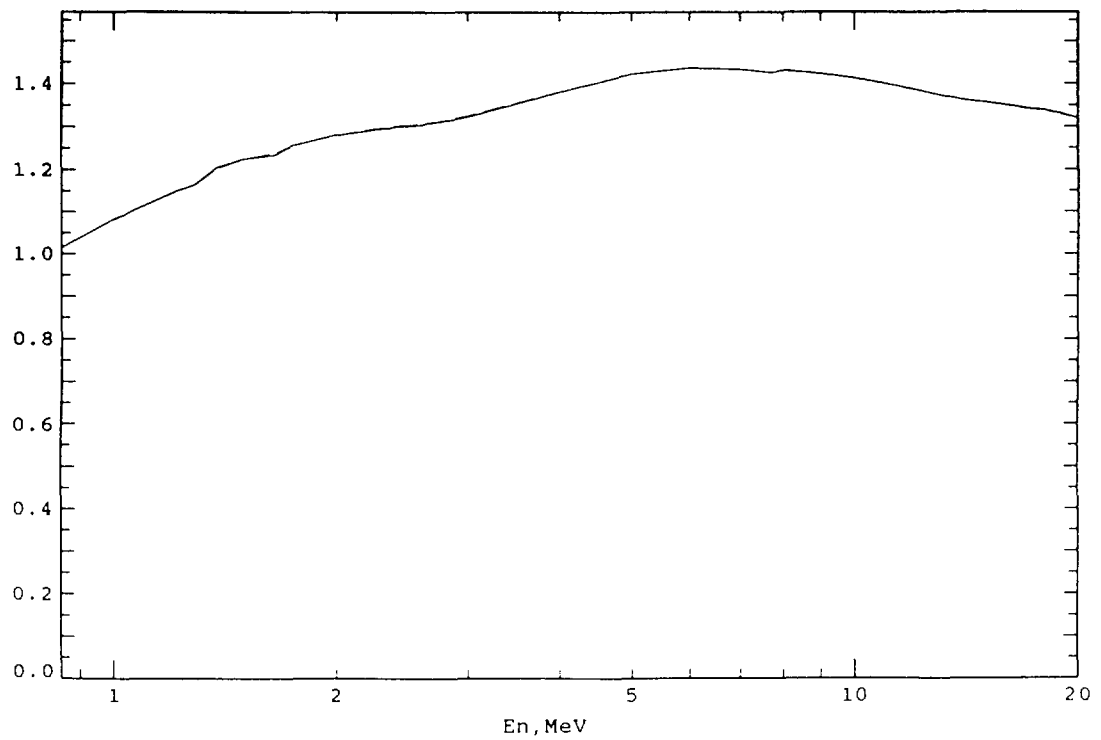


Fig.8.3 Adjusting of ^{57}Fe nonelastic cross section

— Adjusted - - - Original

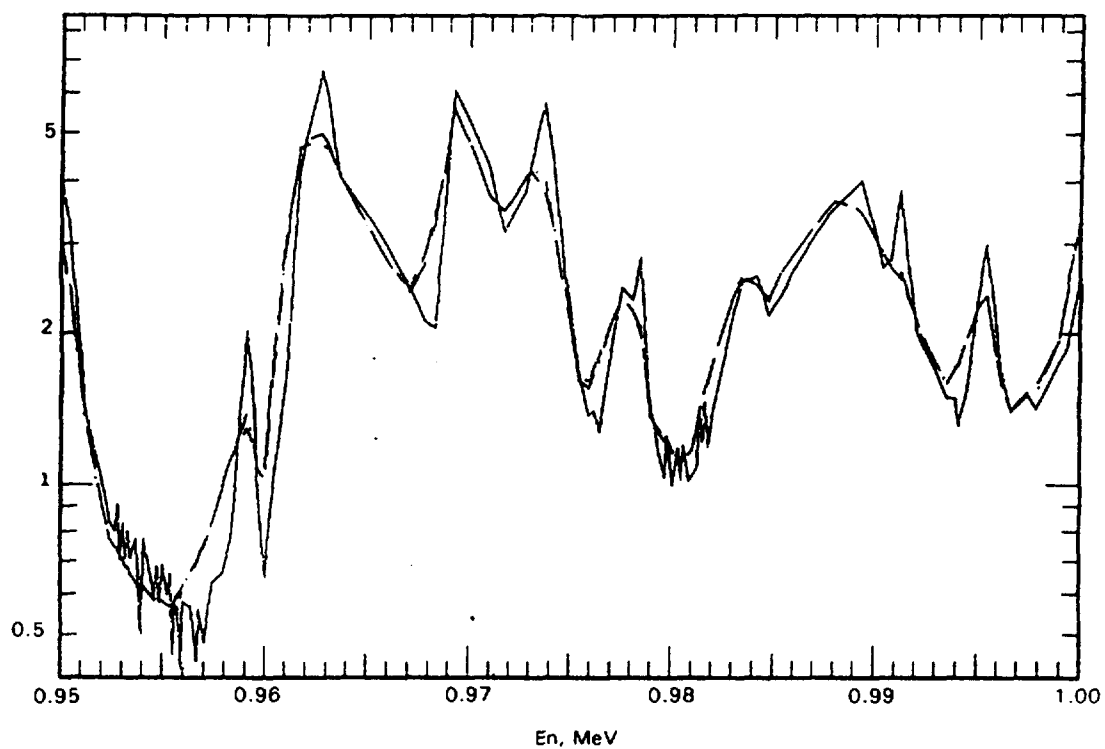


Fig.9 An example of iteration effect on adjusted result: ^{56}Fe total cross section

— Original - - - iteration 3 times - - - iteration 5 times

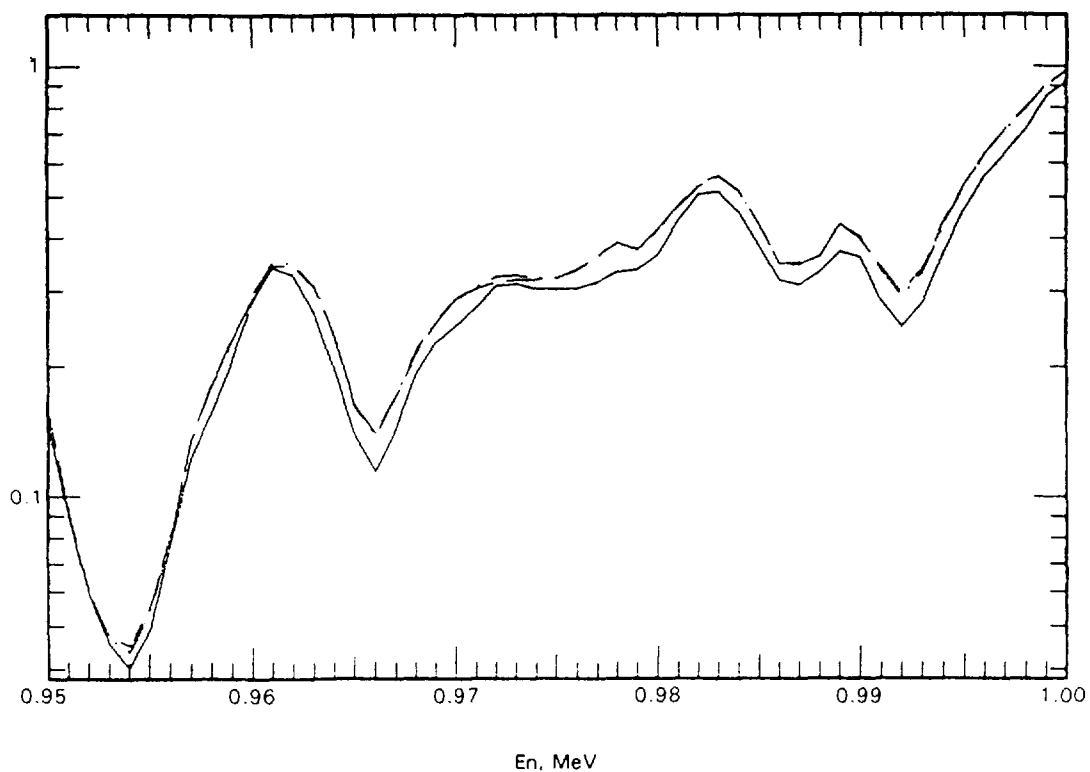


Fig.10 An example of iteration effect on adjusted result: ^{56}Fe nonelastic cross section

— Original - - - iteration 2 times - - - iteration 3 times

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